Universidad de Granada

# Entanglement, complexity and entropic properties of quantum systems

TESIS DOCTORAL

por

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MANIFIESTA:

Que la presente Memoria titulada "Entanglement, complexity and entropic properties of quantum systems", presentada por Irene Valero Toranzo para optar al Grado de Doctora en Física, ha sido realizada bajo mi dirección en el Departamento de Física Atómica, Molecular y Nuclear de la Universidad de Granada y el Instituto Carlos I de Física Teórica y Computacional de la Universidad de Granada.

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Con el fin de obtener la Mención Internacional en el Título de Doctor, se han cumplido, en lo que atañe a esta Tesis Doctoral y a su Defensa, los siguientes requisitos:

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4. Una parte de esta Tesis Doctoral se ha realizado en Grenoble, en GIPSA-Lab, Départment Images et Signal, del Instituto Politécnico de Grenoble, Francia.

A la Vida...

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> *One looks back with appreciation to the brilliant teachers, but with gratitude to those who touched our human feelings. The curriculum is so much necessary raw material, but warmth is the vital element for the growing plant and for the soul of the child.*
> **Carl Gustav Jung**

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# Contents

# Summary

In this Thesis we use the notions of information entropy, statistical complexity and quantum entanglement, together with the methods of Classical and Quantum Information [43, 119] and the algebraic and asymptotic techniques of the theory of orthogonal polynomials and special functions of Applied Mathematics and Mathematical Physics [88, 120, 151], to study and quantify the multiple facets of the spatial delocalization of the charge and matter distributions of the multidimensional quantum systems of bosonic and fermionic character. These facets, which determine both the uncertainty measures of the systems and their physical and chemical properties, are manifested in the enormous diversity of multidimensional geometries of the single-particle densities which characterize the non-relativistic mechano-quantically allowed states of such systems, according to the Density Functional Theories based on the Hohenberg-Kohn theorem and generalizations [64, 123, 124, 132].

The aim of this Thesis is to contribute to the emergent informational representation of the quantum systems [45, 49, 119, 162], which complements the standard representation based on energetic concepts. The analytical determination of the entropy-, complexity- and entanglement-like measures and their associated uncertainty relations [40, 76, 142, 155] is a fundamental task (not yet solved except for the ground state and a few low-lying excited states) even for the very small number of elementary quantum-mechanical potentials which are utilized to approach and model the self-consistent mean-field of the physical systems (atoms, molecules,...), as this work shows. Basically, this is because the quantum manifestations of the multidimensional physical systems are generally inaccessible as the associated Schrödinger equation cannot be exactly solved except for a few cases where the quantum-mechanical potential has a known symmetry [4, 56].

In this work we determine the entropy and complexity-like measures (and their associated uncertainty relations) of the multidimensional quantum systems with central or spherically-symmetric potentials, as well as the quantum entanglement measures of the many-body systems of *Harmonium* [28, 116, 117] and *Spherium* types [101, 102, 156]. The Harmonium-like systems are many-particle systems subject to a harmonic (i.e.,

quadratic) potential, while the Spherium-like systems refer to two-electron systems interacting by means of a Coulomb potential and confined to the surface of a multidimensional ball. Since the wavefunctions of the quantum states of the harmonic and Coulombian systems are controlled by orthogonal hypergeometric polynomials (mainly, Laguerre and Gegenbauer polynomials) and by hyperspherical harmonics [20], the determination of the informational measures of such systems requires necessarily the consideration of novel integral functionals whose computation and asymptotics have been tackled and solved to a great extent in this Thesis.

The Thesis is composed by three chapters (Introduction, Methodology, Applications) followed by some Conclusions and open problems, and Bibliography. Chapter 1, Introduction, is devoted to the presentation and brief explanation of the basic notions (uncertainty, complexity and entanglement) that have been used in the research work about the quantum systems considered in this Thesis (multidimensional blackbody, harmonic and Coulombian systems). In addition, it contains the physico-mathematical motivation about the interest and relevance of the selected systems. Chapter 2, Methodology, includes (i) the mathematical techniques based on orthogonal polynomials that we have derived to determine analytically the informational measures of the quantum states of the harmonic and Coulombian systems including the extreme high-energy (Rydberg) and high-dimensional (pseudoclassical) cases, (ii) a number of inequality-based physico-mathematical methods and informational extremization techniques used to improve the uncertainty relations of the quantum multidimensional systems, and (iii) a brief description of the computational methods used in this work to calculate the wavefunctions and physical observables of the atomic and molecular systems.

The results of the Thesis are given in sections 2.2, 2.3 and 2.4, as well as in the eleven sections of chapter 3. These sections correspond to the different methodological and quantum-physical issues considered in this work which gave rise to the scientific articles gathered in the paragraph *Author's Publications*. Sections 2.2, 2.3 and 2.4 contain the various mathematical theorems and propositions we have found relative to the various entropic functionals of orthogonal hypergeometric polynomials, which are closely related to the weighted analytical norms of $L_q$ type of these functions. The corresponding results allow, among other issues, for the determination of the asymptotics of various entropic integrals of these polynomials when their degree or the parameters of their associated weight function tend towards infinity.

In Sections 3.1, 3.2 and 3.3 we use various physico-mathematical methods (the Lieb-Thirring and Daubechies-Thakkar inequalities and the informational extremization technique) to determine the combined spatial and spin dimensionality effects on the following two mathematical formulations of the Uncertainty Principle of quantum physics: the Heisenberg-like uncertainty relations and the Fisher-information-based uncertainty relation of the multidimensional fermionic systems. Moreover, we study the accuracy of the subsequent uncertainty relations for a large number of neutral atoms, singly-ionized ions and light and heavy molecular systems. In Section 3.4 we determine in an analytical way the generalized Heisenberg-like measures based on the radial expectation values of arbitrary order for the bound non-relativistic stationary states of the high-dimensional hydrogenic systems in the position and momentum spaces; this is done by use of a wide spectrum of mathematical techniques which include the parametric asymptotics of the generalized hypergeometric functions of ${}_{p+1}F_p$ type and the asymptotics of the Laguerre and Gegenbauer polynomials.

In Section 3.5 we investigate the conditions that an informational quantity must fulfill to be considered as a true statistical complexity measure of a complex physical system. Moreover, the notion of monotonicity of a complexity measure of a probability distribution is discussed and applied to the most popular measures of complexity (LMC, Fisher-Shannon and Crámer-Rao) and some of their generalizations. In Section 3.6 we propose a novel monoparametric complexity measure of Fisher-Rényi type and we study their analytical properties; moreover, we calculate explicitly the values of this measure for the quantum states of the hydrogen atom. In Section 3.7 we determine analytically the basic quantities of entropy (Shannon, Rényi,...) and complexity (LMC, Fisher-Shannon and Crámer-Rao) types for the frequency distribution of the multidimensional blackbody radiation, and we discuss their potential relevance on the cosmic microwave background (CMB in short) which baths our universe.

In Sections 3.8 y 3.9 we explicitly calculate the Rényi entropies of arbitrary order for the highly-excited (Rydberg) states of the multidimensional systems of harmonic and Coulomb types in position space in terms of the hyperquantum numbers and the potential strength; to this aim we use the strong asymptotics of the Laguerre polynomials when the polynomial degree becomes very high. In Sections 3.10 y 3.11 we study the quantum entanglement features of the bosonic and fermionic multidimensional systems of Harmonium and Spherium types, respectively; the resulting values are later compared with the corresponding ones in other realistic (helium) and model (Moshinsky, Hooke, Crandall,...) systems analyzed by other authors in recent years.

Finally, the conclusions of the Thesis are briefly given and a few open problems that have emerged throughout the present research are highlighted.

The results of the Thesis are contained in thirteen articles published in the following reviews: Chemical Physics Letters, Entropy, European Physical Journal B: Condensed Matter and Complex Systems, European Physical Journal D: Atomic, Molecular, Optical and Plasma Physics, Europhysics Letters (EPL), Journal of Mathematical Physics, Journal of Mathematical Chemistry, Journal of Physics B: Atomic, Molecular and Optical Physics, Journal of Physics A: Mathematical and Theoretical (3), Physics Letters

A and Physical Review A.

Eight publications of the author, related to but not included in this Thesis, have appeared (as indicated in the paragraph *Author's Publications*) in the following reviews: Entropy, International J. Quantum Chemistry, Journal of Mathematical Physics, Journal of Statistical Mechanics: Theory and Experiment (2), Physica A (2) and IEEE Xplore: IEEE Transactions on Information Theory.

# Resumen

En esta Tesis se utilizan las nociones de entropía de información, complejidad estadística y entrelazamiento cuántico junto con los métodos de la Información Clásica y Cuántica [43, 119] y las técnicas algebraicas y asintóticas de la teoría de los polinomios ortogonales y las funciones especiales de la Matemática Aplicada y la Física Matemática [88, 120, 151], para investigar y cuantificar las múltiples facetas de la deslocalización espacial de las distribuciones de carga y de materia de los sistemas físicos multidimensionales de carácter bosónico y fermiónico. Tales facetas, que determinan tanto las medidas de incertidumbre de tipo entrópico y de complejidad como sus propiedades físicas y químicas, se manifiestan en la enorme diversidad de geometrías multidimensionales de las densidades monoparticulares que caracterizan los estados mecano-cuánticos permitidos no-relativistas de tales sistemas, según la Teoría Funcional de la Densidad de Hohenberg-Kohn y generalizaciones [64, 123, 124, 132].

El objetivo de esta Tesis es contribuir a la descripción teórico-informacional emergente de los sistemas cuánticos multidimensionales [45, 49, 119, 162], que complementa la representación estándar basada en los conceptos energéticos. La determinación analítica de las magnitudes entrópicas, de complejidad y de entrelazamiento y sus relaciones de incertidumbre [40, 76, 142, 155] asociadas es una tarea básica (aún no resuelta salvo para el estado fundamental y unos pocos estados excitados de baja energía), incluso para el escaso número de potenciales mecano-cuánticos elementales que suelen usarse para aproximar y modelizar el potencial de campo medio autoconsistente de los sistemas físicos (átomos, moléculas,...), tal como se muestra en este trabajo. Esto se debe a que las manifestaciones cuánticas de los sistemas físicos multidimensionales son básicamente inaccesibles porque la ecuación de Schrödinger asociada no puede resolverse exactamente salvo para unos pocos casos que corresponden a un potencial cuántico con alguna simetría conocida [4, 56].

En este trabajo se determinan las medidas teórico-informacionales de tipo entrópico y de complejidad de los dos prototipos principales de la física de los sistemas cuánticos multidimensionales con potenciales esféricamente simétricos (a saber, los sistemas armónico y coulombiano) y de la distribución de frecuencias del cuerpo negro en dimensiones

estándar y no-estándar, así como las medidas de entrelazamiento cuántico (entropía de von Neumann,...) de sistemas de tipo *Harmonium* [28, 116, 117] (i.e., sistemas de muchas partículas que interaccionan armónicamente) y de tipo *Spherium* [101, 102, 156](i.e., sistemas de dos electrones interaccionando coulombianamente sobre la superficie de una esfera multidimensional). Habida cuenta de que las funciones de onda de los estados cuánticos de los sistemas armónicos y coulombianos están controladas por polinomios hipergeométricos ortogonales (particularmente, los polinomios de Laguerre y de Gegenbauer) y por armónicos hiperesféricos [20], la determinación de las medidas teórico-informacionales de tales sistemas requiere necesariamente la consideración de funcionales integrales de nuevo cuño de tales polinomios y funciones cuyo cálculo y asintótica hemos abordado y en gran medida resuelto en este trabajo.

La Tesis consta de tres capítulos (Introducción, Metodología y Aplicaciones), seguidos de algunas Conclusiones y problemas abiertos, y Bibliografía. El capítulo 1, Introducción, está dedicado a la presentación y breve explicación de las nociones básicas (incertidumbre, complejidad y entrelazamiento) que han sido usadas en el trabajo de investigación sobre los sistemas y fenómenos cuánticos considerados en esta Tesis, tales como los sistemas armónicos y coulombianos multidimensionales y la radiación de cuerpo negro en universos de dimensiones estándar y no-estándar. Además, contiene la motivación físico-matemática acerca del interés y la relevancia de los sistemas seleccionados. En el capítulo 2, Metodología, se describen (i) las técnicas matemáticas basadas en polinomios ortogonales que hemos tenido que desarrollar para la determinación analítica de las medidas entrópicas y de complejidad de los sistemas armónicos y coulombianos incluyendo los casos extremos correspondientes a los estados altamente excitados (Rydberg) y a los estados pseudosiclásicos o de alta dimensionalidad, (ii) algunos métodos físico-matemáticos de tipo desigualdad y ciertas técnicas de extremización informacional usadas para la extensión y mejora de las relaciones de incertidumbre de los sistemas cuánticos multidimensionales, y (iii) los métodos computacionales usados en este trabajo para calcular las funciones de onda y los observables físicos de los sistemas atómicos y moleculares.

Los resultados de la Tesis se hallan en las secciones 2.2, 2.3 y 2.4, así como en las once secciones del capítulo 3. Estas secciones corresponden a los diferentes tópicos metodológicos y físico-cuánticos abordados, y en gran medida resueltos, en este trabajo que han dado lugar a la publicación de los artículos científicos que se recogen en el apartado *Author's Publications*. En las secciones 2.2, 2.3 y 2.4 se demuestran diversos teoremas y proposiciones matemáticas relativos a varios funcionales entrópicos de polinomios hipergeométricos ortogonales, que están estrechamente relacionados con las normas analíticas ponderadas de tipo $L_q$ de estas funciones. Estos resultados permiten, entre otras cosas, la determinación de la asintótica de las integrales entrópicas de tales polinomios cuando su grado y/o los parámetros de su función peso asociada se hacen muy grandes.

En las Secciones 3.1, 3.2 y 3.3 se utilizan varios métodos físico-matemáticos (e.g., las desigualdades de Lieb-Thirring y de Daubechies-Thakkar así como las técnicas de extremización informacionales) para determinar el efecto combinado de las dimensionalidades espaciales y de espín sobre los dos siguientes tipos de formalizaciones matemáticas del Principio de Incertidumbre de posición-momento de la física cuántica: las relaciones de incertidumbre de tipo Heisenberg generalizadas y las relaciones de incertidumbre basadas en la información de Fisher. Se estudia y discute tambien la precisión de las relaciones de incertidumbre resultantes en todos los átomos neutros e iones simplemente-ionizados de la tabla periódica, así como en numerosos sistemas moleculares ligeros y pesados. En la Sección 3.4 se determinan analíticamente las medidas generalizadas de tipo Heisenberg basadas en los valores esperados radiales de orden arbitrario para los estados estacionarios no-relativistas del sistema hidrogenoide de alta dimensionalidad en los espacios de posiciones y momentos. Para ello se utilizan una amplia gama de técnicas matemáticas que incluyen la asintótica paramétrica de las funciones hipergeométricas generalizadas de tipo ${}_{p+1}F_p$ y la asintótica de los polinomios de Laguerre y Gegenbauer.

En la Sección 3.5 se investigan las propiedades que una magnitud informacional debe satisfacer para que pueda considerarse como medida de complejidad de un sistema físico complejo. Además se propone la noción de monotonía de la medida de complejidad de una distribución de probabilidad y se discute la aplicabilidad de esta propiedad en las tres medidas de complejidad básicas (LMC, Fisher-Shannon and Crámer-Rao) y algunas de sus generalizaciones. En la Sección 3.6 se propone una nueva medida de complejidad monoparamétrica de tipo Fisher-Rényi, cuyas propiedades son estudiadas; posteriormente se calcula detalladamente esta medida en los estados cuánticos del atómo de hidrógeno. En la Sección 3.7 se determinan analíticamente las magnitudes entrópicas (Shannon, Rényi,...) y de complejidad (LMC, Fisher-Shannon and Crámer-Rao) fundamentales de la distribución de frecuencias de la radiación de cuerpo negro multidimensional y se discute su potencial relevancia sobre el fondo cósmico de microondas que baña nuestro universo.

En las Secciones 3.8 y 3.9 se determinan analíticamente en el espacio de posiciones las entropías de Rényi de orden arbitrario para los estados altamente excitados (i.e., Rydberg) de los sistemas multidimensionales de tipo armónico y coulombiano en términos de los números hipercuánticos y de la intensidad del potencial; para ello se usa la asintótica fuerte de los polinomios de Laguerre cuando el grado se hace muy grande. En las Secciones 3.10 y 3.11 se estudia el comportamiento del entrelazamiento cuántico de los sistemas bosónicos y fermiónicos multidimensionales de tipo Harmonium y Spherium, respectivamente; además, las características encontradas son comparadas con lo observado en sistemas similares investigados por otros autores, tales como los modelos de

Hooke y de Crandall, así como en átomos helioides.

Finalmente, se dan algunas Conclusiones y se señalan los problemas abiertos que han surgido a lo largo de la labor investigadora llevada a cabo.

Los resultados de esta Tesis han dado lugar a trece artículos publicados en las revistas: Chemical Physics Letters, Entropy, European Physical Journal B: Condensed Matter and Complex systems, European Physical Journal D: Atomic, Molecular, Optical and Plasma Physics, Europhysics Letters (EPL), Journal of Mathematical Physics, Journal of Mathematical Chemistry, Journal of Physics B: Atomic, Molecular and Optical Physics, Journal of Physics A: Mathematical and Theoretical (3), Physics Letters A and Physical Review A.
Ocho publicaciones del autor relacionadas con los tópicos de esta Tesis pero no incluidas en ella han aparecido, tal como se detalla en el apartado *Author's Publications*, en las revistas siguientes: Entropy, International J. Quantum Chemistry, Journal of Mathematical Physics, Journal of Statistical Mechanics: Theory and Experiment (2), Physica A (2) and IEEE Xplore: IEEE Transactions on Information Theory.

# Author's publications

Publications of the author upon which this Thesis are based. The numbers in brackets at the end of each reference indicate the Section where it is located.

- **I. V. Toranzo**, P. Sánchez-Moreno and J. S. Dehesa
  *Frequency moments, $L_q$ norms and Rényi entropies of general hypergeometric polynomials*
  J. Math. Chem. **52**, 1372-1385 (**2014**) [Section 2.4]

- C. L. Benavides-Riveros, **I. V. Toranzo** and J. S. Dehesa
  *Entanglement in $N$-Harmonium: bosons and fermions*
  J. Phys. B: At. Mol. Opt. Phys. **47**, 195503 (**2014**) [Section 3.10]

- **I. V. Toranzo**, P. Sanchez-Moreno, R.O. Esquivel and J. S. Dehesa
  *Pauli effects in uncertainty relations*
  Chem. Phys. Lett. **614**, 1-4 (**2014**) [Section 3.1]

- **I. V. Toranzo** and J. S. Dehesa
  *Entropy and complexity properties of the $d$-dimensional blackbody radiation*
  Eur. Phys. J. D **68**, 316 (**2014**) [Section 3.7]

- **I. V. Toranzo**, S. López-Rosa, R. O. Esquivel and J. S. Dehesa
  *Heisenberg-like and Fisher-information-based uncertainty relations for $N$-electron $d$-dimensional systems*
  Phys. Rev. A **91**, 062122 (**2015**) [Section 3.2]

- **I. V. Toranzo**, A. R. Plastino and J. S. Dehesa
  *Quantum entanglement in $(d-1)$-Spherium*
  J. Phys. A: Math. Theor. **48**, 475302 (**2015**) [Section 3.11]

- **I. V. Toranzo**, S. López-Rosa, R. O. Esquivel and J. S. Dehesa
  *Extremum-entropy-based Heisenberg-like uncertainty relations*
  J. Phys. A: Math. Theor. **49**, 025301 (**2016**) [Section 3.3]

- Ł. Rudnicki, **I. V. Toranzo**, P. Sánchez-Moreno and J. S. Dehesa
  *Monotone measures of statistical complexity*
  Phys. Lett. A **380**, 377–380 (**2016**) [Section 3.5]

- A. I. Aptekarev, D. N. Tulyakov, **I. V. Toranzo** and J. S. Dehesa
  *Rényi entropies of the highly-excited states of multidimensional harmonic oscillators by use of strong Laguerre asymptotics*
  Eur. Phys. J. B **89**, 85 (**2016**) [Section 3.8]

- **I. V. Toranzo** and J. S. Dehesa
  *Rényi, Shannon and Tsallis entropies of Rydberg hydrogenic systems*
  Europhysics Letters (EPL) **113**, 48003 (**2016**) [Section 3.9]

- **I. V. Toranzo**, A. Martínez-Finkelshtein and J. S. Dehesa
  *Heisenberg-like uncertainty measures for $D$-dimensional hydrogenic systems at large $D$*
  J. Math. Phys. **57**, 082109 (**2016**) [Section 3.4]

- **I. V. Toranzo**, P. Sánchez-Moreno, Ł. Rudnicki and J. S. Dehesa
  *One-parameter Fisher–Rényi complexity: Notion and hydrogenic applications*
  Entropy **19**(1), 16 (**2017**) [Section 3.6]

- N. M. Temme, **I. V. Toranzo**, J. S. Dehesa
  *Entropic functionals of Laguerre and Gegenbauer polynomials with large parameters*
  J. Phys. A: Math. Theor. **50**, 215206 (**2017**) [Section 2.3]

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Other publications, related to but not included in this Thesis, are the following:

- J. S. Dehesa, P. Sánchez-Moreno, S. López-Rosa and **I. V. Toranzo**
  *Entropy and complexity analysis of hydrogenic Rydberg atoms*
  J. Math. Phys. **54**, 052109 (**2013**)

- **I. V. Toranzo**, A. R. Plastino and J. S. Dehesa
  *Quasi-stationary states of the NRT nonlinear Schrödinger equation*
  Physica A **392**, 39453951 (**2013**)

- **I. V. Toranzo**, D. Puertas-Centeno and J. S. Dehesa
  *Entropic properties of $D$-dimensional Rydberg systems*
  Physica A **462**, 1197–1206 (**2016**)

- J. S. Dehesa, **I. V. Toranzo**, D. Puertas-Centeno
  *Entropic measures of Rydberg-like harmonic states*
  Int. J. Quantum Chem. **117**(1), 48–56 (**2017**)

- D. Puertas-Centeno, **I. V. Toranzo**, J. S. Dehesa
  *The biparametric Fisher–Rényi complexity measure and its application to the multidimensional blackbody radiation*
  J. Stat. Mech..: Theory and Experiment (**2017**) 043408

- D. Puertas-Centeno, **I. V. Toranzo**, J. S. Dehesa
  *Heisenberg and entropic uncertainty measures for large-dimensional harmonic systems*
  Entropy **19**, 164 (**2017**)

- N. Sobrino-Coll, D. Puertas-Centeno, **I. V. Toranzo** and J. S. Dehesa
  *Complexity measures and uncertainty relations of the high-dimensional harmonic and hydrogenic systems*
  J. Stat. Mech.: Theory and Experiment (**2017**) 083102

- **I. V. Toranzo**, Steeve Zozor, Jean-Marc Brossier
  *Generalization of the de Bruijn's identity to general $\phi$-entropies and $\phi$-Fisher informations*
  IEEE Xplore: IEEE Transactions on Information Theory. Accepted (**2017**)

# Chapter 1

# Introduction

> *Science cannot solve the ultimate mystery of nature. And that is because, in the last analysis, we ourselves are part of nature and therefore part of the mystery that we are trying to solve.*
> **Max Planck**

The spatial delocalization of the charge and matter distribution of a quantum many-electron system, which controls its physical and chemical properties, is closely related to the notions of uncertainty, complexity and entanglement of the system. These notions are expressed by means of informational functionals of the electron probability density which characterizes the system according to the density functional methods based on the Hohenberg-Kohn methods and its generalizations [64, 123, 124, 132].

### Uncertainty

The Heisenberg uncertainty principle prevents us to measure with arbitrary accuracy all the physical quantities which are classically within our reach. The first mathematical formulation of the uncertainty principle (i.e., the Heisenberg uncertainty relation) was done by using the standard deviations of the electron density in position and momentum spaces as basic uncertainty variables [79]. Later on, it was expressed in terms of the moments with arbitrary order of the electron distribution (the Heisenberg-like uncertainty relations; see e.g., [50, 172]) and in a most appropriate way via the Shannon information entropy and its Rényi and Tsallis generalizations (the entropic uncertainty relations; see e.g. [30, 50, 172]).

The uncertainty principle has numerous relevant consequences, being the stability of matter one of the most distinguised ones [97]. Indeed, atomic electrons operate as small radiating classical antennas that should fall on the nucleus at the time of a few billionths of a second, causing unstable atoms. The uncertainty principle comes to your rescue, enabling, together with the Pauli exclusion principle [114, 146] (i.e., two identical fermions cannot occupy the same quantum state simultaneously), the existence of electronic shells and subshells, and thus the periodic table and all the wealth of structural atomic and molecular physics and chemistry. In fact, the uncertainty principle is more than that. When we talk about the stability of microscopic systems [96**?** ] (e.g., the stability of hydrogen), we simply mean that the total energy of the system cannot be arbitrarily negative. If the system would not have such lower bound to the energy, it would be possible to extract an infinite amount of energy, at least in principle. This stability of the first kind admits a generalization to the macroscopic systems, referred as stability of second kind. In this second type of stability, the lowest posible energy of the macroscopic systems depends at most linearly on the number of particles; or, in other terms, the lowest posible energy per particle cannot be arbitrarily negative as the number of particle increases. These two stability problems have a crucial relevance to understand the world around us. Both of them rely on the fermionic property of electrons; more specifically, they rely on the uncertainty principle and the Pauli principle.

In fact, the influence of the Pauli principle on the mathematical formulations of the uncertainty principle (i.e., the uncertainty relations) has been previously perceived (see e.g., [23]) but it has never been explicitly described, to the best of our knowledge. In this Thesis we tackle this issue. To be more specific, in our work we explore the effects of the Pauli exclusion principle on the Heisenberg-like and entropic uncertainty relations of $d$-dimensional systems; namely, a generalized Heisenberg relation valid for general finite fermion systems (i.e., for all antisymmetric $N$-fermion wavefunctions), and various entropic uncertainty relations of finite fermion systems subject to central potentials. In other words, we investigate the combined balance of the effects of spatial and spin dimensionalities on these fundamental uncertainty relations. We do this way because of the relevant role that space dimensionality plays in the analysis of the structure and dynamics of natural systems and phenomena, from atomic and molecular systems and $d$-dimensional systems (see e.g. the excellent monographs of Herschbach et al [82], Sen [142] and Dong [55]), quantum optics [62] to condensed matter (see e.g., [1, 108, 112]) and quantum information and computation (see e.g.,[93, 144]).

Moreover, Herschbach et al [37, 82, 159] 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 $(D \to \infty)$-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 [80, 82, 159]. Most important here is that the electronic structure for the $(D \to \infty)$-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 $(D \to \infty)$-limit. Indeed, in this high-dimensional 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 $(D \to \infty)$-limit is called *pseudoclassical*, tantamount to $h \to 0$ and/or $m_e \to \infty$ in the kinetic energy, being $h$ and $m_e$ the Planck constant and the electron mass, respectively. This limit is not the same as the conventional classical limit obtained by $h \to 0$ for a fixed dimension [82, 165, 166]. 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., [81]).

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 [2, 13–16, 32, 36, 41, 47, 55, 56, 68, 89], quantum chromodynamics and elementary particle physics [149, 163], atomic and molecular physics [39, 100], heat transport [18, 95, 118], information theory [11, 19, 38, 136, 170], fluids [42, 147], quantum crystals [57], fractality [136] and entanglement [69, 128]. 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 [149]. In addition, a recent effort [136] 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 exit a deep knowledge about the Heisenberg and entropy-like uncertainty measures of the $D$-dimensional harmonic and hydrogenic systems (i.e., a particle moving under the action of a quadratic and a Coulombian potential, respectively) in both quantum-pseudoclassical and quantum-semiclassical borders although a few works have been carried out [3, 11, 19, 36, 44, 51, 52, 67, 74, 76, 77, 110, 131, 139, 170, 172]. These measures, which quantify the spreading properties of the harmonic and hydrogenic probability densities, 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. Unfortunately, the determination of the entropic measures of the $D$-dimensional harmonic and hydrogenic systems, which describe most appropriately the electronic uncertainty of the system, is a formidable task not yet solved except for the lowest-lying energy states despite some efforts [11, 19, 51, 52, 67, 74, 170]. 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 $n$ [31]. Therefore, one of the main goals of this Thesis is the explicit determination of the Heisenberg-like and entropic properties of the high dimensional (pseudoclassical) and high energy (i.e., Rydberg) harmonic and hydrogenic states (namely, the Rényi, Shannon and Tsallis entropies) by use of modern techniques of approximation theory based on the pseudoclassical ($\alpha \to \infty$) [150, 152, 153] and strong ($n \to \infty$) [12, 51, 52] asymptotics of the Laguerre $\mathcal{L}_n^{(\alpha)}(x)$ and Gegenbauer $\mathcal{C}_n^{(\alpha)}(x)$ polynomials which control the state's wavefunctions in position and momentum spaces, respectively .

## Complexity

We all have an intuitive sense of what *complexity* means. In the last two decades, an increasing number of efforts have been published [21, 24, 66, 71–73, 75, 105, 141, 142, 173], to refine our intuitions about complexity into precise, scientific concepts, pointing out a large amount of open problems. Nevertheless, there is neither a consensus on the term *complexity* nor whether there is a simple core to *complexity*. Contrary to the Boltzmann–Shannon entropy, which is ever increasing according to the second law of thermodynamics, the complexity seems to behave very differently.

Indeed, 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 order and randomness, respectively), the ultimate goal of complexity theory is to find an operationally meaningful, yet nevertheless computable, quantifier of complexity [71]. Many efforts have been done to understand it by using concepts extracted from information theory and density functional methods (see e.g., [17, 66, 123, 142]). First, they used information entropies (Fisher information [65] and Shannon, Rényi and Tsallis entropies [133, 143, 157]) 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, they are not enough to describe and quantify the multiple aspects of the complexity of natural systems from particle physics to cosmology [21, 141, 142]. In fact there is no general axiomatic formalization for the term *complexity*, 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 [9, 137], Fisher-Shannon [7, 134] and LMC (López-Ruiz-Mancini-Calvet)[8, 35, 105] 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 [53, 76], invariant under translation and scaling transformation [167, 168]), and monotone in a certain sense.
In this Thesis, these basic measures of complexity are applied to the multidimensional spectral frequency density of a blackbody at temperature $T$, since 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 [5, 34, 70, 94, 121, 129, 130, 145, 158, 171] and experimental [60, 63, 109, 113, 115] standpoints.

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 [9, 10, 134, 135] and LMC-Rényi [105, 106, 127, 137] types.
In this Thesis we introduce a novel monoparametric measure of complexity for continuous probability densities, which is qualitatively different from all the previously known ones, generalizing the well-known Fisher-Shannon. Then, we discuss its main properties and we illustrate its usefulness by applying it to the main prototype of Coulombian systems, the real hydrogenic atom.

## Entanglement

Nowadays the electron correlation in atomic and molecular systems is widely and implicitly believed to be a purely methodical effect coming from the inadequate use of a trial wavefunction of multiconfiguration Hartree-Fock type; so, lacking of physical reality (see e.g., [83, 84]). The application of quantum information ideas and techniques in electronic structure theory has recently allowed to conclude that the electron correlation is closely related to entanglement of electrons. Indeed, it has been proved that while the single Slater determinant in the monoconfigurational Hartree-Fock approximation is a disentangled state, the wavefunction of the multiconfiguration Hartree-Fock approximations (such as, e.g. FCI) accounts for entanglement effects. Therefore, entanglement plays an essential role not only in quantum communication between parties separated by macroscopic distances (see e.g., [85, 119]), but also it is essential to characterize quantum correlations at short distances. The latter problem, where one should necessarily consider the indistinguishable character of the involved particles, has received relatively less attention until a short time ago [25, 26, 86, 140, 155, 160]. This is a serious lack because of its relevance for quantum information processing in various physical systems (see e.g., [6, 140]), to gain deeper insight into non-classical correlations of atomic and molecular systems as well as to fully understand the course of their dissociation processes and chemical reactions [6, 59, 155].

The main difficulty, however, stems from the fact that the Schrödinger equation of most quantum many-body systems cannot be solved analytically. Even numerically, the determination of the wavefunction is, in general, a serious problem. In the last three years an intense effort has been made to determine the entanglement of some real atomic and molecular species such as helium-like atoms [29, 84, 98, 111, 169], of a few processes of diatomic molecules [48] and elementary chemical reactions [58]. These works basically focus on the entanglement of bipartite systems, mainly because the characterization of this phenomenon for systems of many indistinguishable constituents is much less known, even at the level of the very notion of entanglement measure [148].

Thus, the quantification of entanglement of bound states for model systems enabling analytic solutions of the associated Schrödinger equation is being a promising way to investigate correlation phenomena. Indeed, entanglement between the constituents of any bound system is most conveniently analyzed in such models, enabling to relate it to the bosonic or fermionic character. Up until now, however, only entanglement of some models of two bound electrons have been determined. We refer to the 2-Harmonium (or Moshinsky) [117, 126, 161], Crandall and Hooke [111] atoms. In all these models the electron confinement is harmonic, and the electron-electron interaction is of harmonic (2-Harmonium), $r_{12}^{-1}$ (Crandall), and Coulombic (Hooke) type. All of them show that when the spin degree of freedom and the indistinguishability of electrons are taken into account, new entanglement aspects [161] are encountered as compared to the model of distinguishable particles, although some further clarification is needed.

In this Thesis we have extended these efforts by calculating the von Neumann and linear entropies of the entanglement of the one-body reduced density matrix of the $N$-Harmonium model for bosons and fermions and the multidimensional two-electron Spherium system in a fully analytical way.

# Chapter 2

# Methodology

> *The best possible knowledge of a whole does not necessarily include the best possible knowledge of all its parts.*
> **Erwin Schrödinger**

The methodology used in this Thesis encompass a wide range of self-consistent computational methods, inequality-based physico-mathematical approaches and mathematical techniques of orthogonal polynomials. In the three sections below we develop the mathematical methodology needed to determine the entropy-, complexity- and entanglement-like measures of the quantum systems of harmonic and Coulomb types, and we briefly point out the computational methods to calculate the self-consistent wavefunctions and the associated single-particle probability densities of the one- and many-particle systems of fermionic character which are considered in this Thesis. Basically, these mathematical procedures allow us for the determination of the modified $L_q$ norms of the orthogonal hypergeometric polynomials which control the wavefunctions of the quantum states for the harmonic and Coulomb potentials as well as the corresponding ones for the highly-excited (Rydberg) and high-dimensional (pseudoclassical) extreme states.

## 2.1 Computational and inequality-based physico-mathematical approaches

The computational strategies used in this work are based on the Koga-Hartree-Fock self-consistent methods [90, 91] for all neutral atoms of the periodic table from Hydrogen ($N = 1$) to Lawrencium ($N = 103$) and their corresponding anions and cations as well as some diatomic molecules. As heavier systems, we have chosen in our numerical study a molecular set which includes different types of chemical organic and inorganic systems (aliphatic and aromatic hydrocarbons, alcohols, ethers, ketones). It represents a variety of closed shell systems, radicals, isomers as well as molecules with heavy atoms such as sulphur, chlorine, magnesium and phosphorous. The electronic structure calculations performed in the present study for the whole set of molecules were obtained with the Gaussian 03 suite of programs [61] at the $CISD/6-311++G(3df,2p)$ level of theory. For this set of molecules we have calculated the position and momentum moments defined previously by employing software developed in our laboratory along with $3D$ numerical integration routines [125] and the DGRID suite of programs [92]. For further details, see e.g. section 3.2 of this Thesis.

In addition, we use various inequality-based physico-mathematical approaches to improve the different mathematical formalizations of the quantum uncertainty principle (i.e., the quantum uncertainty relations); namely, the Lieb-Thirring [87, 97] and Daubechies-Thakkar [46, 154] inequalities and the extremization technique of the entropic measures of a probability distribution [103, 104]. See sections 3.1, 3.2 and 3.3 for further details.

## 2.2 Laguerre entropic integrals: Strong asymptotics

In this section we briefly describe an analytical technique to determine the asymptotic behavior of the following Rényi-like integral functional of Laguerre polynomials of degree $n$ when $n \to \infty$:

$$N_n(D,p) = \int_0^\infty \left( \left[ \hat{L}_n^{(\alpha)}(x) \right]^2 \omega_\alpha(x) \right)^p x^\beta \, dx, \quad p > 0, \quad n \to \infty \tag{2.1}$$

with $\alpha = l + \frac{D}{2} - 1$, $l = 0, 1, 2, \ldots$ and $\beta = (p-1)\left(1 - \frac{D}{2}\right)$, where the condition $\beta + p\alpha > -1$ is required for the proper convergence of the integral, $D$ refers to the spatial dimension and $\hat{L}_n^{(\alpha)}(x)$ denotes the orthonormal Laguerre polynomials (see e.g., [122])[1] with respect to the weight function $\omega_\alpha(x) = x^\alpha e^{-x}$ on the interval $[0, \infty)$.

The application of the mathematical technique requires the split of the integral (2.1) into different regions where the Laguerre polynomials present a specific asymptotical regime with the corresponding dominant contribution. Altogether, there exist five asymptotical regimes which give the dominant constribution in the asymptotics of $N_n(D,p)$. Three of them, known as the Bessel, cosine and Airy regimes, depend on $n$ in a power law form with an exponent that depends on the parameters $D$ and $p$ and have associated a particular constant. Besides, there exist two more asymptotical regimes which act as the transition regions between the former ones, called cosine-Bessel and cosine-Airy regimes. When they dominate in the integral, the leading term of the asymptotics of $N_n(D,p)$

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[1] Also called associated Laguerre polynomials or Sonine polynomials in different contexts.

goes with $\ln n$ plus the power law in $n$. The final asymptotic behavior is summarized in the form of the three following theorems:

*Theorem* 1. Let $D \in (2, \infty)$. The weigthed $\mathcal{L}_p$-norms of Laguerre polynomials $N_n(D,p)$, given by (2.1), have the following asymptotical $(n \to \infty)$ values:

$$N_n(D,p) = \begin{cases} C(\beta,p)\,(2n)^{(1-p)\frac{D}{2}}\,(1+\bar{\bar{o}}(1)), & p \in (0,p^*) \\ \dfrac{2}{\pi^{p+1/2} n^{p/2}} \dfrac{\Gamma(p+1/2)}{\Gamma(p+1)}\,(\ln n + \underline{\underline{O}}(1))\,, & p = p^* \\ C_B(\alpha,\beta,p)\,n^{(p-1)\frac{D}{2}-p}\,(1+\bar{\bar{o}}(1)), & p > p^* \end{cases}, \tag{2.2}$$

where $p^* := \frac{D}{D-1}$.

*Theorem* 2. Let $D = 2$. The weigthed $\mathcal{L}_p$-norms of Laguerre polynomials $N_n(D,p)$, given by (2.1), have the following asymptotical $(n \to \infty)$ values:

$$N_n(D,p) = \begin{cases} C(0,p)\,(2n)^{(1-p)}\,(1+\bar{\bar{o}}(1))\,, & p \in (0,2) \\ \dfrac{\ln n + \underline{\underline{O}}(1)}{\pi^2 n}\,, & p = 2 \\ \dfrac{C_B(\alpha,0,p)}{n}\,(1+\bar{\bar{o}}(1))\,, & p > 2 \end{cases}. \tag{2.3}$$

*Theorem* 3. Let $D \in [0, 2)$. The weigthed $\mathcal{L}_p$-norms of Laguerre polynomials $N_n(D,p)$, given by (2.1), have the following asymptotical $(n \to \infty)$ values:

- For $p \in (0, 2]$,

$$N_n(D,p) = \begin{cases} C(\beta,p)\,(2n)^{(1-p)\frac{D}{2}}\,(1+\bar{\bar{o}}(1))\,, & p \in (0,2) \\ \dfrac{\ln n + \underline{\underline{O}}(1)}{\pi^2 (4n)^{1-\beta}}\,, & p = 2 \end{cases}. \tag{2.4}$$

- For $p > 2$ and $\frac{4}{3} < D < 2$,

$$N_n(D,p) = \begin{cases} \dfrac{C_A(p)}{\pi^p}\,(4n)^{(\frac{1-2p}{3}+\beta)}(1+\bar{\bar{o}}(1))\,, & p \in (2,\widetilde{p}) \\ \left(\dfrac{C_A(p)}{\pi^p}\,4^{(\frac{1-2p}{3}+\beta)} + C_B(\alpha,\beta,p)\right) n^{-\beta-1}\,, & p = \widetilde{p} \\ C_B(\alpha,\beta,p)\,n^{-\beta-1}\,, & p \in (\widetilde{p},\infty) \end{cases}, \tag{2.5}$$

where $\widetilde{p} := \frac{-2+3D}{-4+3D}$, and

- For $p > 2$ and $D \leqslant \frac{4}{3}$,

$$N_n(D,p) = \frac{C_A(p)}{\pi^p}\,(4n)^{\left(\frac{1-2p}{3}+\beta\right)}(1+\bar{o}(1))\,, \qquad p \in (2,\infty)\,. \tag{2.6}$$

The constants $C$, $C_A$ and $C_B$ are defined as

$$C_B(\alpha,\beta,p) := 2\int_0^\infty t^{2\beta+1}|J_\alpha(2t)|^{2p}\,dt \tag{2.7}$$

for the Bessel regime,

$$C_A(p) := \int_{-\infty}^{+\infty}\left[\frac{2\pi}{\sqrt[3]{2}}\,\mathrm{Ai}^2\left(-\frac{t\sqrt[3]{2}}{2}\right)\right]^p dt \tag{2.8}$$

for the Airy regime, and

$$C(\beta,p) := \frac{2^{\beta+1}}{\pi^{p+1/2}}\,\frac{\Gamma(\beta+1-p/2)\,\Gamma(1-p/2)\,\Gamma(p+1/2)}{\Gamma(\beta+2-p)\,\Gamma(1+p)} \tag{2.9}$$

for the cosine regime, respectively. The symbols $J_\alpha(z)$ and $\mathrm{Ai}(-z)$ denote the known Bessel and Airy functions [122].

This technique has been developed in section II of the article with coordinates *A. I. Aptekarev, D. N. Tulyakov, I. V. Toranzo y J. S. Dehesa, European Physical Journal B: Condensed Matter and Complex Systems* ***89****, 85 (****2016****)*, as included in the paragraph *Author's Publications* and explicitly attached at the end of the section 3.8 of this Thesis.

## 2.3 Laguerre and Gegenbauer entropic integrals: Parameter asymptotics

In this section we describe the mathematical *modus operandi* developed to determine the $(\alpha \to \infty)$-asymptotics of some entropic integrals and logarithmic functionals of the Laguerre ($\mathcal{L}_m^{(\alpha)}(x)$) and Gegenbauer ($\mathcal{C}_m^{(\alpha)}(x)$) polynomials as given below. These asymptotical functionals control the entropy-like uncertainty measures (Rényi, Shannon) of the quantum states of the high-dimensional physical systems of harmonic and Coulomb types, as is discussed in the following chapter of this Thesis.

The concrete achievements of this technique are the following:

- Determination of the asymptotics of the power and logarithmic integral functionals of Laguerre and Gegenbauer polynomials when the parameter $\alpha \to \infty$ and the rest of parameters, including the polynomial degree $m$, are fixed, and

- derivation of new Hermite-type expansions of the Laguerre and Gegenbauer polynomials, which are useful in the analysis of certain special cases of the functionals.

Specifically we will consider here the following integral functionals of the Laguerre and Gegenbauer polynomials:

$$I_1(m,\alpha) = \int\limits_0^\infty x^{\mu-1} e^{-\lambda x} \left|\mathcal{L}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{2.10}$$

$$I_2(m,\alpha) = \int_0^\infty x^{\mu-1} e^{-\lambda x} \big(\mathcal{L}_m^{(\alpha)}(x)\big)^2 \log\big(\mathcal{L}_m^{(\alpha)}(x)\big)^2 dx, \tag{2.11}$$

$$I_3(m,\alpha) = \int_{-1}^1 (1-x)^{c\alpha+a}(1+x)^{d\alpha+b} \left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{2.12}$$

$$I_4(m,\alpha) = \int_{-1}^1 (1-x^2)^{\alpha-\frac{1}{2}} [\mathcal{C}_m^{(\alpha)}(x)]^2 \log\big(\mathcal{C}_m^{(\alpha)}(x)\big)^2 dx, \tag{2.13}$$

where $\mathcal{L}_m^{(\alpha)}(x)$ and $\mathcal{C}_m^{(\alpha)}(x)$ are the standard Laguerre and Gegenbauer polynomials, $m = 0,1,2,\ldots$, $\mu > 0$, $\lambda > 0$, $\kappa > 0$, $c > 0$, $d > 0$.

Briefly, let us advance the ($\alpha \to \infty$)-asymptotical behavior of the integrals (2.10), (2.11), (2.12) and (2.13) in the form of the two following propositions:

*Proposition* 1. Let $\alpha, \lambda, \kappa$, and $\mu$ be positive real numbers, and $m$ a positive natural number. Then, for the Rényi-like integral

$$I_1(m,\alpha) = \int\limits_0^\infty x^{\mu-1} e^{-\lambda x} \left|\mathcal{L}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{2.14}$$

we have the asymptotic expansion

$$I_1(m,\alpha) \sim \frac{\alpha^{\kappa m}\Gamma(\mu)}{\lambda^\mu (m!)^\kappa} \sum_{k=0}^\infty \frac{D_k}{\alpha^k}, \quad \alpha \to \infty. \tag{2.15}$$

The first coefficients are

$$D_0 = 1, \quad D_1 = \frac{\kappa m(-2\mu + m\lambda + \lambda)}{2\lambda}, \tag{2.16}$$

and

$$\begin{aligned} D_2 = \kappa m\big(&-12\mu\lambda\kappa m^2 + 24\mu\lambda - 12\mu\lambda\kappa m - 4m^2\lambda^2 - 6m\lambda^2 + 3m^3\lambda^2\kappa \\ &-12\mu^2 + 12\mu^2\kappa m - 12\mu + 12\mu\kappa m + 6\lambda^2\kappa m^2 - 2\lambda^2 + 3\lambda^2\kappa m\big)/(24\lambda^2). \end{aligned} \tag{2.17}$$

To obtain a result for the Shannon-like integrals $I_2(m,\alpha)$ defined in (2.11), we differentiate the expansion in (2.15) with respect to $\kappa$, and take $\kappa = 2$ afterwards. We have

$$I_2(m,\alpha) = 2\,\frac{\partial}{\partial\kappa} I_1(m,\alpha)\Big|_{\kappa=2} \sim \frac{\alpha^{2m}\Gamma(\mu)}{\lambda^{\mu}(m!)^2}\big(\log\frac{\alpha^{2m}}{(m!)^2}\sum_{k=0}^{\infty}\frac{D_k}{\alpha^k} + 2\sum_{k=0}^{\infty}\frac{D'_k}{\alpha^k}\big), \tag{2.18}$$

for $\alpha \to \infty$ and the rest of parameters are fixed. The derivatives in $D_k$ are with respect to $\kappa$.

For the case $\mu = O(\alpha)$ in the special form $\mu = \sigma + \alpha$, with $\sigma$ a fixed real number, we rewrite (2.10) as

$$I_1^{*}(m,\alpha) = \int\limits_{0}^{\infty} x^{\alpha+\sigma-1} e^{-\lambda x} \left|\mathcal{L}_m^{(\alpha)}(x)\right|^{\kappa} dx, \tag{2.19}$$

whose asymptotics is given by

$$I_1^{*}(m,\alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha-\sigma-\kappa m} \left|\lambda - 1\right|^{\kappa m} \sqrt{\frac{2\pi}{\alpha}}\,\frac{\alpha^{\kappa m}}{(m!)^{\kappa}} \sum_{j=0}^{\infty}\frac{D_j}{\alpha^j}, \qquad \lambda \neq 1 \tag{2.20}$$

with first coefficients $D_0 = 1$ and

$$\begin{aligned} D_1 = \tfrac{1}{12(\lambda-1)^2}\Big(&1 - 12\kappa m\sigma\lambda + 6\sigma^2\lambda^2 - 12\sigma^2\lambda - 6\sigma\lambda^2 + 12\sigma\lambda + \\ &6\kappa^2 m^2 + 12\kappa m\sigma - 12\kappa m^2\lambda - 12\kappa m\lambda + 6\kappa m\lambda^2 + \\ &6\kappa m^2\lambda^2 + \lambda^2 + 6\sigma^2 - 2\lambda - 6\sigma + 6\kappa m^2\Big) \end{aligned} \tag{2.21}$$

and

$$I_1^{*}(m,\alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \frac{1}{(m!)^{\kappa}} \left(\frac{\alpha}{2}\right)^{\frac{1}{2}\kappa m} \int\limits_{-\infty}^{\infty} e^{-\frac{1}{2}\alpha y^2} \left|H_m\left(\sqrt{\frac{\alpha}{2}}\,y\right)\right|^{\kappa} dy, \qquad \lambda = 1, \tag{2.22}$$

for the integral functional (2.19) when $\alpha \to \infty$ and the rest of parameters $(\sigma, \kappa, m)$ are fixed. In this case, at first sight, it seems not to be possible to give a large-$\alpha$ expansion for the integral $I_2$.

*Proposition* 2. Let $a, b, c, d$, and $\kappa$ be positive real numbers, $c < d$, and $m$ a positive natural number. Then, for the integral functional

$$I_3(m,\alpha) = \int_{-1}^{1} (1-x)^{c\alpha+a}(1+x)^{d\alpha+b} \left|\mathcal{C}_m^{(\alpha)}(x)\right|^{\kappa} dx, \tag{2.23}$$

we have that the asymptotic expansion has the form

$$I_3(m,\alpha) \sim e^{-\alpha\phi(x_m)} \sqrt{\frac{2\pi}{\alpha}}\,\frac{2^{\kappa m}\big((\alpha)_m\big)^{\kappa}}{(m!)^{\kappa}} \sum_{k=0}^{\infty}\frac{D_k}{\alpha^k}, \qquad \alpha \to \infty, \tag{2.24}$$

with coefficients $D_k$ not depending on $\alpha$. The first coefficient is

$$D_0 = C_0 = a_1 \left(\frac{2c}{c+d}\right)^a \left(\frac{2d}{c+d}\right)^b \left(\frac{d-c}{c+d}\right)^{\kappa m}, \tag{2.25}$$

where $a_1 = 2\sqrt{\frac{cd}{(c+d)^3}}$.

A result for the Shannon-like integral $I_4(m,\alpha)$ defined in (2.13) follows from differentiating the expansion in (2.24) with respect to $\kappa$, and taking $\kappa = 2$ afterwards. We have

$$\begin{aligned} I_4(m,\alpha) = 2\,\tfrac{\partial}{\partial\kappa} I_3(m,\alpha)\big|_{\kappa=2} \sim \\ e^{-\alpha\phi(x_m)}\sqrt{\tfrac{2\pi}{\alpha}}\,\tfrac{2^{2m}\left((\alpha)_m\right)^2}{(m!)^2}\left(\log\tfrac{2^{2m}\left((\alpha)_m\right)^2}{(m!)^2}\textstyle\sum_{k=0}^{\infty}\frac{D_k}{\alpha^k} + 2\sum_{k=0}^{\infty}\frac{D_k'}{\alpha^k}\right), \end{aligned} \tag{2.26}$$

for $\alpha \to \infty$ and the rest of parameters are fixed. Here again, the derivatives in $D_k$ are with respect to $\kappa$.

When $c = d = 1$, one has the following asymptotics for the integral (2.12)

$$I_3(m,\alpha) \sim \frac{\alpha^{\frac{1}{2}\kappa m}}{\sqrt{2}\,(m!)^\kappa}\int_{-\infty}^{\infty} e^{-\frac{1}{2}\alpha y^2}\left|H_m\left(y\sqrt{\alpha/2}\right)\right|^\kappa dy, \tag{2.27}$$

for $\alpha \to \infty$ and the rest of parameters are fixed. Here again, at first sight, it seems not to be possible to give a large-$\alpha$ expansion for the integral $I_4$.

This mathematical procedure has been given in the article with coordinates *N. M. Temme, I. V. Toranzo and J. S. Dehesa, Journal of Physics A: Mathematical and Theoretical* ***50****, 215206 (****2017****)*, which is attached at the end of this section.

# Entropic functionals of Laguerre and Gegenbauer polynomials with large parameters

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The determination of the physical entropies (Rényi, Shannon, Tsallis) of high-dimensional quantum systems subject to a central potential requires the knowledge of the asymptotics of some power and logarithmic integral functionals of the hypergeometric orthogonal polynomials which control the wavefunctions of the stationary states. For the $D$-dimensional hydrogenic and oscillator-like systems, the wavefunctions of the corresponding bound states are controlled by the Laguerre ($\mathcal{L}_m^{(\alpha)}(x)$) and Gegenbauer ($\mathcal{C}_m^{(\alpha)}(x)$) polynomials in both position and momentum spaces, where the parameter $\alpha$ linearly depends on $D$. In this work we study the asymptotic behavior as $\alpha \to \infty$ of the associated entropy-like integral functionals of these two families of hypergeometric polynomials.

## I. INTRODUCTION

Let us define the integral functionals

$$I_1(m,\alpha) = \int_0^\infty x^{\mu-1} e^{-\lambda x} \left|\mathcal{L}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{1.1}$$

$$I_2(m,\alpha) = \int_0^\infty x^{\mu-1} e^{-\lambda x} \left(\mathcal{L}_m^{(\alpha)}(x)\right)^2 \log\left(\mathcal{L}_m^{(\alpha)}(x)\right)^2 dx, \tag{1.2}$$

$$I_3(m,\alpha) = \int_{-1}^1 (1-x)^{c\alpha+a}(1+x)^{d\alpha+b} \left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{1.3}$$

$$I_4(m,\alpha) = \int_{-1}^1 (1-x^2)^{\alpha-\frac{1}{2}} [\mathcal{C}_m^{(\alpha)}(x)]^2 \log\left(\mathcal{C}_m^{(\alpha)}(x)\right)^2 dx, \tag{1.4}$$

where $\mathcal{L}_m^{(\alpha)}(x)$ and $\mathcal{C}_m^{(\alpha)}(x)$ are the standard Laguerre and Gegenbauer polynomials, $m = 0, 1, 2, \ldots$, $\mu > 0$, $\lambda > 0$, $\kappa > 0$, $c > 0$, $d > 0$. In certain information-theoretic contexts these integrals are called Rényi ($I_1, I_3$) and Shannon ($I_2, I_4$) entropic functionals of Laguerre and Gegenbauer polynomials, respectively. This is because they describe the Rényi and Shannon information entropies of the probability densities (squared wave functions) which characterize the physical states of the $D$-dimensional quantum systems subject to spherically symmetric potentials. It happens that the solutions (wave functions) of the Schrödinger equation of some of these systems are controlled by the Laguerre and Gegenbauer polynomials in the conjugated position and momentum spaces, respectively, being the parameter $\alpha$ of the polynomials a linear function of the dimension $D$.

Indeed, e.g. the wave functions of the stationary states of a three-dimensional single-particle system subject to a central potential $V(\vec{r},t) = V(r)$ are known to have the form $\Psi(\vec{r},t) = \psi(\vec{r})\, e^{-\frac{i}{\hbar}Et}$, where $E$ denotes the state's energy and the corresponding eigenfunction can be expressed in spherical coordinates as

$$\psi_{nlm}(\vec{r}) = R_{nl}(r)\, Y_{lm}(\theta,\phi) \tag{1.5}$$

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with the quantum numbers $n = 0, 1, 2, \ldots$, $l = 0, 1, 2, \ldots$, and $m = -l, -l+1 \ldots, l$. The angular part is given by the spherical harmonics

$$Y_{lm}(\theta,\phi) = \frac{1}{\sqrt{2\pi}} C^{(l+m)}_{l-m}(\cos\theta)\,(\sin\theta)^m\, e^{im\phi} \tag{1.6}$$

with $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. The symbol $C^{(\alpha)}_k(x)$ denotes the ultraspherical or Gegenbauer polynomials [1]. The radial part $R_{nl}(r)$ can be often expressed as $\omega^{1/2}(r) y_n(r)$, where $\{y_n(r)\}$ denotes a system of hypergeometric polynomials orthogonal with respect to the weight function $\omega(r)$ in an interval support of the real line. Then, the quantum probability density of the system is given by

$$\rho_{nlm}(\vec{r}) = |\psi_{nlm}(\vec{r})|^2 = \omega(r)\,[y_n(r)]^2 \, \left[C^{(l+m)}_{l-m}(\cos\theta)\right]^2 [\sin\theta]^{2m}, \tag{1.7}$$

where the radial part denotes the Rakhmanov density of the polynomials $y_n(r)$, $\omega(r)\,[y_n(r)]^2$, and the angular part is controlled by the Rakhmanov density of the Gegenbauer polynomials $C^{(\alpha)}_k(x)$, $\omega^*_\alpha(x)\left[C^{(\alpha)}_k(x)\right]^2$, where $\omega^*_\alpha(x) = (1-x^2)^{\alpha-\frac{1}{2}}$ on the interval $[-1,+1]$ denotes the associated weight function. In the case of hydrogenic and oscillator-like systems (where the potential $V(r)$ is of the form $r^{-1}$ and $r^2$, respectively) the radial part is given by the Rakhmanov density of the Laguerre polynomials $\mathcal{L}^{(\alpha)}_m(r)$ [1], $\omega_\alpha(r)\left[\mathcal{L}^{(\alpha)}_m(r)\right]^2$, where $\omega_\alpha(r) = r^\alpha e^{-r}$ on the interval $[0,\infty)$ is the corresponding associated weight function.

The multiple facets of the spreading of the quantum probability density $\rho_{nlm}(\vec{r})$, which include the intrinsic randomness (uncertainty) and the geometrical profile of the quantum system, can be quantified by means of the dispersion measures (e.g., the variance) and the entropy-like measures (e.g., Rényi, Shannon, Tsallis) of the radial and angular densities. The variance $V[\rho_{nlm}] = \langle \vec{r}^2\rangle - \langle\vec{r}\rangle^2 = \langle r^2\rangle$ (since $\langle\vec{r}\rangle = 0$ for any central potential) is given by

$$V\left[\rho_{nlm}\right] = \int_0^\infty r^4 |R_{nl}(r)|^2 dr \tag{1.8}$$

and the Shannon entropy $S[\rho_{n,l,m}] := -\int \rho_{n,l,m}(\vec{r}) \ln[\rho_{n,l,m}(\vec{r})]\, d\vec{r}$ can be decomposed as $S[\rho_{n,l,m}] = S[R_{n,l}] + S[Y_{l,m}]$, where the radial and angular Shannon entropies are given by

$$S[R_{nl}] = -\int_0^\infty |R_{nl}(r)|^2 \ln|R_{nl}(r)|^2 r^2 dr \tag{1.9}$$

and

$$S[Y_{lm}] = -\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, |Y_{lm}(\theta,\phi)|^2 \ln|Y_{lm}(\theta,\phi)|^2, \tag{1.10}$$

respectively. Moreover the Rényi entropies of the quantum state $(n,l,m)$, $\mathcal{R}_p[\rho_{n,l,m}] = \frac{1}{1-p}\ln\int_{\mathbb{R}^3}[\rho_{n,l,m}(\vec{r})]^p\, d\vec{r}, \quad 0 < p < \infty, p \neq 1$, can be expressed as

$$\mathcal{R}_p[\rho_{n,l,m}] = \mathcal{R}_p[R_{n,l}] + \mathcal{R}_p[Y_{l,m}], \tag{1.11}$$

where $\mathcal{R}_p[R_{n,l}]$ denotes the radial part

$$\mathcal{R}_p[R_{n,l}] = \frac{1}{1-p}\ln\int_0^\infty [R_{n,l}(r)]^{2p} r^2\, dr, \tag{1.12}$$

and $\mathcal{R}_p[Y_{l,m}]$ denotes the angular part

$$\mathcal{R}_p[Y_{l,m}] = \frac{1}{1-p}\ln\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\phi\, |Y_{l,m}(\theta,\phi)|^{2p}. \tag{1.13}$$

Now it is straightforward to see that for three-dimensional hydrogenic and oscillator-like systems the integrals required for the determination of the variance and the angular Rényi entropy are of the type $I_1$ given by Eq. (1.1), and the integrals involved in the determination of the angular Rényi entropy are of the type $I_3$ given by Eq. (1.3). Moreover the integrals needed to calculate the radial and angular Shannon entropies belong to the family of functionals $I_2$ and $I_4$ given by Eqs. (1.2) and (1.4), respectively. The extension of all these physical entropies from 3 to $D$ ($D > 3$)

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dimensions is direct and then the parameter $\alpha$ of the involved orthogonal polynomials is directly proportional to $D$. The usefulness of high- and very high-dimensional quantum systems and phenomena has been amply shown in the the literature from general quantum mechanics and quantum field theory[2–12] to quantum information [13–16].

In this work we first study the asymptotic behavior of these integral functionals for large positive values of the parameter $\alpha$, while the other parameters are fixed. Then, as a separate case, we take $\mu = O(\alpha)$ as an additional large parameter. These integrals arise in the study of entropy-like functionals of Rényi and Shannon types which describe various facets of the electronic spreading of the quantum probability density of the $D$-dimensional hydrogenic and harmonic systems in both position and momentum space with large and very large dimensionalities [10–12]. These entropic measures are closely related to various fundamental and/or experimentally accessible quantities (e.g., charge and momentum average densities, Thomas-Fermi and exchange potential energies, ...) of electronic systems (see e.g., [11]). Moreover, they characterize some uncertainty measures which have allowed to find the position-momentum uncertainty relations of entropic type [17, 18]. These relations are the mathematical formalizations of the uncertainty principle of quantum mechanics which generalize the Heisenberg uncertainty relation [19, 20].

The structure of this work is the following. First, in Section 2 we give the basic asymptotics of Laguerre and Gegenbauer polynomials needed in the rest of the paper. Then, in Sections 3 and 4 we obtain the asymptotic expansions of the Laguerre and Gegenbauer integral functionals for large positive values of the parameter $\alpha$, while the other parameters are fixed. Finally, in Section 5 we consider the asymptotic expansion of the Laguerre functionals for large positive values of the parameters $\alpha$ and $\mu$.

## II. BASIC ASYMPTOTICS OF LAGUERRE AND GEGENBAUER POLYNOMIALS

In this section we gather some well-known limits and we give some further details of these limits. We begin with the limits ([22, Eqn. (18.6.5)])

$$\lim_{\alpha\to\infty} \alpha^{-m}\mathcal{L}_m^{(\alpha)}(\alpha t) = \frac{(1-t)^m}{m!}, \tag{2.1}$$

and ([22, Eqn. (18.6.4)])

$$\lim_{\alpha\to\infty} \frac{1}{(2\alpha)_m}\mathcal{C}_m^{(\alpha)}(x) = \frac{x^m}{m!}, \tag{2.2}$$

These relations can be used to obtain first approximations of the four integrals $I_j(m,\alpha)$ for large values of $\alpha$. Before showing more details, we give more information about these limits and we derive complete asymptotic expansions of $\mathcal{L}_m^{(\alpha)}(\alpha t)$ and $\mathcal{C}_m^{(\alpha)}(x)$ as $\alpha \to +\infty$.

We have the Taylor expansion

$$\mathcal{L}_m^{(\alpha)}(x) = \sum_{n=0}^{m} \frac{(x-\alpha)^n}{n!} \left(\frac{d^n}{dx^n}\mathcal{L}_m^{(\alpha)}(x)\right)\Big|_{x=\alpha}. \tag{2.3}$$

We have the relation for the derivative ([22, Eqn. (18.9.23)])

$$\frac{d}{dx}\mathcal{L}_m^{(\alpha)}(x) = -\mathcal{L}_{m-1}^{(\alpha+1)}(x), \tag{2.4}$$

and this gives

$$\mathcal{L}_m^{(\alpha)}(x) = \sum_{n=0}^{m} (-1)^n \frac{(x-\alpha)^n}{n!}\mathcal{L}_{m-n}^{(\alpha+n)}(\alpha). \tag{2.5}$$

We write this in the form

$$\mathcal{L}_m^{(\alpha)}(\alpha t) = \sum_{n=0}^{m} \frac{\alpha^{m-n}(1-t)^{m-n}}{(m-n)!} f_n(m;\alpha), \quad f_n(m;\alpha) = \mathcal{L}_n^{(\alpha+m-n)}(\alpha), \tag{2.6}$$

and we see that, because $f_0(m;\alpha) = 1$, the term $n = 0$ corresponds to the limit in (2.1).

A few other values of $f_n(m;\alpha)$ are

$$\begin{aligned}
&f_1(m;\alpha) = m, \quad f_2 = \tfrac{1}{2}\bigl(m(m-1)-\alpha\bigr),\\
&f_3(m;\alpha) = \tfrac{1}{6}\bigl(m(m-1)(m-2)+2\alpha-3m\alpha\bigr),\\
&f_4(m;\alpha) = \tfrac{1}{24}\bigl(m(m-1)(m-2)(m-3)-2\alpha(3m^2-7m+3)+3\alpha^2\bigr).
\end{aligned} \tag{2.7}$$

A recurrence relation for $f_n(m;\alpha)$ with respect to $n$ reads

$$(n+1)f_{n+1}(m;\alpha) = (m-n)f_n(m;\alpha) - \alpha f_{n-1}(m;\alpha). \tag{2.8}$$

This follows from the representations in terms of the Kummer function (see ([22, Eqn. (18.11.2)])

$$\begin{aligned}
f_n(m;\alpha) &= \binom{\alpha+m}{n}\ {}_1F_1(-n;\alpha+m+1-n;\alpha)\\
&= \binom{\alpha+m}{n} e^{\alpha}\ {}_1F_1(\alpha+m+1;\alpha+m+1-n;-\alpha),
\end{aligned} \tag{2.9}$$

and the recursion of ${}_1F_1(a;b;z)$ in the second representation with respect to the $b$-direction (see ([22, Eqn. (13.3.2)]).

With mathematical induction, using (2.8), we conclude that

$$f_{2n}(m;\alpha) = \mathcal{O}\left(\alpha^n\right), \quad f_{2n+1}(m;\alpha) = \mathcal{O}\left(\alpha^n\right), \quad \alpha\to\infty, \tag{2.10}$$

and that the representation in (2.6) has an asymptotic character for large $\alpha$, because of the decreasing order with respect to large $\alpha$ of pairs of successive terms.

We can rearrange the representation in (2.6) into a series with negative powers of $\alpha$, but the present form with powers of $(1-t)$ is more convenient when using it to obtain asymptotic information of the integrals in (1.1) and (1.2).

For the Gegenbauer polynomials a similar result is straightforward by using the explicit representation (see ([22, Eqn. (18.5.10)])

$$\mathcal{C}_m^{(\alpha)}(x) = \sum_{n=0}^{\lfloor m/2\rfloor} \frac{(-1)^n\,(\alpha)_{m-n}}{n!\,(m-2n)!}(2x)^{m-2n}, \tag{2.11}$$

and the term with $n=0$ corresponds to the limit in (2.2). In addition, successive terms are of lower order with respect to large values of $\alpha$. That is, denoting the terms by $T_n$, then one has $T_{n+1}/T_n = \mathcal{O}\left(\alpha^{-1}\right)$ as $\alpha\to\infty$.

## III. ASYMPTOTIC EXPANSIONS OF THE LAGUERRE INTEGRALS

In this section we obtain the asymptotic expansion of the Rényi and Shannon-like integral functionals of Laguerre polynomials given by Eqs. (1.1) and (1.2), respectively, for large positive values of the parameter $\alpha$, while the other parameters are fixed. For the integral in (1.1) we change the variable of integration by writing $x=\alpha t$, and obtain

$$I_1(m,\alpha) = \alpha^{\mu}\int_0^{\infty} t^{\mu-1}e^{-\lambda\alpha t}\left|\mathcal{L}_m^{(\alpha)}(\alpha t)\right|^{\kappa}\,dt. \tag{3.1}$$

For large values of $\alpha$, it follows from (2.1) that

$$\mathcal{L}_m^{(\alpha)}(\alpha t) \sim \frac{\alpha^m(1-t)^m}{m!}, \tag{3.2}$$

and that $I_1(m,\alpha)\sim I_1^{(0)}(m,\alpha)$, where

$$I_1^{(0)}(m,\alpha) = \alpha^{\mu}\frac{\alpha^{\kappa m}}{(m!)^{\kappa}}\int_0^{\infty} t^{\mu-1}e^{-\lambda\alpha t}|1-t|^{\kappa m}\,dt. \tag{3.3}$$

An asymptotic expansion can be obtained by expanding

$$(1-t)^{\kappa m} = \sum_{n=0}^{\infty} \frac{(-\kappa m)_n}{n!} t^n, \tag{3.4}$$

and invoking Watson's lemma ([26, Chapter 3]). This gives

$$I_1^{(0)}(m,\alpha) \sim \frac{\alpha^{\kappa m}\Gamma(\mu)}{\lambda^\mu (m!)^\kappa} \sum_{n=0}^{\infty} \frac{(\mu)_n(-\kappa m)_n}{n!(\alpha\lambda)^n}. \tag{3.5}$$

When we use more terms of the representation in (2.6), we write

$$\mathcal{L}_m^{(\alpha)}(\alpha t) = \frac{\alpha^m(1-t)^m}{m!} \sum_{n=0}^{m} \frac{m!}{(m-n)!\,\alpha^n} f_n(m;\alpha)(1-t)^{-n}. \tag{3.6}$$

We expand

$$\left|\mathcal{L}_m^{(\alpha)}(\alpha t)\right|^\kappa = \frac{\alpha^{\kappa m}}{(m!)^\kappa}|1-t|^{\kappa m} \left| \sum_{j=0}^{\infty} \frac{A_j}{\alpha^j}(1-t)^{-j} \right|, \tag{3.7}$$

where the first coefficients are

$$\begin{aligned} &A_0 = 1, \quad A_1 = \kappa m f_1(m;\alpha), \\ &A_2 = \tfrac{1}{2}\kappa m\big(2mf_2(m;\alpha) - 2f_2(m;\alpha) - mf_1(m;\alpha)^2 + \kappa m f_1(m;\alpha)^2\big). \end{aligned} \tag{3.8}$$

The series in (3.6) has an asymptotic character for large $\alpha$ starting with the first term equal to 1, and for using it in (3.1) we assume that we can skip the absolute values. This gives

$$I_1(m,\alpha) \sim \sum_{j=0}^{\infty} \frac{A_j}{\alpha^j} I_1^{(j)}(m,\alpha), \tag{3.9}$$

where

$$I_1^{(j)}(m,\alpha) = \alpha^\mu \frac{\alpha^{\kappa m}}{(m!)^\kappa} \int_0^\infty t^{\mu-1} e^{-\lambda\alpha t}|1-t|^{\kappa m - j}\,dt. \tag{3.10}$$

**Remark III.1.** It should be observed that the expansion in (3.7) contains negative powers of $(1-t)$. This gives divergent integrals in (3.10) when $\kappa m - j \le -1$. For the asymptotic results this is not relevant, because in the application of Watson's lemma we can concentrate on small intervals $[0, t_0]$, $t_0 \in (0,1)$, of the Laplace integrals, even in the starting integral in (3.1). △

With this in mind, we can expand the functions defined in (3.10) in the form

$$I_1^{(j)}(m,\alpha) \sim \frac{\alpha^{\kappa m}\Gamma(\mu)}{\lambda^\mu (m!)^\kappa} \sum_{n=0}^{\infty} \frac{B_{j,n}}{\alpha^n}, \quad B_{j,n} = \frac{(\mu)_n (j-\kappa m)_n}{n!\,\lambda^n}, \tag{3.11}$$

and when using this in (3.9) we obtain

$$I_1(m,\alpha) \sim \frac{\alpha^{\kappa m}\Gamma(\mu)}{\lambda^\mu (m!)^\kappa} \sum_{k=0}^{\infty} \frac{C_k}{\alpha^k}, \quad C_k = \sum_{j=0}^{k} A_j B_{j,k-j}. \tag{3.12}$$

In this expansion the coefficients $C_k$ are in terms of $f_j(m;\alpha)$, which are polynomials of $\alpha$; see (2.7) and (3.8). By rearranging the expansion in (3.12) we can obtain an expansion in negative powers of $\alpha$.

We summarize the above results in the following theorem.

**Theorem III.2.** *Let $\alpha, \lambda, \kappa$, and $\mu$ be positive real numbers, and $m$ a positive natural number. Then, for the Rényi-like integral*

$$I_1(m,\alpha) = \int_0^\infty x^{\mu-1} e^{-\lambda x} \left|\mathcal{L}_m^{(\alpha)}(x)\right|^\kappa \, dx, \tag{3.13}$$

*we have the asymptotic expansion*

$$I_1(m,\alpha) \sim \frac{\alpha^{\kappa m}\Gamma(\mu)}{\lambda^\mu (m!)^\kappa} \sum_{k=0}^\infty \frac{D_k}{\alpha^k}, \quad \alpha \to \infty. \tag{3.14}$$

*The first coefficients are*

$$D_0 = 1, \quad D_1 = \frac{\kappa m(-2\mu + m\lambda + \lambda)}{2\lambda}, \tag{3.15}$$

*and*

$$\begin{aligned} D_2 = \kappa m\big(&-12\mu\lambda\kappa m^2 + 24\mu\lambda - 12\mu\lambda\kappa m - 4m^2\lambda^2 - 6m\lambda^2 + 3m^3\lambda^2\kappa \\ &-12\mu^2 + 12\mu^2\kappa m - 12\mu + 12\mu\kappa m + 6\lambda^2\kappa m^2 - 2\lambda^2 + 3\lambda^2\kappa m\big)/(24\lambda^2). \end{aligned} \tag{3.16}$$

**Remark III.3.** To obtain a result for the Shannon-like integrals $I_2(m,\alpha)$ defined in (1.2), we differentiate the expansion in (3.14) with respect to $\kappa$, and take $\kappa = 2$ afterwards. We have

$$I_2(m,\alpha) = 2\,\frac{\partial}{\partial\kappa} I_1(m,\alpha)\Big|_{\kappa=2} \sim \frac{\alpha^{2m}\Gamma(\mu)}{\lambda^\mu (m!)^2}\big(\log\frac{\alpha^{2m}}{(m!)^2}\sum_{k=0}^\infty \frac{D_k}{\alpha^k} + 2\sum_{k=0}^\infty \frac{D_k'}{\alpha^k}\big), \tag{3.17}$$

for $\alpha \to \infty$ and the rest of parameters are fixed. The derivatives in $D_k$ are with respect to $\kappa$. △

**Example III.4.** We have the special case for $\kappa = 2$ and $\lambda = 1$ (see [24, Page 478])

$$\begin{aligned} I_1(m,\alpha) = \int_0^\infty x^{\mu-1} e^{-x} \mathcal{L}_m^{(\alpha)}(x)^2 \, dx = \frac{(\alpha+1)_m(\alpha+1-\mu)_m\Gamma(\mu)}{m!\,m!} \times \\ {}_3F_2\left(-m, \mu, \mu-\alpha; \alpha+1, \mu-\alpha-m; 1\right). \end{aligned} \tag{3.18}$$

We can expand the finite ${}_3F_2$-function term by term in negative powers of $\alpha$, and the Pochhammer symbols can be expanded as well:

$$\begin{aligned} (\alpha+1)_m &= \frac{\Gamma(\alpha+1+m)}{\Gamma(\alpha+1)} \sim \alpha^m\left(1 + \frac{m(m+1)}{2\alpha} + \dots\right), \\ (\alpha+1-\mu)_m &= \frac{\Gamma(\alpha+1-\mu+m)}{\Gamma(\alpha+1-\mu)} \sim \alpha^m\left(1 + \frac{m(m+1-\mu)}{2\alpha} + \dots\right). \end{aligned} \tag{3.19}$$

More terms follow from [26, §6.5.1]. We obtain the expansion as in (3.14), with coefficients $D_0 = 1$, $D_1 = m(1+m-2\mu)$ and

$$D_2 = \tfrac{1}{6}m\left(-1 + 6\mu - 6\mu^2 + 12\mu^2 m - 12m^2\mu + 4m^2 + 3m^3\right), \tag{3.20}$$

which confirms those for (3.14) when $\kappa = 2$ and $\lambda = 1$. ♢

## IV. ASYMPTOTIC EXPANSIONS OF THE GEGENBAUER INTEGRALS

In this section we obtain the asymptotic expansion of the Rényi and Shannon-like integral functionals of Gegenbauer polynomials given by Eqs. (1.3) and (1.4), respectively, for large positive values of the parameter $\alpha$, while the other parameters are fixed. For the integral in (1.3) we need to consider separately the following two cases: $c \neq d$ and $c = d$.

### A. The case $c \neq d$

We assume that $c < d$, and we observe that $c > d$ follows from interchanging $a$ and $b$ and $c$ and $d$.

The limit in (2.2) can be written in the equivalent form

$$\lim_{\alpha\to\infty} \frac{1}{(\alpha)_m} \mathcal{C}_m^{(\alpha)}(x) = \frac{(2x)^m}{m!}, \tag{4.1}$$

and we write the representation given in (2.10) in the form

$$\begin{aligned} \mathcal{C}_m^{(\alpha)}(x) &= \frac{(2x)^m(\alpha)_m}{m!} \sum_{n=0}^{\lfloor m/2 \rfloor} \frac{(-1)^n m!\,(\alpha)_{m-n}}{(\alpha)_m n!\,(m-2n)!}(2x)^{-2n} \\ &= \frac{(2x)^m(\alpha)_m}{m!} \sum_{n=0}^{\lfloor m/2 \rfloor} \frac{f_n(m;\alpha)}{\alpha^n} x^{-2n} \\ &= \frac{(2x)^m(\alpha)_m}{m!} \left(1 - \frac{m(m-1)}{4x^2(\alpha+m-1)} + \mathcal{O}\left(\alpha^{-2}\right)\right). \end{aligned} \tag{4.2}$$

Because successive terms are of lower order of $\alpha$, this is an asymptotic representation, if $x \neq 0$. Observe that $f_n(m;\alpha) = \mathcal{O}(1)$ as $\alpha \to \infty$.

We expand

$$\left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa = \frac{(2x)^{\kappa m}\big((\alpha)_m\big)^\kappa}{(m!)^\kappa} \left|\sum_{j=0}^{\infty} \frac{A_j}{\alpha^j} x^{-2j}\right| \tag{4.3}$$

where the first coefficients are

$$\begin{aligned} &A_0 = 1, \quad A_1 = \kappa f_1(m;\alpha), \\ &A_2 = \tfrac{1}{2}\kappa\big(2f_2(m;\alpha) - f_1(m;\alpha)^2 + \kappa f_1(m;\alpha)^2\big). \end{aligned} \tag{4.4}$$

This gives for the integral in (1.3) the expansion

$$I_3(m,\alpha) \sim \frac{2^{\kappa m}\big((\alpha)_m\big)^\kappa}{(m!)^\kappa} \sum_{j=0}^{\infty} \frac{A_j}{\alpha^j} I_3^{(2j)}(m,\alpha), \tag{4.5}$$

where[33]

$$I_3^{(2j)}(m,\alpha) = \int_{-1}^{1} (1-x)^{c\alpha+a}(1+x)^{d\alpha+b}\,|x|^{\kappa m-2j}\,dx, \quad j = 0,1,2,\ldots. \tag{4.6}$$

We write this in the form

$$I_3^{(2j)}(m,\alpha) = \int_{-1}^{1} (1-x)^{a}(1+x)^{b}\,|x|^{\kappa m-2j}\,e^{-\alpha\phi(x)}\,dx, \tag{4.7}$$

where

$$\phi(x) = -c\log(1-x) - d\log(1+x). \tag{4.8}$$

This function assumes a minimum at the internal point $x_m = (d-c)/(d+c)$, the saddle point, and we can apply Laplace's method (see, for example, [26, Chapter 3]) to obtain an asymptotic representation.

When $c < d$ we have $x_m \in (0,1)$ and the contribution of the interval $(-1,0)$ is exponentially small compared with that of $(0,1)$. Hence, we replace the interval $(-1,1)$ by $(0,1)$ and introduce the new variable of integration $y$ by writing

$$\phi(x) - \phi(x_m) = \tfrac{1}{2}y^2, \quad \operatorname{sign}(y) = \operatorname{sign}(x - x_m). \tag{4.9}$$

In addition we extend the $y$-interval into $(-\infty,\infty)$. We obtain

$$I_3^{(2j)}(m,\alpha) \sim e^{-\alpha\phi(x_m)} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\alpha y^2} f_j(y)\, dy, \tag{4.10}$$

where

$$f_j(y) = (1-x)^a (1+x)^b x^{\kappa m - 2j} \frac{dx}{dy}. \tag{4.11}$$

With the expansion $f_j(y) = \sum\limits_{k=0}^{\infty} c_k^{(2j)} y^k$ the asymptotic result follows:

$$I_3^{(2j)}(m,\alpha) \sim e^{-\alpha\phi(x_m)} \sqrt{\frac{2\pi}{\alpha}} \sum_{k=0}^{\infty} c_{2k}^{(2j)} \frac{2^k \left(\frac{1}{2}\right)_k}{\alpha^k}, \quad \alpha \to \infty, \tag{4.12}$$

where

$$\phi(x_m) = -c \log \frac{2c}{c+d} - d \log \frac{2d}{c+d}. \tag{4.13}$$

To evaluate the coefficients $c_k^{(2j)}$ we derive from (4.9) those in the expansion $x = x_m + \sum\limits_{k=1}^{\infty} a_k y^k$. We have

$$a_1 = 2\sqrt{\frac{cd}{(c+d)^3}}, \quad a_2 = \frac{2(c-d)}{3(c+d)^2}, \quad a_3 = \frac{c^2 - 11cd + d^2}{9a_1(c+d)^4}, \tag{4.14}$$

and next

$$\begin{aligned} c_0^{(2j)} &= a_1 \left(\frac{2c}{c+d}\right)^a \left(\frac{2d}{c+d}\right)^b \left(\frac{d-c}{c+d}\right)^{\kappa m - 2j}, \\ c_1^{(2j)} &= c_0^{(2j)} a_1 \frac{(c+d)\big(6cd(\kappa m - 2j) + (d-c)(3bc - 3ad + 2c - 2d)\big)}{6cd(d-c)}. \end{aligned} \tag{4.15}$$

Using the expansions of (4.12) in (4.5) we obtain

$$I_3(m,\alpha) \sim e^{-\alpha\phi(x_m)} \sqrt{\frac{2\pi}{\alpha}} \frac{2^{\kappa m}\big((\alpha)_m\big)^\kappa}{(m!)^\kappa} \sum_{k=0}^{\infty} \frac{C_k(\alpha)}{\alpha^k}, \tag{4.16}$$

with first coefficients

$$\begin{aligned} &C_0(\alpha) = A_0 c_0^{(0)}, \quad C_1(\alpha) = A_0 c_2^{(0)} + A_1 c_0^{(2)}, \\ &C_2(\alpha) = 3A_0 c_4^{(0)} + A_1 c_2^{(2)} + A_2 c_0^{(4)}. \end{aligned} \tag{4.17}$$

These coefficients are $\mathcal{O}(1)$ as $\alpha \to \infty$. If we wish we can expand them, rearrange the series in (4.16), and obtain an expansion in negative powers of $\alpha$.

We summarize the above results in the following theorem.

**Theorem IV.1.** *Let $a, b, c, d$, and $\kappa$ be positive real numbers, $c < d$, and $m$ a positive natural number. Then, for the Rényi-like integral*

$$I_3(m,\alpha) = \int_{-1}^{1} (1-x)^{c\alpha + a} (1+x)^{d\alpha + b} \left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{4.18}$$

*we have the asymptotic expansion given in (4.16), which can be converted into the form*

$$I_3(m,\alpha) \sim e^{-\alpha\phi(x_m)} \sqrt{\frac{2\pi}{\alpha}} \frac{2^{\kappa m}\big((\alpha)_m\big)^\kappa}{(m!)^\kappa} \sum_{k=0}^{\infty} \frac{D_k}{\alpha^k}, \quad \alpha \to \infty, \tag{4.19}$$

*with coefficients $D_k$ not depending on $\alpha$. The first coefficient is*

$$D_0 = C_0 = a_1 \left(\frac{2c}{c+d}\right)^a \left(\frac{2d}{c+d}\right)^b \left(\frac{d-c}{c+d}\right)^{\kappa m}, \tag{4.20}$$

*where $a_1$ is given in (4.14).*

**Remark IV.2.** A result for the Shannon-like integral $I_4(m,\alpha)$ defined in (1.4) follows from differentiating the expansion in (4.19) with respect to $\kappa$, and taking $\kappa = 2$ afterwards. We have

$$\begin{aligned} I_4(m,\alpha) = 2\,\frac{\partial}{\partial\kappa} I_3(m,\alpha)\Big|_{\kappa=2} \sim \\ e^{-\alpha\phi(x_m)}\sqrt{\frac{2\pi}{\alpha}}\,\frac{2^{2m}\left((\alpha)_m\right)^2}{(m!)^2}\left(\log\frac{2^{2m}\left((\alpha)_m\right)^2}{(m!)^2}\sum_{k=0}^{\infty}\frac{D_k}{\alpha^k} + 2\sum_{k=0}^{\infty}\frac{D'_k}{\alpha^k}\right), \end{aligned} \tag{4.21}$$

for $\alpha \to \infty$ and the rest of parameters are fixed. Here again, the derivatives in $D_k$ are with respect to $\kappa$. For the corresponding logarithmic case when $c = d$ we refer to Remark IV.5. The special form of $I_4(m,\alpha)$ in (1.4) with $a = b = -\frac{1}{2}$ and $c = d = 1$ does not follow from (4.21). For the case $c = d = 1$ we refer to §IV B.

△

**Example IV.3.** We have the special case (see [24, Eqn. 6, Page 562]) for $\kappa = 2$, $a = -\frac{1}{2}$, $b = 2m - \frac{3}{2}$, $c = 1$, $d = 3$,

$$\begin{aligned} I_3(m,\alpha) &= \int_{-1}^{1} (1-x)^{\alpha-\frac{1}{2}}(1+x)^{3\alpha+2m-\frac{3}{2}}\left(\mathcal{C}_m^{(\alpha)}(x)\right)^2 dx \\ &= \frac{\sqrt{\pi}(2\alpha)_{2m}}{\left(2^m\left(\alpha+\frac{1}{2}\right)_m m!\right)^2}\,\frac{\Gamma\left(\alpha+2m+\frac{1}{2}\right)\Gamma\left(3\alpha+2m-\frac{1}{2}\right)}{\Gamma(2\alpha)\,\Gamma\left(2\alpha+2m+\frac{1}{2}\right)}. \end{aligned} \tag{4.22}$$

Expanding this for large $\alpha$, we obtain the first-order approximation

$$I_3 \sim \sqrt{\frac{\pi}{\alpha}}\,\frac{3^{3\alpha+2m-1}\alpha^{2m}}{2^{4\alpha+2m}\left(m!\right)^2}. \tag{4.23}$$

The same result follows from (4.19) with the first term $D_0$ and the special choice of the parameters. ◇

### B. The case $c = d = 1$

In this case we write (1.3) in the form

$$I_3(m,\alpha) = \int_{-1}^{1} (1-x)^a(1+x)^b e^{-\alpha\phi(x)}\left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa dx, \tag{4.24}$$

where $\phi(x)$ is defined in (4.8). It is symmetric on $(-1,1)$ and has a saddle point $x_m$ at $x = 0$, with $\phi(0) = 0$. We use the transformation given in (4.9), and obtain

$$I_3(m,\alpha) = \int_{-\infty}^{\infty} f(y)e^{-\frac{1}{2}\alpha y^2}\left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa dy, \quad f(y) = (1-x)^a(1+x)^b\frac{dx}{dy}. \tag{4.25}$$

In this case, with the saddle point at the origin, we cannot use the relation that follows from the limit given in (4.1), that is, $\mathcal{C}_m^{(\alpha)}(x) \sim \dfrac{(2x)^m}{m!}(\alpha)_m$. This relation is useless in a small interval around the origin; it does not hold uniformly with respect to small values of $x$. Instead, we may consider an expansion in ascending powers of $x$, for example in the notation of the Gauss hypergeometric function,

$$\begin{aligned} \mathcal{C}_{2m}^{(\alpha)}(x) &= (-1)^m\frac{(\alpha)_m}{m!}\,{}_2F_1\left(-m; m+\alpha; \tfrac{1}{2}; x^2\right), \\ \mathcal{C}_{2m+1}^{(\alpha)}(x) &= (-1)^m\frac{(\alpha)_{m+1}}{m!}2x\,{}_2F_1\left(-m; m+\alpha+1; \tfrac{3}{2}; x^2\right), \end{aligned} \tag{4.26}$$

which are rearrangements of the representation in the first line of (4.2). These forms clearly show that the expansions in powers of $x$ do not give asymptotic representations for large $\alpha$, unless $x = o(1/\sqrt{\alpha})$. Because $x \sim y/\sqrt{2}$ (see coefficient $a_1$ in (4.14)), an expansion of $\left|\mathcal{C}_m^{(\alpha)}(x)\right|^\kappa$ in powers of $y$ is useless for obtaining the large $\alpha$ expansion of the integral given in (4.25).[34]

From the literature (see, for example, [26, §24.2] we know that large $\alpha$ approximations of $\mathcal{C}_m^{(\alpha)}(x)$ can be given in terms of Hermite polynomials, and these are uniformly valid in an $x$-interval around the origin. We also know the simple relation (see [22, Eqn. (18.7.24)]

$$\lim_{\alpha\to\infty} \alpha^{-\frac12 m}\mathcal{C}_m^{(\alpha)}\left(\alpha^{-\frac12}\,x\right) = \frac{H_m(x)}{m!}. \tag{4.27}$$

When we use this as a first order asymptotic relation in (4.25) and observe that $x = y/\sqrt{2} + \mathcal{O}\left(y^3\right)$, and replace $f(y)$ by $f(0) = 1/\sqrt{2}$, we obtain the following asymptotics of the Rényi-like integral

$$I_3(m,\alpha) \sim \frac{\alpha^{\frac12\kappa m}}{\sqrt{2}\,(m!)^\kappa}\int_{-\infty}^{\infty} e^{-\frac12\alpha y^2}\left|H_m\left(y\sqrt{\alpha/2}\right)\right|^\kappa\,dy. \tag{4.28}$$

for $\alpha \to \infty$ and the rest of parameters are fixed. Using the orthogonality relation of the Hermite polynomials, we can evaluate the integral when $\kappa = 2$ and find

$$I_3(m,\alpha) \sim \sqrt{\frac{\pi}{\alpha}}\frac{(2\alpha)^m}{m!}, \quad \alpha \to \infty. \tag{4.29}$$

This result is not very detailed; for example, it does not show the parameters $a$ and $b$. In fact we can try an expansion of the form

$$\begin{aligned} I_3(m,\alpha) &\sim \sqrt{\frac{\pi}{\alpha}}\frac{(2\alpha)^m}{m!}\sum_{k=0}^{\infty}\frac{D_k}{\alpha^k}, \quad D_0 = 1,\\ D_1 &= \tfrac18\left(2(2m+1)\big((a-b)^2-(a+b)\big)+2m^2-14m-3\right). \end{aligned} \tag{4.30}$$

In §IV C we explain how to obtain $D_1$ and more coefficients.

**Example IV.4.** For $\kappa = 2$, $a = -\frac12$, $b = -\frac32$ , $c = d = 1$, the corrected result of [24, Eqn. 7, Page 562] is

$$I_3(m,\alpha) = \int_{-1}^{1}(1-x)^{\alpha-\frac12}(1+x)^{\alpha-\frac32}\left(\mathcal{C}_m^{(\alpha)}(x)\right)^2 dx = \frac{\sqrt{\pi}\,(2\alpha)_m}{m!}\frac{\Gamma\left(\alpha-\frac12\right)}{\Gamma\left(\alpha\right)}. \tag{4.31}$$

When we expand the right-hand side for large values of $\alpha$, we obtain

$$I_3(m,\alpha) \sim \sqrt{\frac{\pi}{\alpha}}\frac{(2\alpha)^m}{m!}\left(1+\frac{2m^2-2m+3}{8\alpha}\right), \tag{4.32}$$

which corresponds to the estimate given in (4.30) when we take $a = -\frac12$ and $b = -\frac32$. It is easy to verify that this correspondence does not happen when we use the asymptotic relation that follows from (4.1) instead of the one that follows from (4.27). ♢

**Remark IV.5.** A result for the Shannon-like integral $I_4(m,\alpha)$ defined in (1.4) follows from differentiating (4.28) with respect to $\kappa$ and putting $\kappa = 2$ afterwards. It seems not to be possible to give a large-$\alpha$ expansion of the resulting integral. △

### C. Hermite-type expansion of the Gegenbauer polynomials

Here we find more asymptotic details of the approximation in (4.30). To do that we expand the Gegenbauer polynomials in an asymptotic representation in terms of the Hermite polynomials of the form

$$\mathcal{C}_m^{(\alpha)}(z) \sim \frac{\alpha^{\frac12 m}}{m!}\left(H_m\left(z\sqrt{\alpha}\right)\sum_{k=0}^{\infty}\frac{c_k}{\alpha^k} + \frac{m}{\sqrt{\alpha}}H_{m-1}\left(z\sqrt{\alpha}\right)\sum_{k=0}^{\infty}\frac{d_k}{\alpha^k}\right). \tag{4.33}$$

The first coefficients are

$$\begin{aligned} &c_0 = 1, \quad d_0 = 0, \\ &c_1 = -\alpha z^2 m, \quad d_1 = \tfrac{1}{3}\alpha z\left(4z^2 + 6\alpha z^2 - 4z^2 m - 3 + 3m\right). \end{aligned} \tag{4.34}$$

This expansion is valid for large $\alpha$ and bounded $m$ and $z\sqrt{\alpha}$. The coefficients $c_k$ and $d_k$ depend on $\alpha$. After rearranging the expansion and putting $z = x/\sqrt{\alpha}$ we find

$$\mathcal{C}_m^{(\alpha)}\left(\alpha^{-\frac{1}{2}}\, x\right) \sim \frac{\alpha^{\frac{1}{2}m}}{m!}\left(H_m(x)\sum_{k=0}^{\infty}\frac{p_k}{\alpha^k} + \frac{m}{\alpha}H_{m-1}(x)\sum_{k=0}^{\infty}\frac{q_k}{\alpha^k}\right). \tag{4.35}$$

The coefficients do not depend on $\alpha$ and the first few are

$$\begin{aligned} &p_0 = 1, \quad q_0 = \tfrac{1}{4}x\left(2x^2 + 2m - 1\right), \quad p_1 = \tfrac{1}{8}m(m - 2x^2 - 2), \\ &q_1 = \tfrac{1}{192}x\Bigl(3 + 24m - 42m^2 + 12m^3 + \left(400m - 48m^2 - 640\right)x^2 + \\ &\qquad\qquad \left(1280 - 384m\right)x^4\Bigr). \end{aligned} \tag{4.36}$$

This expansion is valid for large $\alpha$ and bounded $x$ and $m$.

For uniform expansions in which $\alpha$ and $m$ may be of the same order, we refer to [26, §24.2]. The simpler asymptotic results given above are not available in the literature, and we show how to find the coefficients.

We start with the representation

$$\mathcal{C}_m^{(\alpha)}(z) = \frac{1}{2\pi i}\int_{\mathcal{C}}\frac{1}{(1 - 2zt + t^2)^{\alpha}}\,\frac{dt}{t^{m+1}}, \tag{4.37}$$

where $\mathcal{C}$ is a circle with radius smaller than 1. We write this the form

$$\begin{aligned} \mathcal{C}_m^{(\alpha)}(z) &= \frac{1}{2\pi i}\int_{\mathcal{C}} e^{-\alpha\left(t^2 - 2zt\right)}h(t)\,\frac{dt}{t^{m+1}}, \\ h(t) &= e^{-\alpha\left(\log\left(1 - 2zt + t^2\right) - t^2 + 2zt\right)}. \end{aligned} \tag{4.38}$$

When we expand $h(t)$ in powers of $t$, we obtain a simple finite expansion in which each successive term contains a Hermite polynomial of lower degree. A slightly different approach is given in [23]. In the problem to find more details of the expansion in (4.33), it is more convenient to use an expansion with only two Hermite polynomials.

When we replace $h(t)$ by its value at the origin, $h(0) = 1$, we obtain

$$\mathcal{C}_m^{(\alpha)}(z) \sim \frac{\alpha^{\frac{1}{2}m}}{m!}H_m\left(z\sqrt{\alpha}\right), \tag{4.39}$$

which corresponds to the limit in (4.27). The next step is writing

$$h(t) = c_0 + d_0 t + t^2 g_0(t), \quad c_0 = h(0) = 1, \quad d_0 = h'(0) = 0, \tag{4.40}$$

and substituting this in (4.38). This gives

$$\begin{aligned} \mathcal{C}_m^{(\alpha)}(z) = {} & \frac{\alpha^{\frac{1}{2}m}}{m!}\left(c_0 H_m\left(z\sqrt{\alpha}\right) + \frac{m}{\sqrt{\alpha}}d_0 H_{m-1}\left(z\sqrt{\alpha}\right)\right) + \\ & \frac{1}{2\pi i}\int_{\mathcal{C}} e^{-\alpha\left(t^2 - 2zt\right)}g_0(t)\,\frac{dt}{t^{m-1}}. \end{aligned} \tag{4.41}$$

Integrating by parts, writing $e^{-\alpha t^2}\,dt = -\dfrac{1}{2\alpha t}\,de^{-\alpha t^2}$, we find

$$\begin{aligned} \mathcal{C}_m^{(\alpha)}(z) = {} & \frac{\alpha^{\frac{1}{2}m}}{m!}\left(c_0 H_m\left(z\sqrt{\alpha}\right) + \frac{m}{\sqrt{\alpha}}d_0 H_{m-1}\left(z\sqrt{\alpha}\right)\right) + \\ & \frac{1}{2\pi i\alpha}\int_{\mathcal{C}} e^{-\alpha\left(t^2 - 2zt\right)}h_1(t)\,\frac{dt}{t^{m+1}}, \end{aligned} \tag{4.42}$$

where

$$h_1(t) = \tfrac{1}{2}e^{-2z\alpha t}t^{m+1}\frac{d}{dt}\frac{e^{2z\alpha t}g_0(t)}{t^m} = \tfrac{1}{2}\bigl(tg_0'(t) + (2z\alpha t - m)g_0(t)\bigr). \tag{4.43}$$

Repeating this procedure, we find an expansion of the form given in (4.33).

**Example IV.6.** For $x = 0$ and even $m = 2n$ we find from

$$H_{2n}(0) = (-1)^n\frac{(2n)!}{n!}, \quad \mathcal{C}_{2n}^{(\alpha)}(0) = (-1)^n\frac{\Gamma(\alpha+n)}{n!\,\Gamma(\alpha)}, \tag{4.44}$$

and from (4.33) we conclude that the first series should be an expansion of $\dfrac{\Gamma(\alpha+n)}{\alpha^n\,\Gamma(\alpha)}$. This function has the expansion

$$\frac{\Gamma(\alpha+n)}{\alpha^n\,\Gamma(\alpha)} \sim 1 + \frac{n(n-1)}{2\alpha} + \ldots, \tag{4.45}$$

which confirms the first values given in (4.36). ♢

Next we explain how the coefficients $D_k$ of expansion (4.30) can be obtained. The Gegenbauer polynomial in (4.25) has argument $x$ and we need the polynomial in terms of $y$. For $c = d = 1$ the relation between $x$ and $y$ is given by (see also (4.9))

$$-\log\left(1 - x^2\right) = \tfrac{1}{2}y^2, \quad x = a_1 y\sqrt{\frac{1 - e^{-\frac{1}{2}y^2}}{\frac{1}{2}y^2}}, \tag{4.46}$$

where the square root is positive and $a_1 = \frac{1}{2}\sqrt{2}$. We write

$$x = z + h, \quad z = \tfrac{1}{2}y\sqrt{2}, \quad h = a_3y^3 + a_5y^5 + \ldots, \tag{4.47}$$

and the coefficients easily follow from (4.46). We expand

$$\mathcal{C}_m^{(\alpha)}(x) = \sum_{k=0}^{\infty}\frac{h^k}{k!}\frac{d^k}{dx^k}\,\mathcal{C}_m^{(\alpha)}(x)\Big|_{x=z}, \tag{4.48}$$

and we obtain expansions of the derivatives from (4.33). The derivatives of the Hermite polynomials can be written in terms of the polynomials used in (4.33). The result of straightforward manipulations is a representation of the form

$$\mathcal{C}_m^{(\alpha)}(x) \sim \frac{\alpha^{\frac{1}{2}m}}{m!}\left(H_m\left(y\sqrt{\alpha/2}\right)P + \frac{m}{\sqrt{\alpha}}H_{m-1}\left(y\sqrt{\alpha/2}\right)Q\right), \tag{4.49}$$

in which $P$ and $Q$ can be expanded in powers of $y$, with coefficients that are finite combinations of the coefficients $c_k$ and $d_k$ and their derivatives. These expansions should be multiplied by that of $f(y)$ given in (4.25). Next, this new compound expansion should be squared and finally we need to evaluate integrals of the form

$$\int_{-\infty}^{\infty} e^{-t^2}t^j H_m(t)H_{m-k}(t)\,dt, \tag{4.50}$$

with $k = 0, 1$ and for even $j + k$. For example,

$$\begin{aligned}
&\int_{-\infty}^{\infty} e^{-t^2}tH_m(t)H_{m-1}(t)\,dt = 2^m(m+1)!\,\sqrt{\pi},\\
&\int_{-\infty}^{\infty} e^{-t^2}t^2\,H_m(t)H_m(t)\,dt = 2^{m-1}(2m+1)m!\,\sqrt{\pi}.
\end{aligned} \tag{4.51}$$

Because of the lengthy calculations, which are all quite straightforward with symbolic calculations, we skip the details.

## V. EXTENDED ASYMPTOTIC EXPANSIONS OF LAGUERRE INTEGRALS

In this section we obtain the asymptotic expansion of the Rényi and Shannon-like integral functionals of Laguerre polynomials given by Eqs. (1.1) and (1.2), respectively, for large positive values of the parameters $\alpha$ and $\mu$, while the other parameter $\lambda$ is fixed. We consider the Rényi-like integral in (1.1) for the case $\mu = \mathcal{O}(\alpha)$ in the special form $\mu = \sigma + \alpha$, with $\sigma$ a fixed real number.

We write

$$I_5(m,\alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-\lambda x} \left|\mathcal{L}_m^{(\alpha)}(x)\right|^\kappa \, dx, \tag{5.1}$$

or

$$I_5(m,\alpha) = \alpha^{\alpha+\sigma} e^{-\alpha} \int_0^\infty x^{\sigma-1} e^{-\alpha\phi(x)} \left|\mathcal{L}_m^{(\alpha)}(\alpha x)\right|^\kappa \, dx, \tag{5.2}$$

where

$$\phi(x) = \lambda x - \log x - 1, \quad \phi'(x) = \frac{\lambda x - 1}{x}. \tag{5.3}$$

There is a saddle point at $x_0 = 1/\lambda$ and we use the transformation

$$\phi(x) - \phi(x_0) = \tfrac{1}{2} y^2, \quad \operatorname{sign}(x - x_0) = \operatorname{sign}(y), \quad \phi(x_0) = \log \lambda. \tag{5.4}$$

For small $y$ we have the expansion

$$x = x_0 + \sum_{k=1}^\infty x_k y^k, \tag{5.5}$$

with first coefficients

$$x_1 = \frac{1}{\lambda}, \quad x_2 = \frac{1}{3\lambda}, \quad x_3 = \frac{1}{36\lambda}, \quad x_4 = -\frac{1}{270\lambda}, \quad x_5 = \frac{1}{4320\lambda}. \tag{5.6}$$

The transformation in (5.4) gives, because $\dfrac{dx}{dy} = \dfrac{xy}{\lambda x - 1}$,

$$I_5(m,\alpha) = \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha} \int_{-\infty}^\infty e^{-\frac{1}{2}\alpha y^2} f(y) \, dy, \tag{5.7}$$

where

$$f(y) = \frac{x^\sigma \, y}{\lambda x - 1} \left|\mathcal{L}_m^{(\alpha)}(\alpha x)\right|^\kappa. \tag{5.8}$$

and the relation between $x$ and $y$ is defined in (5.4). We need to distinguish between $\lambda = 1$ and $\lambda \neq 1$.

### A. The case $\lambda \neq 1$

We use the expansion given in (3.7) and write

$$f(y) = \frac{x^\sigma \, y}{\lambda x - 1} \frac{\alpha^{\kappa m}}{(m!)^\kappa} |1 - x|^{\kappa m} \left| \sum_{j=0}^\infty \frac{A_j}{\alpha^j} (1 - x)^{-j} \right|. \tag{5.9}$$

Using the expansion given in (5.5) in the form

$$1 - x = (1 - x_0) \left(1 - \frac{x_1 y}{1 - x_0} - \frac{x_2 y^2}{1 - x_0} - \ldots \right), \tag{5.10}$$

we expand

$$f(y) \sim x_0^\sigma \left|1-x_0\right|^{\kappa m} \frac{\alpha^{\kappa m}}{(m!)^\kappa} \sum_{j=0}^{\infty} C_j y^j, \tag{5.11}$$

and obtain for the integral $I_5(m,\alpha)$ given in (5.7) the expansion

$$I_5(m,\alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha} x_0^\sigma \left|1-x_0\right|^{\kappa m} \sqrt{\frac{2\pi}{\alpha}}\, \frac{\alpha^{\kappa m}}{(m!)^\kappa} \sum_{j=0}^{\infty} C_{2j} \frac{2^j \left(\frac{1}{2}\right)_j}{\alpha^j}. \tag{5.12}$$

The coefficients $C_{2j}$ can expand them for large $\alpha$ and we can rearrange the series to obtain an expansion in negative powers of $\alpha$. This gives the asymptotics

$$I_5(m,\alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha-\sigma-\kappa m} \left|\lambda-1\right|^{\kappa m} \sqrt{\frac{2\pi}{\alpha}}\, \frac{\alpha^{\kappa m}}{(m!)^\kappa} \sum_{j=0}^{\infty} \frac{D_j}{\alpha^j}, \tag{5.13}$$

with first coefficients $D_0 = 1$ and

$$\begin{aligned} D_1 = \frac{1}{12(\lambda-1)^2}\Big(&1 - 12\kappa m\sigma\lambda + 6\sigma^2\lambda^2 - 12\sigma^2\lambda - 6\sigma\lambda^2 + 12\sigma\lambda + \\ &6\kappa^2 m^2 + 12\kappa m\sigma - 12\kappa m^2\lambda - 12\kappa m\lambda + 6\kappa m\lambda^2 + \\ &6\kappa m^2\lambda^2 + \lambda^2 + 6\sigma^2 - 2\lambda - 6\sigma + 6\kappa m^2\Big). \end{aligned} \tag{5.14}$$

for the Rényi-like integral functional (5.1) when $\alpha \to \infty$ and the rest of parameters $(\sigma, \lambda \neq 1, \kappa, m)$ are fixed.

**Example V.1.** We have the special case for $\kappa = 2$ and $\sigma = 1$ (see [24, Page 477])

$$\begin{aligned} I_5(m,\alpha) = \int_0^\infty x^\alpha e^{-\lambda x} \mathcal{L}_m^{(\alpha)}(x)^2\, dx = \frac{(\alpha+1)_m (\alpha+1)_m \Gamma(\alpha+1)(\lambda-1)^{2m}}{m!\, m!\, \lambda^{2m+\alpha+1}} \times \\ {}_2F_1\left(-m,-m;\alpha+1;\frac{1}{(\lambda-1)^2}\right). \end{aligned} \tag{5.15}$$

We can expand the Pochhammer symbols as in (3.19), the gamma function, and the ${}_2F_1$-function term by term in negative powers of $\alpha$. We obtain

$$\begin{aligned} I_5(m,\alpha) \sim \frac{\alpha^{2m+1+\alpha} e^{-\alpha} (\lambda-1)^{2m}}{m!\, m!\, \lambda^{2m+\alpha+1}} \sqrt{\frac{2\pi}{\alpha}} \times \\ \left(1 + \frac{m(m+1)}{2\alpha} + \ldots\right)^2 \left(1 + \frac{1}{12\alpha} + \ldots\right) \left(1 + \frac{m^2}{\alpha(\lambda-1)^2} + \ldots\right). \end{aligned} \tag{5.16}$$

We obtain the expansion as in (5.13), with the same front factor and coefficients $D_0 = 1$ and

$$D_1 = \frac{24m^2 + \lambda^2 - 2\lambda + 1 + 12m^2\lambda^2 - 24m^2\lambda + 12m\lambda^2 - 24m\lambda + 12m}{12(\lambda-1)^2}, \tag{5.17}$$

which confirms $D_1$ given in (5.14) when $\kappa = 2$ and $\lambda = 1$. ♢

**Remark V.2.** The Shannon-like integral

$$I_5^*(m,\alpha) = \int_0^\infty x^{\alpha+\sigma-1} e^{-\lambda x} \left(\mathcal{L}_m^{(\alpha)}(x)\right)^2 \log\left(\mathcal{L}_m^{(\alpha)}(x)\right)^2 dx \tag{5.18}$$

follows from differentiating (5.13) with respect to $\kappa$ and putting $\kappa = 2$ afterwards. The result is

$$\begin{aligned} I_5^*(m,\alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \lambda^{-\alpha-\sigma-2m} (\lambda-1)^{2m} \sqrt{\frac{2\pi}{\alpha}}\, \frac{\alpha^{2m}}{(m!)^2} \times \\ \left(\log \frac{\alpha^{2m}(\lambda-1)^{2m}}{\lambda^{2m}(m!)^{2m}} \sum_{j=0}^{\infty} \frac{D_j}{\alpha^j} + 2\sum_{j=0}^{\infty} \frac{D_j'}{\alpha^j}\right), \end{aligned} \tag{5.19}$$

where the derivatives of $D_j$ are with respect to $\kappa$. △

### B. The case $\lambda = 1$

The limit given in (2.1) cannot be used in this case, because it does not give enough information in the immediate neighborhood of $x = 1$, that is, $y = 0$. The asymptotic relation in (3.2) that follows from the limit is not uniformly valid at $t = 1$. A similar form of nonuniform behavior is considered in §IV B for the Gegenbauer polynomial.

In this case we use the limit (see [22, Eqn. 18.7.26])

$$\lim_{\alpha\to\infty} \left(\frac{2}{\alpha}\right)^{\frac{1}{2}m} \mathcal{L}_m^{(\alpha)}\left(\sqrt{2\alpha}\,x + \alpha\right) = \frac{(-1)^m}{m!} H_m(x), \tag{5.20}$$

and we write it as the asymptotic relation

$$\mathcal{L}_m^{(\alpha)}(\alpha x) \sim \left(\frac{\alpha}{2}\right)^{\frac{1}{2}m} \frac{(-1)^m}{m!} H_m\left(\sqrt{\frac{\alpha}{2}}(x-1)\right). \tag{5.21}$$

We use this estimate in (5.6), replace $x - 1$ by $y$ and $x^\sigma\, y/(x-1)$ by 1, and obtain the first approximation

$$I_5(m,\alpha) \sim \alpha^{\alpha+\sigma} e^{-\alpha} \frac{1}{(m!)^\kappa} \left(\frac{\alpha}{2}\right)^{\frac{1}{2}\kappa m} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\alpha y^2} \left|H_m\left(\sqrt{\frac{\alpha}{2}}\, y\right)\right|^\kappa dy, \tag{5.22}$$

for the Rényi-like integral functional (5.1) when $\alpha \to \infty$ and the rest of parameters $(\sigma, \lambda = 1, \kappa, m)$ are fixed.. In particular, for $\kappa = 2$ we can evaluate this integral by using a standard result for the orthogonal Hermite polynomials; we finally have

$$I_5(m,\alpha) \sim \frac{\alpha^{\alpha+\sigma+m} e^{-\alpha}}{m!} \sqrt{\frac{2\pi}{\alpha}}. \tag{5.23}$$

We can obtain more details of the asymptotic estimate by using an approach similar to that described for the Gegenbauer polynomials in §IV C.

**Example V.3.** We take $\sigma = 1$, and have, by the orthogonality relation of the Laguerre polynomials,

$$I_5(m,\alpha) = \int_0^\infty x^\alpha e^{-x} \mathcal{L}_m^{(\alpha)}(x)^2\, dx = \frac{\Gamma(m+\alpha+1)}{m!}. \tag{5.24}$$

The large-$\alpha$ asymptotic result in the right-hand side of (5.10) corresponds to that of (5.11). It is easy to verify that this correspondence does not happen when we use the asymptotic relation in (3.2) instead of the one in (5.8). ♢

**Remark V.4.** A result for the Shannon-like integral in (5.18) with $\lambda = 1$ follows from differentiating (5.22) with respect to $\kappa$ and putting $\kappa = 2$ afterwards. It seems not to be possible to give a large-$\alpha$ expansion of the resulting integral. △

### C. Hermite-type expansion of the Laguerre polynomials

We can find more asymptotic details of the approximation in (5.23) when we expand the Laguerre polynomials in an asymptotic representation in terms of the Hermite polynomials of the form

$$\begin{aligned} &\mathcal{L}_m^{(\alpha)}(\alpha x) \sim \left(\frac{\alpha}{2}\right)^{\frac{1}{2}m} \frac{(-1)^m}{m!} \times \\ &\left(H_m\left(\sqrt{\frac{\alpha}{2}}(x-1)\right) \sum_{k=0}^\infty \frac{c_k}{\alpha^k} - m\sqrt{\frac{2}{\alpha}} H_{m-1}\left(\sqrt{\frac{\alpha}{2}}(x-1)\right) \sum_{k=0}^\infty \frac{d_k}{\alpha^k}\right). \end{aligned} \tag{5.25}$$

The first coefficients are

$$\begin{aligned} &c_0 = 1, \quad d_0 = 1, \\ &c_1 = m\left(\alpha(x-1) - 1\right), \\ &d_1 = \tfrac{1}{3}\left(3 + 7\alpha - 3m - 9\alpha x + 3\alpha^2(x-1)^2 - 4\alpha m + 6\alpha x m\right). \end{aligned} \tag{5.26}$$

The expansion is valid for bounded values of the argument of the Hermite polynomials. Information on Hermite-type uniform expansions for large $\alpha$ and degree $m$ can be found in [25] and in [26, §32.4].

The expansion in (5.25) can be derived by using the well-known integral representation

$$\mathcal{L}_m^{(\alpha)}(x) = \frac{1}{2\pi i}\int_{\mathcal{C}} (1-t)^{-\alpha-1} e^{-xt/(1-t}\,\frac{dt}{t^{n+1}} \tag{5.27}$$

where $\mathcal{C}$ is a circle with radius 1 around the origin. We write this in the form

$$\mathcal{L}_m^{(\alpha)}(\alpha x) = \frac{1}{2\pi i}\int_{\mathcal{C}} h(t) e^{\alpha(1-x)t-\frac{1}{2}\alpha t^2}\,\frac{dt}{t^{n+1}}, \tag{5.28}$$

where

$$h(t) = \frac{1}{(1-t)} e^{\alpha\left(-\log(1-t)-xt/(1-t)-(1-x)t+\frac{1}{2}t^2\right)}. \tag{5.29}$$

Integrating by parts, starting with $e^{\frac{1}{2}\alpha t^2}\,dt = \dfrac{1}{\alpha t}\,de^{\frac{1}{2}\alpha t^2}$, and using the procedure described in §IV C, we can obtain the expansion given in (5.25).

Next, we need to expand this expansion in terms of $y$ (see (5.5) with $x_0 = 1$ and $\lambda = 1$), and we can obtain more details of the asymptotic relation in (5.23) when we use the method used for the Gegenbauer polynomials. Again, see §IV C. We skip further details.

## VI. CONCLUDING REMARKS

We have investigated in a detailed manner the asymptotics of the power and logarithmic integral functionals of Laguerre and Gegenbauer polynomials $I_j(m,\alpha), j = 1-4$ when the parameter $\alpha \to \infty$ and the rest of parameters, including the polynomial degree $m$, are fixed. These asymptotic functionals of power and logarithmic kind characterize the Rényi and Shannon entropies, respectively, of numerous quantum systems with a large dimensionality $D$.

Because of the many parameters in some of the integrals only a limited number of coefficients of the expansions have been given, and we have used special cases of these variables as examples for which analytic closed forms can be found in the literature. We have used these analytic forms to show how their simple asymptotic results correspond to the derived expansions, and confirm our (in some cases rather formal) approach.

We have derived new Hermite-type expansions of the Laguerre and Gegenbauer polynomials, which in fact are not as powerful as known uniform expansions, but the expansions are useful in the analysis of certain special cases of the functionals.

As always, certain problems remain to be studied. We have not been able to determine the large-$\alpha$ expansion of the Shannon-like integral in (5.18) with $\lambda = 1$ within our approach. Moreover, the determination of the asymptotics of the Laguerre and Gegenbauer polynomials for large values of the degree of the polynomials is most important from both fundamental and applied standpoints. Indeed, it would allow for the analytical calculation of the physical entropies of the highly-excited (i.e., Rydberg) states of numerous hydrogenic and harmonic systems. Let us just point out that the underlying asymptotic analysis for large degree is essentially more difficult than the large-parameter case studied in the present paper and it requires other asymptotical tools. Nevertheless, some remarkable results have been obtained [12, 27–30] (see also the reviews [31, 32]).

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[33] We refer to Remark III.1 for an interpretation of the possibly divergent integrals.

[34] See also the discussion in [21, §5.1] about the range of a saddle point.

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## 2.4 Entropic functionals of general hypergeometric polynomials

In this section we describe the mathematical techniques to determine the unweighted and weighted $L_q$-norms of the orthogonal hypergeometric polynomials (Jacobi, Laguerre, Hermite, Bessel) as well as their $(q \to \infty)$-asymptotics. These functional norms are useful for the analytical calculation of the entropic uncertainty measures of the quantum systems subject to a central potential whose wavefunctions are controlled by some orthogonal hypergeometric polynomials [138].

The main achievements applying these techniques have been the following:

- Compute the unweighted and weighted $L_q$ norms ($q \in \mathbb{Z}^+$) of general hypergeometric polynomials of a real variable $y_n(x)$, and their explicit values for the canonical families of Hermite, Laguerre and Jacobi types. The results are given in terms of $q$ and the parameters of the corresponding weight function,
- determine the asymptotical behaviour ($q \to \infty$) of the unweighted $L_q$-norms of the Jacobi orthogonal polynomials via the Laplace method. Let us comment that this method is not applicable to the Hermite and Laguerre polynomials, and
- compute the entropy-like integrals for the Bessel hypergeometric polynomials $\mathcal{B}_n^{(\alpha)}(z)$, $\alpha = 1, 2, \ldots$

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# Frequency moments, $L_q$ norms and Rényi entropies of general hypergeometric polynomials

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The basic variables of the information theory of quantum systems (e.g., frequency or entropic moments, Rényi and Tsallis entropies) can be expressed in terms of $L_q$ norms of general hypergeometrical polynomials. These polynomials are known to control the radial and angular parts of the wavefunctions of the quantum-mechanically allowed states of numerous physical systems. The computation of the $L_q$ norms of these polynomials is presently an interesting issue *per se* in the theory of special functions; moreover, these quantities are closely related to the frequency moments and other information-theoretic properties of the associated Rakhmanov probability density. In this paper we calculate the unweighted and weighted $L_q$-norms ($q = 2k, k \in \mathbb{N}$) of general hypergeometric real orthogonal polynomials (Hermite, Laguerre and Jacobi) and some entropy-like integrals of Bessel polynomials, in terms of $q$ and the parameters of the corresponding weight function by using their explicit expression and second order differential equation. In addition, the asymptotics ($q \to \infty$) of the unweighted $L_q$ norms of the Jacobi polynomials is determined by the Laplace method.

## I. INTRODUCTION

Let us consider the polynomials $y_n(x)$ of hypergeometric type, which are solutions of

$$\sigma(x)y_n'' + \tau(x)y_n' + \lambda_n y_n = 0, \tag{1}$$

with $\lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma''$, and $\sigma(x)$ and $\tau(x)$ are polynomials of degrees, at most, 2 and 1, respectively. Moreover, $\omega(x)$ $(x \in \Delta)$ denotes the symmetrization function which satisfies the Pearson differential equation

$$[\sigma(x)\omega(x)]' = \tau(x)\omega(x), \tag{2}$$

so that Eq.(1) can be written in the self-adjoint form $(\sigma\omega y_n')' + \lambda_n \omega y_n = 0$. See [19] for further mathematical details and physical applications.
Throughout this paper, we set

$$N_q(n) \equiv \int_\Delta \omega(x)|y_n(x)|^q \, dx \quad , \; q \in \mathbb{R}_+, \tag{3}$$

and

$$W_q(n) \equiv \int_\Delta |\omega(x)y_n^2(x)|^q \, dx \quad , \; q \in \mathbb{R}_+, \tag{4}$$

for the unweighted and weighted $L_q$ norms of the polynomials $y_n(x)$. The $L_q$ norms of hypergeometric polynomials have been recently shown to be closely connected with some combinatorial objects [14] and to have some interesting

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information-theoretic characterizations [13, 24, 26]. It is worth pointing out here that these quantities are closely connected to several information-theoretic properties of the Rakhmanov probability density associated to the polynomial $y_n(x)$, which is defined by $\rho_n(x) = \omega(x)y_n^2(x)$. Indeed, the quantities

$$R_q[\rho_n] = \frac{1}{1-q}\ln W_q(n) \qquad ;q>0, q\neq 1,$$

and

$$T_q[\rho_n] = \frac{1}{q-1}(1-W_q(n)) \qquad ;q>0, q\neq 1,$$

describe the Rényi entropy [22, 23] and the Tsallis entropy [29, 30] of $\rho_n(x)$, respectively.

The $R_q$ and $T_q$ quantities, which include the celebrated Shannon information entropy $S[\rho_n] = -\int \rho_n(x)\ln\rho_n(x)\,dx$ in the limiting case $q \to 1$, grasp different aspects of the distribution of the probability density $\rho_n(x)$ along the interval $\Delta$ when the order $q$ is varying. Moreover, the $L_q$ norms have been used to define various spreading measures of the polynomials $y_n(x)$ over the support interval $\Delta$; in particular the Rényi lengths $L_q^R[\rho_n]$ for the Hermite [24], Laguerre [26] and Jacobi [13] cases, which allow us to know how these polynomials are effectively distributed on the orthogonality interval in a quantitative manner.

Physically, the Rakhmanov density $\rho_n(x)$ describes the probability density of the ground and excited states of the physical systems whose non-relativistic wavefunctions are controlled by the polynomials $y_n(x)$. The frequency moments of this density, which are given by the corresponding weighted $L_q$ norms, allow us to gain insight into the internal disorder of the quantum systems and, moreover, they represent various fundamental and/or experimentally measurable quantities of the systems; e.g., the frequency moments of order $p = 1, 2, 4/3, 5/3$ are, at times up to a proportionality factor, the number of constituents, the average electron density, and the Dirac exchange and Thomas-Fermi energies (see e.g. [1, 10]), respectively. In addition, they can be represented by functionals of the single-particle density of the physical systems [17–19]. For further details, see e.g. the recent review [10].

Since the times of S.N. Bernstein [4] and V.A. Steklov [28] it is known that the $L_q$ norm of measurable functions is known to be a very useful concept in various mathematical fields ranging from classical analysis to applied mathematics and quantum physics. However, by the end of 1990's the only theoretical knowledge to calculate the $L_q$ norms of special functions was the asymptotics ($n \to \infty$) results of the weighted $L_q$ norms of Aptekarev et al [2, 3] for the hypergeometric polynomials $y_n(x)$, and some elegant inequalities for $L_q$ norms of specific orthogonal polynomials [5, 15]. Recently, two analytical procedures to calculate weighted $L_q$ norms for orthogonal polynomials with arbitrary degree $n$ have been proposed [13, 24, 26]. One uses the expansion of $|y_n(x)|^q$ in terms of the powers of the variable, being the expansion coefficients given by some multivariate Bell polynomials. The other method linearizes $[y_n(x)]^q$ in terms of $y_k(x)$, being the linearization coefficients given by some multivariate special functions of Lauricella and Srivastava types [20, 27].

In this paper we extend these works in a three-fold sense. First, we calculate not only the weighted norms but also the unweighted ones. Second, we compute these two norms not only for the classical orthogonal polynomials in a real variable but also for the larger family of the hypergeometric polynomials. In turn, we calculate the unweighted and weighted $L_q$ norms of the hypergeometric polynomial of degree $n$ in terms of the expansion coefficients $c_k$ ($k = 0, 1, \ldots, n$) of its explicit expression and the polynomial coefficients $\sigma(x)$ and $\tau(x)$ of the second order differential equation that it satisfies. Third, we determine the asymptotics ($q \to \infty$) of the unweighted $L_q$ norms of the general orthogonal polynomials by means of the Laplace method [31], following a similar procedure recently used for the corresponding weighted norms [9]. This method works for Jacobi polynomials but it does not apply in Hermite, Laguerre and Bessel cases for reasons discussed later.

The structure of this paper is the following. In sections II and III we calculate the unweighted and weighted $L_q$ norms ($q \in \mathbb{N}$), respectively, of the three canonical families of real hypergeometric orthogonal polynomials; namely, the Hermite, Laguerre and Jacobi polynomials. In section IV we obtain the asymptotics ($q \to \infty$) of the unweighted $L_q$ norms of the Jacobi orthogonal polynomials using the Laplace asymptotic method [31]. Then, in section V we compute some entropy-like integrals for the Bessel polynomials [6, 11, 12, 16].

## II. $L_q$ NORMS OF GENERAL HYPERGEOMETRIC POLYNOMIALS

In this section we first determine the (unweighted) $L_q$ norms, $N_q(n)$ with $q \in \mathbb{N}$, of general hypergeometric polynomials $y_n(x)$. Then, we apply them to the three canonical families of real continuous orthogonal hypergeometric polynomials: Hermite, Laguerre and Jacobi. Let us assume that the polynomials $y_n(x)$ have the explicit expression

$$y_n(x) = \sum_{k=0}^{n} c_k x^k \tag{5}$$

and fulfill the second-order hypergeometric differential equation (1).

To calculate the quantities $N_q(n)$ defined by (3) for $q = 2k$, $k \in \mathbb{N}$, we begin with the following power expansion [24] (see also [8])

$$[y_n(x)]^q = \left[\sum_{k=0}^{n} c_k x^k\right]^q = \sum_{t=0}^{nq} \frac{q!}{(t+q)!} B_{t+q,q}(c_0, 2!c_1, \ldots, (t+1)!c_t) x^t \tag{6}$$

with $c_i = 0$ for $i > n$, and where the $B$-symbols denote the Bell polynomials of combinatorics [7], which are given by

$$B_{m,l}(c_1, c_2, \ldots, c_{m-l+1}) = \sum_{\pi(m,l)} \frac{m!}{j_1! j_2! \ldots j_{m-l+1}!} \left(\frac{c_1}{1!}\right)^{j_1} \left(\frac{c_2}{2!}\right)^{j_2} \ldots \left(\frac{c_{m-l+1}}{(m-l+1)!}\right)^{j_{m-l+1}} \tag{7}$$

where the sum runs over all partitions $\pi(m,l)$ such that

$$j_1 + j_2 + \ldots + j_{m-l+1} = l, \tag{8}$$

and

$$j_1 + 2j_2 + \ldots + (m-l+1) j_{m-l+1} = m \tag{9}$$

Then, taking (6) in (3) we obtain that

$$N_q(n) = \sum_{t=0}^{nq} \frac{q!}{(t+q)!} B_{t+q,q}(c_0, 2!c_1, \ldots, (t+1)c_t) \mu_t \tag{10}$$

where $\mu_t$ denotes the moment of order $t$ of the symmetrization function $\omega(x)$; i.e.

$$\mu_t = \int_\Delta x^t \omega(x)\, dx \qquad ; t = 0, 1, \ldots \tag{11}$$

To calculate these moments, we multiply the Pearson equation (2) by $x^t$ and we integrate over the support interval $\Delta \equiv (a,b)$ of $\omega(x)$; so that,

$$\int_a^b x^t (\sigma\omega)'\, dx = \int_a^b x^t \tau\omega\, dx$$

Integrating by parts we have

$$\int_a^b [x^t \tau(x) + t x^{t-1} \sigma(x)] \omega(x)\, dx - A(t,a,b) = 0,$$

with

$$A(t,a,b) = x^t \sigma(x)\omega(x)|_a^b = b^t \sigma(b)\omega(b) - a^t \sigma(a)\omega(a) \tag{12}$$

From this expression it is straightforward to obtain the following recurrence relation

$$\left(\frac{t}{2}\sigma'' + \tau'\right) \mu_{t+1} + [t\sigma'(0) + \tau(0)]\, \mu_t + t\sigma(0)\mu_{t-1} - A(t,a,b) = 0 \tag{13}$$

which allows us to determine the wanted moments $\mu_t$, with the initial conditions
$\mu_0 = \int_\Delta \omega(x)\, dx$ and $\mu_{-1} = 0$.

|  | Hermite | Laguerre | Jacobi | Bessel |
|---|---|---|---|---|
| $\Delta$ | $(-\infty,+\infty)$ | $(0,+\infty)$ | $(-1,+1)$ | Unit circle |
| $\omega(z)$ | $e^{-z^2}$ | $z^\alpha e^{-z}$ | $(1-z)^\alpha(1+z)^\beta$ | $z^\alpha e^{-2/z}$ |
| $\sigma(z)$ | $1$ | $z$ | $1-z^2$ | $z^2$ |
| $\tau(z)$ | $-2z$ | $1+\alpha-z$ | $-(\alpha+\beta+2)z+\beta-\alpha$ | $(\alpha+2)z+2$ |
| $\lambda_n$ | $2n$ | $n$ | $n(n+\alpha+\beta+1)$ | $-n(n+\alpha+1)$ |
| $y_n(z)$ | $H_n(z)$ | $L_n^{(\alpha)}(z)$ | $P_n^{(\alpha,\beta)}(z)$ | $\mathcal{B}_n^{(\alpha)}(z)$ |

TABLE I: Classical orthogonal polynomials of Hermite, Laguerre, Jacobi and Bessel types

In turn, Eqs.(10), (11) and (13) allow us to determine the $L_q$ norms $N_q(x)$ of the polynomials of hypergeometric type $y_n(x)$ in terms of the expansion coefficients $c_k$ $(k=0,1,\ldots,n)$ and the coefficients $\sigma(x)$ and $\tau(x)$ of the corresponding differential equation (1). Moreover, when these polynomials are orthogonal with respect to $\omega(x)$ on the interval $\Delta$ so that

$$\int_a^b y_n(x)y_m(x)\omega(x)\,dx = d_n^2\delta_{m,n} \tag{14}$$

(where $d_n^2$ is the normalization constant), it happens that $A(t,a,b)=0$. The classical orthogonal polynomials of Hermite, Laguerre and Jacobi satisfy this condition (see e.g. [19] and main data in Table I).

Thus, the unweighted $L_q$ norms, $N_q(n)$, of these orthogonal polynomials are determined by Eqs. (10) and (13), where the expansion coefficients $c_k$ are well-known in the literature (see e.g. [19]) the moments $\mu_t$ can be obtained by the following recursion relation with constant coefficients

$$\left(\frac{t}{2}\sigma''+\tau'\right)\mu_{t+1}+\left[t\sigma'(0)+\tau(0)\right]\mu_t+t\sigma(0)\mu_{t-1}=0 \tag{15}$$

Taking into account the polynomial coefficients $\sigma(x)$ and $\tau(x)$ given in Table 1 for each of the classical orthogonal polynomials, the recursion relation (15) boils down as follows:

$$\begin{aligned} -2\mu_{t+1}+t\mu_{t-1} &= 0 \quad \text{for} \quad H_n(x)\\ -\mu_{t+1}+(t+\alpha+1)\mu_t &= 0 \quad \text{for} \quad L_n^{(\alpha)}(x)\\ -(t+\alpha+\beta+2)\mu_{t+1}+(\beta-\alpha)\mu_t+t\mu_{t-1} &= 0 \quad \text{for} \quad P_n^{(\alpha,\beta)}(x)\end{aligned}$$

These recurrence relations can be solved, giving rise to the following explicit expressions

$$\begin{aligned}\mu_{2t+1}(H) &= 0,\ \mu_{2t}(H)=\Gamma\left(t+\frac{1}{2}\right) &(16)\\ \mu_t(L) &= \Gamma(1+\alpha+t) &(17)\\ \mu_t(P) &= \Gamma(1+t)\Big[(-1)^t\frac{\Gamma(1+\beta)}{\Gamma(2+t+\beta)}{}_2F_1(-\alpha,t+1;2+t+\beta;-1)\\ &\quad+\frac{\Gamma(1+\alpha)}{\Gamma(2+t+\alpha)}{}_2F_1(-\beta,t+1;2+t+\alpha;-1)\Big] &(18)\end{aligned}$$

for the moments $\mu_t$, $t=0,1,2,\ldots$ of the Hermite, Laguerre and Jacobi polynomials. Needless to say that the values (16)-(18) for the moments of classical orthogonal polynomials can be obtained either from relation (15) or from (11), respectively.

Summarizing, the expressions (10) and (16)-(18) allow one to compute the unweighted $L_q$ norms ($q\in\mathbb{N}$) of the (Rakhmanov probability density associated to the) three classical families of orthogonal hypergeometric polynomials in terms of their expansion coefficients, whose values are well-known in the literature (see e.g. [14, 19, 21]).

## III. WEIGHTED $L_q$ NORMS OF GENERAL HYPERGEOMETRIC POLYNOMIALS

In this section we determine the weighted $L_q$ norms $W_q(n)$, $q\in\mathbb{N}$, of the general hypergeometric polynomials $y_n(x)$. Then, we apply them to the three classical families of real orthogonal hypergeometric polynomials.

According to the definition (4) and making use of expansion formula (6) of $[y_n(x)]^q$, we obtain that the weighted $L_q$ norms $W_q(n)$ for $q \in \mathbb{N}$ can be expressed as

$$\begin{aligned} W_q(n) &= \int_\Delta [\omega(x)]^q \, [y_n(x)]^{2q} \, dx \\ &= \sum_{t=0}^{2nq} \frac{(2q)!}{(t+2q)!} B_{t+2q,2q}(c_0, 2!c_1, \ldots, (t+1)c_t) \cdot \Omega_q(t) \end{aligned} \tag{19}$$

with the expansion coefficients $c_k$ (see (5)) and the $\Omega$-functional

$$\Omega_q(t) \equiv \int_\Delta x^t [\omega(x)]^q \, dx \,, \tag{20}$$

where $\omega(x)$ is the symmetrization function of the polynomials as defined by means of the Pearson equation and $\Delta \equiv (a,b)$. These generalized moments $\Omega_q(t)$ can be determined recurrently in terms of the coefficients $\tau(x)$ and $\sigma(x)$ of (1) by means of a procedure similar to that already used for the moments $\mu_t$ in the previous section. Indeed, integrating (20) by parts we have that

$$\int_a^b x^t [\omega(x)]^q \, dx = \frac{x^{t+1}}{t+1} [\omega(x)]^q \Big|_a^b - \int_a^b x^t \cdot x \frac{1}{t+1} q \cdot \omega'(x) \, [\omega(x)]^{q-1} \, dx \tag{21}$$

Now we use the Pearson equation in the following way,

$$(\sigma(x)\omega(x))' = \tau(x)\omega(x) \xrightarrow{\times [\omega(x)]^{q-1}} \sigma'(x) \, [\omega(x)]^q + \sigma(x)\omega'(x) \, [\omega(x)]^{q-1} = \tau(x) \, [\omega(x)]^q$$

Taking the last term of the left side alone, i.e.

$$\sigma(x)\omega'(x) \, [\omega(x)]^{q-1} = \tau(x) \, [\omega(x)]^q - \sigma'(x) \, [\omega(x)]^q \to \omega'(x) \, [\omega(x)]^{q-1} = \frac{1}{\sigma(x)} \left(\tau(x) - \sigma'(x)\right) [\omega(x)]^q \,,$$

we can write (20)

$$\begin{aligned} \int_a^b x^t [\omega(x)]^q \, dx &= \frac{x^{t+1}}{t+1} [\omega(x)]^q \Big|_a^b - \int_a^b x^t \cdot x \frac{1}{t+1} q \frac{1}{\sigma(x)} \left(\tau(x) - \sigma'(x)\right) \cdot [\omega(x)]^q \, dx \\ &= B(t,a,b) - \int_a^b x^t \cdot \left[ \frac{q}{t+1} x \frac{\tau(x) - \sigma'(x)}{\sigma(x)} \right] \cdot [\omega(x)]^q \, dx \end{aligned}$$

So, finally we have the following equation

$$\int_a^b x^t \cdot \left[ 1 + \frac{q}{t+1} x \frac{\tau(x) - \sigma'(x)}{\sigma(x)} \right] \cdot [\omega(x)]^q \, dx - B(t,a,b) = 0 \tag{22}$$

where

$$B(t,a,b) = \frac{1}{t+1} \left( b^t \, [\omega(b)]^q - a^t \, [\omega(a)]^q \right)$$

Remark that, since $\tau(x)$ and $\sigma(x)$ are polynomials of degrees 1 and 2 at most, the expression (22) is actually a recurrence relation of the generalized moments $\Omega_q(t)$. Thus, (19) and (22) allow us to determine analytically the weighted $L_q$-norm of the hypergeometric polynomials $y_n(x)$ in terms of their expansion coefficients $c_k$ and their differential-equation coefficients $\tau(x)$ and $\sigma(x)$. To illustrate this procedure we apply it to the three classical families of orthogonal hypergeometric polynomials which satisfy the orthogonality condition (14). In these cases, it is fulfilled that $B(t,a,b) = 0$, so that (22) simplifies as

$$\int_a^b x^t \cdot \left[ 1 + \frac{q}{t+1} x \frac{\tau(x) - \sigma'(x)}{\sigma(x)} \right] \cdot [\omega(x)]^q \, dx = 0 \tag{23}$$

Then, taking into account the data of Table I, this expression provides us with the following recurrence relation for the generalized moments $\Omega_q(t)$ of the Hermite, Laguerre and Jacobi polynomials:

$$\Omega_q^{(H)}(t) - \frac{2q}{t+1}\Omega_q^{(H)}(t+2) = 0 \tag{24}$$

$$\left(1 + \frac{\alpha q}{t+1}\right)\Omega_q^{(L)}(t) - \frac{q}{t+1}\Omega_q^{(L)}(t+1) = 0 \tag{25}$$

$$(t+1)\Omega_q^{(P)}(t) - q(\alpha-\beta)\Omega_q^{(P)}(t+1) - [t+3+q(\alpha+\beta)]\Omega_q^{(P)}(t+2) = 0, \tag{26}$$

respectively. Remark that the expressions (24) and (25) are two-term recurrence relation which can be solved, giving rise to the values

$$\begin{aligned} \Omega_q^{(H)}(2t+1) &= 0, \quad \Omega_q^{(H)}(2t) = q^{-t-\frac{1}{2}}\Gamma\left(t+\frac{1}{2}\right) && (27)\\ \Omega_q^{(L)}(t) &= q^{-(1+\alpha q+t)}\Gamma(1+\alpha q+t) && (28) \end{aligned}$$

for the Hermite and Laguerre cases, respectively. As well, these values easily follow from (20). In the Jacobi case one can solve the recurrence relation (26), or better (20), to obtain the value

$$\begin{aligned} \Omega_q^{(P)}(t) = \Gamma(1+t)\Big[(-1)^t \frac{\Gamma(1+\beta q)}{\Gamma(2+t+\beta q)}\, {}_2F_1(-\alpha q, t+1; 2+t\beta q; -1) \\ + \frac{\Gamma(1+\alpha q)}{\Gamma(2+t+\alpha q)}\, {}_2F_1(-\beta q, t+1; 2+t+\alpha q; -1)\Big] \end{aligned} \tag{29}$$

In summary, the expressions (19) and (27)-(29) provide a procedure to determine the weighted $L_q$ norms ($q \in \mathbb{N}$) of the Hermite, Laguerre and Jacobi polynomials in terms of their expansion coefficients, which are well-known in the literature [19].

## IV. $L_q$-NORMS OF GENERAL ORTHOGONAL POLYNOMIALS: ASYMPTOTICS ($q \to \infty$)

In this section we apply the Laplace method to obtain the asymptotic behaviour ($q \to \infty$) of the unweighted $L_q$-norms, $N_q(n)$, of the classical orthogonal polynomials, as given by (3). Since the Laplace method [31] demands the existence of a global maximum of the function $|y_n(x)|$, it is not applicable to the Hermite and Laguerre polynomials because the functions $|H_n(x)|$ and $|L_n^{(\alpha)}(x)|$ do not have such maximum in the intervals of orthogonality $(-\infty, +\infty)$ and $(0, +\infty)$, respectively. This is not the case for the Jacobi polynomials, which achieve the maximum

$$|P_n^{(\alpha,\beta)}(-1)| = \frac{(\beta+1)_n}{n!} \tag{30}$$

at $x = -1$ if $\beta \geq \alpha > -1$, $\beta \geq -\frac{1}{2}$ [21, Eq. 18.14.2], and

$$|P_n^{(\alpha,\beta)}(1)| = \frac{(\alpha+1)_n}{n!} \tag{31}$$

at $x = 1$ if $\alpha \geq \beta > -1$, $\alpha \geq -\frac{1}{2}$ [21, Eq. 18.14.1].

The use of an extended Laplace formula given by Theorem 1 [31, Chapter 2] allows us to obtain the following result:

**Theorem 1.** *The unweighted $L_q$ norm for the Jacobi polynomials, i.e.*

$$N_q(n) = \int_{-1}^{1} (1-x)^\alpha (1+x)^\beta \left|P_n^{(\alpha,\beta)}(x)\right|^q dx$$

*has the asymptotic behaviour*

$$N_q(n) = \left(\frac{(\beta+1)_n}{n!}\right)^q \left(2^\alpha \Gamma(\beta+1)\left(\frac{2(\beta+1)}{(n+\alpha+\beta+1)n}\right)^{\beta+1} q^{-\beta-1} + O\left(q^{-\beta-2}\right)\right), \tag{32}$$

*if* $\beta \geq \alpha > -1$, $\beta \geq -\frac{1}{2}$, *and*

$$N_q(n) = \left(\frac{(\alpha+1)_n}{n!}\right)^q \left(2^\beta \Gamma(\alpha+1)\left(\frac{2(\alpha+1)}{(n+\alpha+\beta+1)n}\right)^{\alpha+1} q^{-\alpha-1} + O\left(q^{-\alpha-2}\right)\right), \tag{33}$$

*if* $\alpha \geq \beta > -1$, $\alpha \geq -\frac{1}{2}$. ☐

*Proof.* We make use of Theorem 1 [31, Chapter 2], where the asymptotic behaviour of the integral

$$I(q) = \int_a^b \phi(x) e^{-qh(x)} dx$$

is considered for $q \to \infty$, where $h(x) > h(a)\ \forall x \in (a,b)$ and the expansions

$$h(x) = h(a) + a_0(x-a)^\mu + \cdots,$$

and

$$\phi(x) = b_0(x-a)^{\gamma-1} + \cdots,$$

hold. Then, the first order of the asymptotic behaviour is given as

$$I(q) = e^{-qh(a)}\left(\Gamma\left(\frac{\gamma}{\mu}\right)\frac{b_0}{\mu a_0^{\gamma/\mu}} q^{-\frac{\gamma}{\mu}} + O\left(q^{-\frac{1+\gamma}{\mu}}\right)\right). \tag{34}$$

In our case we have that

$$\phi(x) = (1-x)^\alpha (1+x)^\beta,$$

and

$$h(x) = -\ln\left|P_n^{(\alpha,\beta)}(x)\right|.$$

Let us consider first the case when $\beta \geq \alpha > -1$, $\beta \geq -\frac{1}{2}$, so that, according to Eq. (30), the maximum occurs at $x = a = -1$, fulfilling the requirement of the Theorem in [31]. Then we obtain the expansions

$$\phi(x) = 2^\alpha (x+1)^\beta + \cdots$$

so that $b_0 = 2^\alpha$, $\gamma = \beta+1$, and

$$h(x) = -\ln\left|P_n^{(\alpha,\beta)}(-1)\right| - \frac{1}{2}(n+\alpha+\beta+1)\frac{P_{n-1}^{(\alpha+1,\beta+1)}(-1)}{P_n^{(\alpha,\beta)}(-1)}(x+1) + \cdots,$$

so that $\mu = 1$ and

$$a_0 = -\frac{1}{2}(n+\alpha+\beta+1)\frac{P_{n-1}^{(\alpha+1,\beta+1)}(-1)}{P_n^{(\alpha,\beta)}(-1)} = \frac{1}{2}(n+\alpha+\beta+1)\frac{n}{\beta+1}.$$

The substitution of these values of $a_0$, $b_0$, $\gamma$ and $\mu$ in Eq. (34) gives rise to the desired result (32) of the Theorem for $\beta \geq \alpha > -1$, $\beta \geq -\frac{1}{2}$. Similarly, with the change of variable $x \to -x$, the result (33) for $\alpha \geq \beta > -1$, $\alpha \geq -\frac{1}{2}$, is obtained.

☐

## V. ENTROPY-LIKE INTEGRALS OF BESSEL POLYNOMIALS

In this section we determine the following parametric families of entropy-like integrals

$$\tilde{N}_q(n) \equiv \frac{1}{2\pi i}\int_\Delta \omega(x)\left(y_n(x)\right)^q\, dx \quad, \; q = 2k, k \in \mathbb{N}, \tag{35}$$

and

$$\tilde{W}_q(n) \equiv \frac{1}{2\pi i}\int_\Delta \left(\omega(x)y_n^2(x)\right)^q \, dx \quad , \; q \in \mathbb{N}, \tag{36}$$

for the Bessel hypergeometric polynomials $\mathcal{B}_n^{(\alpha)}(z)$ [6, 11, 12, 16]. Since the Bessel polynomials take complex values, these integrals have not the probabilistic interpretation of unweighted (Eq. (3)) and weighted (Eq. (4)) $L_q$ norms of these polynomials, respectively. Nevertheless, they can be evaluated by means of expansions (6) and (19), respectively.

To evaluate $\tilde{N}_q(n)$, we follow the procedure developed in Section II to reach the recurrence relation (13). The condition $A(t,a,b) = 0$ is also fulfilled by the Bessel polynomials because they are orthogonal in the unit circle of the complex plain so that $a = b$. Finally we obtain that

$$\tilde{N}_q(n) = \sum_{t=0}^{nq} \frac{q!}{(t+q)!} B_{t+q,q}(c_0, 2!c_1, \ldots, (t+1)c_t)\mu_t(\mathcal{B}), \tag{37}$$

where $c_i$ are the coefficients of the expansion of the polynomial in terms of ordinary powers, and $\mu_t$ denotes the Krall-Frink moment [16] of order $t$ of the weight function $\omega(x)$; i.e.

$$\mu_t(\mathcal{B}) = \frac{1}{2\pi i}\int_\Delta x^t \omega(x)\, dx \qquad ; t = 0, 1, \ldots \tag{38}$$

These moments satisfy the two-term recurrence relation

$$(t+\alpha+2)\mu_{t+1}(\mathcal{B}) + 2\mu_t(\mathcal{B}) = 0,$$

where we have operated as done in Section II and we have taken into account the main data of Bessel polynomials given in Table I. This recurrence relation can be exactly solved, giving rise to the following explicit expression:

$$\mu_t(\mathcal{B}) = \frac{(-2)^{\alpha+t+1}}{\Gamma(\alpha+t+2)}.$$

For the entropy-like integrals $\tilde{W}_q(n)$, defined in Eq. (36), we now follow an analogous procedure to that shown in Section III, yielding the expression

$$W_q(n) = \sum_{t=0}^{2nq} \frac{(2q)!}{(t+2q)!} B_{t+2q,2q}(c_0, 2!c_1, \ldots, (t+1)c_t) \cdot \Omega_q^{(\mathcal{B})}(t),$$

where

$$\Omega_q^{(\mathcal{B})}(t) = \frac{1}{2\pi i}\int_\Delta x^t [\omega(x)]^q \, dx.$$

These generalized moments $\Omega_q(t)$ satisfy the recurrence relation

$$\left(1 + \frac{\alpha q}{t+1}\right)\Omega_q^{(\mathcal{B})}(t) + \frac{2q}{t+1}\Omega_q^{(\mathcal{B})}(t-1) = 0,$$

that yields the following expression for the Bessel polynomials.

$$\Omega_q^{(\mathcal{B})}(t) = (-1)^{\alpha q+t+1} \frac{2^{\alpha q+t+1} q^{\alpha q+t+1}}{\Gamma(\alpha q+t+2)}. \tag{39}$$

In doing so, we have operated as in Section III and we have taken into account the main data of Bessel polynomials given in Table I.

Finally, let us point out that the calculation of the leading term of the asymptotics of the integrals $\tilde{N}_q(n)$ and $\tilde{W}_q(n)$ for $q \to \infty$ of Bessel polynomials requires the use of an approach of the steepest descents type, what lies beyond the scope of this paper.

## VI. CONCLUSIONS

The $L_q$-norms of probability distributions play an important role in various mathematical fields ranging from harmonic analysis to approximation theory. Moreover, the $L_q$-norms of the Rakhmanov probability density associated to the orthogonal hypergeometric polynomials $y_n(x)$ describe some entropic or information-theoretic quantities of these functions which measure their spreading over their orthogonality interval in different manners. In this work we have given a procedure to determine the unweighted and weighted $L_q$-norms ($q$ positive integer) of the general hypergeometric polynomials in terms of $q$ and the parameters of the corresponding weight function. It is mainly based on the expansion (6) of the powers of the involved polynomials $y_n(x)$, whose coefficients are multivariate Bell polynomials with variables given by the coefficients $c_k$ of the explicit expression (5) of the polynomials $y_n(x)$, which are well known in the literature (see e.g. [14, 21]). Then we have applied this procedure to the classical real orthogonal polynomials (Hermite, Laguerre and Jacobi), so that the $L_q$-norms are expressed in terms of the known expansion coefficients of the polynomials, whose values are well-known in the literature (see e.g. [14, 19, 21]).

In the case of the Bessel polynomials we have used the same techniques employed previously for the real hypergeometric polynomials to obtain some entropy-like integrals, formally related to the weighted and unweighted $L_q$-norms, but they do not possess a probabilistic interpretation due to the complex character of the polynomials.

In addition, since the resulting expression may be highbrow for large and very large values of $q$, we have used the extended Laplace method [31] to tackle the asymptotics ($q \to \infty$) of the unweighted $L_q$-norms of the classical orthogonal polynomials of Jacobi type. This method does not work in the Hermite and Laguerre cases, as already discussed. Moreover, in the Bessel case we need to use an approach of the steepest descents type, what is beyond the scope of this work.

Let us underline that since the orthogonal hypergeometric polynomials control the physical solutions of the Schrödinger equation of numerous quantum-mechanical potentials, this work contributes to pave the way to determine the entropic moments and the entropies of Rényi and Tsallis types of a great deal of quantum systems in an analytical manner.

Finally, we are aware that it would be desirable (almost mandatory, because of its mathematical and physical interest) to find the $L_q$-norms of the hypergeometric orthogonal polynomials for any real positive number $q$. However this would require a completely different approach than the one presented in this work, which is still unknown in the literature. The only alternative method [25] existing by now is also valid for integer positive values of $q$; it is based on some extended linearization formulas of $y_n(x)$, which allow us to express the $L_q$-norms in terms of some generalized Lauricella and Srivastava-Daoust functions with parameters and variables given by $n$, $q$ and the parameters of the weight function of the involved polynomials.

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# Chapter 3

# Applications

> *The meaning of life consists in the fact that it makes no sense to say that life has no meaning.*
> **Niels Bohr**

This chapter is structured in eleven sections. Each section begins with a brief description of the results of its quantum-physical topic followed by the scientific article published in an international review.

Shortly, the main results of each section are the following:

3.1 We show the effects of the Pauli exclusion principle on a generalized Heisenberg relation valid for general finite fermion systems (i.e., for all antisymmetric $N$-fermion wavefunctions), and various entropic uncertainty relations for finite fermion systems subject to central potentials.

3.2 We use various semiclassical inequalities and the informational extremization technique to determine the interplay effect between the spatial and spin dimensionalities on the Heisenberg-like uncertainty relation and the Fisher-information-based uncertainty relation of the multidimensional fermionic systems.

3.3 We develop a novel approach to obtain generalized position-momentum Heisenberg-like uncertainty relations, which take into account both the effects of the spatial and spin dimensionalities, for $d$-dimensional systems of $N$-fermions with spin $s$, and shown that they often improve the existing ones in the literature.

3.4 We analytically determine the Heisenberg-like uncertainty measures (radial expectation values) together with their corresponding uncertainty relations of the high dimensional hydrogenic systems in both position and momentum spaces. In addition, we explicitly bound some entropic uncertainty measures by means of the former measures.

3.5 We introduce the mathematical notion of monotonocity of the complexity measure of a probability function and we explore whether this property is satisfied by the basic measures of complexity, that is, Crámer-Rao, Fisher-Shannon and LMC as well as some generalizations of them.

3.6 We introduce a new complexity quantifier for the finite quantum many-particle systems, the monoparametric Fisher-Rényi complexity measure, and we examine its properties and applicability to hydrogenic systems.

3.7 We investigate the entropy and complexity properties of the spectral energy density of the blackbody radiation in $d$-dimensional universes by means of the dimensionality of the space and the temperature of the system.

3.8 We analytically determine the Rényi entropies of all orders for the Rydberg states of a $D$-dimensional harmonic oscillator in position space by developing a method to calculate the leading term of the asymptotics of the associated Laguerre polynomials (which control the harmonic oscillator wavefunctions) norms for very high polynomial's degree.

3.9 We explicitly calculate the dominant term of the Rényi, Shannon and Tsallis entropies for the Rydberg hydrogenic states in position space in terms of the nuclear charge and the quantum numbers that characterize the associated wavefunctions.

3.10 We show that some entanglement features (von Neumann and linear entropies) of finite many-particle systems can be comprehended by solely kinematical considerations. This is done by analytically analyzing the ground-state entanglement of a single particle of the $N$-boson and $N$-fermion Harmonium systems.

3.11 We investigate the entanglement features exhibited by the $s$-states of the quasi-exactly solvable $(d-1)$-Spherium system, which are given in terms of the physical and energetic parameters of the system.

## 3.1 Pauli effects in uncertainty relations

The Heisenberg uncertainty principle and the Pauli exclusion principle are two fundamental pillars of Quantum Physics. Nevertheless, the influence of the second principle on the mathematical formulations of the position-momentum Heisenberg principle (i.e., on the uncertainty relations), although they were intuited long time ago, had never yet been explicitly described until now.

In this section, it is shown the spin effects of the Pauli principle on two kind of fundamental uncertainty relations: the Heisenberg uncertainty relation (i.e., which uses the standard deviation as a measure of uncertainty) and the translationally invariant Fisher information-based uncertainty relation.

Specifically:

- We find the modifications that the Heisenberg and Fisher information uncertainty relations undergo due to take into account the effects of the spin in the general and central (i.e., the ones subject to a spherically symmetric mechano-quantical potential) finite multifermionic systems of arbitrary dimension, respectively, and
- we study the precision of these spin-dependent uncertainty relations in all the neutral atoms and single ions of the periodic table, from Hydrogen to Lawrencium by means of the self-consistent mean-field methods of Hartree-Fock type.

These results have been published in the article with coordinates: *I. V. Toranzo, P. Sánchez-Moreno, R. O. Esquivel and J. S. Dehesa, Chemical Physics Letters* ***614****, 1-4* ***(2014)****,* which is attached in the following.

# Pauli effects in uncertainty relations

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In this letter we analyze the effect of the spin dimensionality of a physical system in two mathematical formulations of the uncertainty principle: a generalized Heisenberg uncertainty relation valid for all antisymmetric N-fermion wavefunctions, and the Fisher-information-based uncertainty relation valid for all antisymmetric N-fermion wavefunctions of central potentials. The accuracy of these spin-modified uncertainty relations is examined for all atoms from Hydrogen to Lawrencium in a self-consistent framework.

## I. INTRODUCTION

The uncertainty principle and the Pauli principle are two fundamental pillars of quantum physics which have relevant consequences for the determination of quantum states of matter systems. Indeed, the former one prevents us to measure with arbitrary accuracy all the physical quantities which are classically within our reach, and the second one states that two identical fermions cannot occupy the same quantum state simultaneously. But perhaps the most distinguished issue of these two principles is the stability of matter [1]: atomic electrons operate as small radiating classical antennas that should fall on the nucleus at the time of a few billionths of a second, causing unstable atoms. The uncertainty principle comes to your rescue, enabling, together with the exclusion principle, the existence of electronic shells and subshells, and thus the periodic table and all the wealth of structural chemistry.

In fact, it is more than that. When we talk about the stability of microscopic systems (e.g., the stability of hydrogen), we simply mean that the total energy of the system cannot be arbitrarily negative. If the system would not have such lower bound to the energy, it would be posible to extract an infinite amount of energy, at least in principle. This stability of the first kind admits a generalization to the macroscopic systems, referred as stability of second kind. In this second type of stability, the lowest posible energy of the macroscopic systems depends at most linearly on the number of particles; or, in other terms, the lowest posible energy per particle cannot be arbitrarily negative as the number of particle increases. These two stability problems have a crucial relevance to understand the world around us. Both of them rely on the fermionic property of electrons; more specifically, they rely on the uncertainty principle and the Pauli principle.

The influence of the Pauli principle on the mathematical formulations of the uncertainty principle (i.e., the uncertainty relations) has been previously perceived (see e.g., [2]) but it has never been explicitly described, to the best of our knowledge. In this paper we tackle this issue. To be more specific, in our work we explore the effects of the

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Pauli exclusion principle on two concrete uncertainty relations of d-dimensional systems: a generalized Heisenberg relation valid for general finite fermion systems (i.e., for all antisymmetric N-fermion wavefunctions), and the Fisher-information-based uncertainty relation of finite fermion systems subject to a central potential. In other words, we investigate the combined balance of the effects of spatial and spin dimensionalities on these two fundamental uncertainty relations. We do this way because of the relevant role that space dimensionality plays in the analysis of the structure and dynamics of natural systems and phenomena, from atomic and molecular systems and d-dimensional systems (see e.g. the excellent monographs of Herschbach et al [3], Sen [4] and Dong [5]), quantum optics [6] to condensed matter (see e.g., [7–9]) and quantum information and computation (see e.g.,[10, 11]).
The structure of the present work is the following. In section II we first show the explicit dependence of a generalized Heisenberg uncertainty relation on the spin degree of freedom. As a particular case, the spin effects on the standard Heisenberg relation are given and the accuracy of the corresponding lower bound is examined for all atoms of the periodic table from Hydrogen to Lawrencium. In Section III, a similar study is carried out for the Fisher-information-based uncertainty relation in quantum systems with a central potential. Finally, some conclusions and open problems are given. Atomic units will be used throughout all the paper.

## II. GENERALIZED HEISENBERG UNCERTAINTY RELATIONS: PAULI EFFECTS

Let us consider a $d$-dimensional system of $N$ independent fermions of spin $s$ moving in an arbitrary potential. Let us denote by $\rho(\vec{r})$ the position probability density of the system, whose moment around the origin or radial expectation value of order $\alpha$ is given by

$$\langle r^\alpha \rangle = \int_{\mathbb{R}_d} \rho(\vec{r})\, r^\alpha \, d^d r, \;\; \alpha \geq 0,$$

and $\langle p^2 \rangle$ denote the corresponding radial momentum expectation value of second order. In this section we find a lower bound to the uncertainty product $\langle r^\alpha \rangle^{\frac{2}{\alpha}} \langle p^2 \rangle$, $\alpha > 0$, which only depends on $d$, $N$ and $\alpha$. Then, for $\alpha = 2$ we obtain the standard Heisenberg uncertainty relation with the spin-dependent effects. Finally, we numerically analyze the accuracy of this relation for all atoms with nuclear charge $Z = 1$ through 103.
First we show the main result: the generalized uncertainty relation of the form

$$\langle r^\alpha \rangle^{\frac{2}{\alpha}} \langle p^2 \rangle \geq A(\alpha, d)(2s+1)^{-\frac{2}{d}} N^{\frac{2}{d}+\frac{2}{\alpha}+1}, \tag{1}$$

with the constant

$$A(\alpha, d) = K(d) \cdot F(\alpha, d) \cdot C_d^{-\frac{2}{d}}\,, \tag{2}$$

where

$$K(d) = \frac{4\pi d}{d+2} \left[\Gamma\left(\frac{d}{2}+1\right)\right]^{2/d}, \tag{3}$$

$$F(\alpha, d) = \frac{2^{\frac{2}{d}+\frac{2}{\alpha}} \alpha^{1+\frac{4}{d}} (1+\frac{2}{d})^{1+\frac{2}{d}}}{\pi \left[\alpha(1+\frac{2}{d})+2\right]^{1+\frac{2}{d}+\frac{2}{\alpha}}} \cdot \left[\frac{\Gamma(\frac{d}{\alpha}+\frac{d}{2}+2)}{d(d+2)\Gamma(\frac{d}{\alpha})}\right]^{2/d}, \tag{4}$$

and $1 \leq C_d \leq 2$ for $d \geq 1$. There is a longstanding conjecture $C_d = 1$ due to Lieb and Thirring, which is now current belief; this is assumed heretoforth.
We will prove this result in two steps. First we use an inequality of Lieb-Thirring type [1] to bound the kinetic energy of the system in terms of the entropic moments

$$W_a[\rho] = \int_{\mathbb{R}_d} \rho(\vec{r})^a \, d^d r, \;\; a \geq 1,$$

and then, we bound these quantities in terms of the position moments $\langle r^\alpha \rangle$ of arbitrary order $\alpha$. Indeed, the Lieb-Thirring inequality appropriately modified [12] tells us that

$$\langle p^2 \rangle \geq K(d)(q\, C_d)^{-\frac{2}{d}} W_{1+\frac{2}{d}}[\rho]\,, \quad \text{with} \quad q = 2s+1 \tag{5}$$

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On the other hand, we can variationally bound the entropic moments $W_a[\rho]$ with the given constraints $\langle r^0 \rangle = 1$ and $\langle r^\alpha \rangle$, $\alpha > 0$. Following the lines of the method of Lagrange's multipliers described in Refs. [13, 14], we obtain the lower bound

$$W_a[\rho] \geq F(\alpha, a, d) \frac{N^{1+\frac{2}{d}+\frac{2}{\alpha}}}{\langle r^\alpha \rangle^{\frac{d}{\alpha}(a-1)}}, \tag{6}$$

with

$$F(\alpha, a, d) = \frac{a^a \alpha^{2a-1}}{\left[\Omega_d B\left(\frac{ad-d}{\alpha(a-1)}, \frac{2a-1}{a-1}\right)\right]^{a-1}} \times \left\{ \frac{(ad-d)^{ad-d}}{[a(\alpha+d)-d]^{a(\alpha+d)-d}} \right\}^{\frac{1}{\alpha}} \tag{7}$$

and $\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}$. The symbols $\Gamma(x)$ and $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ denote the well-known gamma and beta functions, respectively.

Now, putting $a = 1 + \frac{2}{d}$ into expressions (6)-(7) and multiplying the subsequent expression by the inequality (5) one finally obtains the wanted generalized uncertainty relation (1).

For the particular case $\alpha = 2$, the generalized uncertainty relation (1) gives the spin-dependent Heisenberg relation for $d$-dimensional $N$-fermion systems

$$\langle r^2 \rangle \langle p^2 \rangle \geq A(2,d)(2s+1)^{-\frac{2}{d}} N^{\frac{2}{d}+2} \tag{8}$$

with

$$A(2,d) = \left\{ \frac{d}{d+1} \left[\Gamma(d+1)\right]^{1/d} \right\}^2. \tag{9}$$

Let us note that the lower bound on the position-momentum Heisenberg product increases when the spatial dimensionality is increasing, so that the uncertainty relation gets improved. Note that for large values of the spatial dimensionality $d$, the bound (8) behaves as $d^2/e^2\, N^2 = 0.13533\, d^2 N^2$. Since the general spinless $d$-dimensional bound is $d^2/4\, N^2 = 0.25\, d^2 N^2$, it is interesting to highlight that there is a delicate balance between the spatial and spin dimensionality effects so that it turns out that the lower bound (8) is better or worse than the spinless bound when $d$ is small or large, respectively. This is because of the relative values of $d$, $s$, and $N$ in (8). Let us realize that for a given d-dimensional $N$-fermion system, the uncertainty relation is less accurate when the Pauli effects (i.e., spin dimensionality) increase.

Moreover, for $d = 3$ one trivially obtains the spin-dependent Heisenberg uncertainty relation for all real $N$-fermion systems

$$\langle r^2 \rangle \langle p^2 \rangle \geq \left( \frac{3}{4} 6^{1/3} \right)^2 (2s+1)^{-2/3} N^{8/3} \tag{10}$$

where the equality is reached for the harmonic oscillator, as previously known [2].

To have an idea of the accuracy of the Heisenberg relation (10), we study the uncertainty product $\langle r^2 \rangle \langle p^2 \rangle / N^{8/3}$ for all neutral atoms of the periodic table from Hydrogen ($N = 1$) to Lawrencium ($N = 103$) in a numerical Hartree-Fock framework. The results are shown in Fig. 1, where the lower bound is $\left(\frac{3}{4}6^{1/3}\right)^2 2^{-2/3} = 1.17005$ since the electron spin $s = 1/2$. Therein we can clearly observe two important phenomena: (i) the atomic shell structure is grasped by the Heisenberg uncertainty relation, and (ii) the accuracy of the inequality globally decreases when the nuclear charge of the atoms is increasing.

## III. FISHER-INFORMATION-BASED UNCERTAINTY RELATION: PAULI EFFECTS

The Fisher information of a $d$-dimensional system of $N$ fermions characterized by the quantum-mechanical probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ in position and momentum spaces are defined [15, 16] by

$$I[\rho] := \int \frac{|\vec{\nabla}\rho(\vec{r})|^2}{\rho(\vec{r})}\, d^d r \quad \text{and} \quad I[\gamma] := \int \frac{|\vec{\nabla}\gamma(\vec{p})|^2}{\gamma(\vec{p})}\, d^d p.$$

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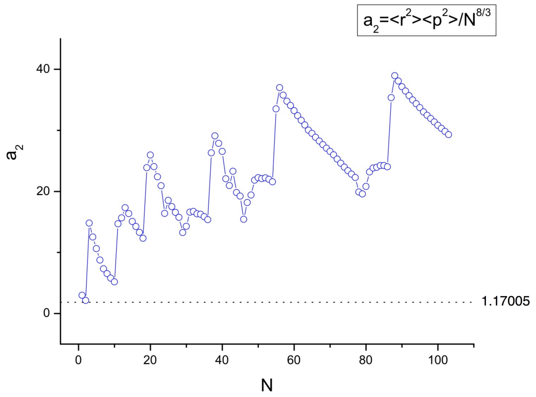

FIG. 1: Numerical study of the Heisenberg uncertainty relation for all neutral atoms with $N = 1$ to 103.

It has been proved that the product of these information-theoretical quantities is known to have an uncertainty character [17–19]. In fact, for the systems subject to central potentials of arbitrary type one knows that the Fisher-information-based uncertainty product is bounded from below by the standard Heisenberg uncertainty product [19] as

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

where $l = 0, 1, 2, ...$ and $m$ are two hyperquantum numbers. We should keep in mind that the angular part of the wavefunctions of a particle in a $d$-dimensional central potential is characterized by $d - 1$ hyperangular quantum numbers $l \equiv \mu_1 \geq \mu_2 \geq \cdots \geq \mu_{d-1} = |m| \geq 0$.

Then, taking into account this inequality together with the expressions (8)-(9) one finds the following spin-modified Fisher-information-based uncertainty relation

$$I[\rho] \times I[\gamma] \geq C(l, m, d)(2s+1)^{-\frac{2}{d}} N^{\frac{2}{d}+2}, \tag{11}$$

with the constant

$$C(l, m, d) = 16 \left[1 - \frac{2|m|}{2l+d-2}\right]^2 \times \left\{\frac{d}{d+1} [\Gamma(d+1)]^{\frac{1}{d}}\right\}^2. \tag{12}$$

This uncertainty relation holds for all $d$-dimensional $N$-fermion systems subject to a central potential of arbitrary type. It is interesting to note that for the values $l \equiv \mu_1 = \ldots = m = 0$, one has

$$I[\rho] \times I[\gamma] \geq \left\{\frac{4d}{d+1} [\Gamma(d+1)]^{\frac{1}{d}}\right\}^2 (2s+1)^{-\frac{2}{d}} N^{\frac{2}{d}+2}, \tag{13}$$

which is the Pauli-modified expression of the general spinless Fisher-information-based uncertainty relation $I[\rho] \times I[\gamma] \geq 4d^2N^2$ recently found [20]. Note that for large values of the spatial dimensionality $d$, the bound (13) behaves as $16e^{-2}d^2N^2 = 2.16536\, d^2N^2$. Again here, it is manifest the delicate balance between the spatial and spin dimensionality effects which makes the lower bound (13) to be better or worse than the spinless bound when $d$ is small or large, respectively. On the other hand, we observe as in the Heisenberg-like case discussed in the previous section, that the lower bound on the position-momentum Fisher-based product increases when the spatial dimensionality is increasing; and it decreases when the spin dimensionality is increasing, so that the Pauli effects worse the uncertainty relation, especially when the spatial dimensionality decreases. The global improvement of the Pauli-modified bound actually comes from the extra $(2/d)$-power which N has with respect to the spinless bound.

Then, for $d = 3$ we obtain the uncertainty relation

$$I[\rho] \times I[\gamma] \geq 9 \times 6^{2/3}\, (2s+1)^{-\frac{2}{3}} N^{\frac{8}{3}}$$

for real $N$-fermion systems. So, for electronic systems ($s = \frac{1}{2}$), one has

$$I[\rho] \times I[\gamma] \geq 3^{\frac{8}{3}} N^{\frac{8}{3}}$$

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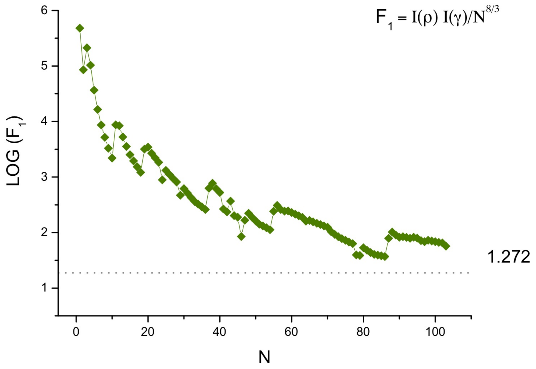

FIG. 2: Numerical study of the Fisher-information-based uncertainty relation for all neutral atoms with $N = 1$ to 103.

The accuracy of this relation is numerically examined in Fig. 2 for all neutral atoms of the periodic table from Hydrogen ($N = 1$) through Lawrencium ($N = 103$) in a Hartree-Fock framework. The lower bound is $\log 3^{8/3} = 1.272\ldots$. Here again we first observe that the known atomic shell structure is grasped by the Fisher-information-based uncertainty product. Moreover, contrary to the Heisenberg uncertainty product, this Fisher-like product globally decreases, and so its accuracy globally increases, when the nuclear charge of the atom is increasing. The different behavior of the Fisher uncertainty relation with respect to the Heisenberg one is due to the local character of the position and momentum Fisher informations; indeed, they are functionals of the gradient of position and momentum densities of the system, respectively.

## IV. CONCLUSIONS AND OPEN PROBLEMS

The Pauli-principle effects in two uncertainty relations (the generalized Heisenberg relations and the Fisher-information-based relation) have been investigated together with the spatial dimensionality contribution. Summarizing, we have explicitly found the effects of the combined contribution of the spatial and spin dimensionalities in two mathematical formulations of the quantum-mechanical uncertainty principle. First, for a system with a fixed number $N$ of fermions we have observed in both Heisenberg-like and Fisher cases that there exists a delicate balance between the contributions due to these two dimensionality effects, so that the lower bound increases or decreases with respect to the spinless general bound depending on whether the spatial dimensionality is small or large, respectively; thus, making more or less accurate the uncertainty relation. Second, when $N$ is increasing, the lower bound on the Heisenberg-like and Fisher-like uncertainty products globally increases; thus, the corresponding uncertainty relations better.

The Pauli effects in the uncertainty relations based on the Shannon, Rényi or the Tsallis entropies remain unknown. To determine them it is necessary to design a *modus operandi* different to the one used in this work. Indeed, here we have expressed the Heisenberg-like and Fisher-like uncertainty products in terms of the standard Heisenberg product $\langle r^2 \rangle \langle p^2 \rangle$, and then we have obtained a lower bound on it. In the Shannon and Rényi cases it is not yet possible to express the corresponding position and momentum sums [21–23] in terms of the standard Heisenberg product, and a similar situation occurs for the position and momentum quotients in the Tsallis or Rajagopal-Maassen-Uffink case [24, 25].

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***Chem. Phys. Lett. 614, 1-4 (2014)***

## 3.2 Heisenberg-like and Fisher-information-based uncertainty relations for multidimensional electronic systems

In this section we have derived some generalized Heisenberg-like uncertainty relations based on radial expectation values with order other than 2, which hold for arbitrary multidimensional fermionic systems. They have been obtained by means of the inequality-based Daubechies-Thakkar relations, semiempirically found by Thakkar for atomic and molecular systems and rigorously proved by Daubechies for $d$-dimensional quantum systems.

In addition:

- We have studied its accuracy for a large set of quantum systems: all the neutral and singly-ionized atoms of the periodic table and a great diversity of molecular systems, and
- we have found a lower bound on the uncertainty product of the position and momentum Fisher information of finite fermionic systems in terms of the number $N$ of its constituents.

These results have been published in the article with coordinates: *I. V. Toranzo, S. Lopez-Rosa, R. O. Esquivel and J. S. Dehesa, Physical Review A **91**, 062122 (**2015**)*, which is attached in the following.

# Heisenberg-like and Fisher-information-based uncertainty relations for $N$-electron $d$-dimensional systems

***Phys. Rev. A 91, 062122 (2015)***

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Heisenberg-like and Fisher-information-based uncertainty relations which extend and generalize previous similar expressions are obtained for $N$-fermion $d$-dimensional systems. The contributions of both spatial and spin degrees of freedom are taken into account. The accuracy of some of these generalized spinned uncertainty-like relations is numerically examined for a large number of atomic and molecular systems.

## I. INTRODUCTION

According to the density functional theory, the physical and chemical properties of atoms and molecules can be described in principle by means of functionals of the position electron density $\rho(\vec{r})$ and/or functionals of the momentum electron density $\gamma(\vec{p})$ [1–3]. Moreover, the qualitative and quantitative understanding of the electronic structure of atoms and molecules require in practice the knowledge of the expressions of the position and momentum space representations of the relevant physico-chemical quantities of these systems [4, 5]. These quantities can be fully determined by the position ordinary and frequency or entropic moments which for $d$-dimensional systems are given by

$$\langle r^k \rangle = \int_{\mathbb{R}_d} r^k \rho(\vec{r})\, d^d r, \tag{1}$$

$$W_q[\rho] = \int_{\mathbb{R}_d} \rho^q(\vec{r})\, d^d r \tag{2}$$

respectively, under certain conditions. A similar statement can be said for the momentum density $\gamma(\vec{p})$ in terms of the corresponding momentum moments $\langle p^k \rangle$ and $Z_q[\gamma]$. The notation $r = |\vec{r}|$ and $p = |\vec{p}|$ is used throughout the paper.

The connections between these moments in the two conjugate position and momentum spaces are very important for both fundamental and practical reasons. Indeed, the position-momentum uncertainty principle for quantum systems that generalizes the seminal variance-based formulation of Heisenberg can be expressed in a more accurate and useful manner by use of ordinary moments of order higher than 2 [6–10] and/or by means of entropic moments [13]. On the other hand, numerous physical and chemical properties can be expressed in terms of some ordinary and entropic moments in both position and momentum representations [4, 10, 11]. Indeed, they describe and/or are closely related to some fundamental and/or experimentally accesible quantities, such as the diamagnetic susceptibility ($\langle r^2 \rangle$), the kinetic energy ($\langle p^2 \rangle$), the Thomas-Fermi kinetic energy ($W_{5/3}$), the Dirac-Slater exchange energy ($W_{4/3}$, $\langle p \rangle$), the

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height peak of the Compton profile ($\langle p^{-1}\rangle$), the relativistic Breit-Pauli energy ($\langle p^4\rangle$), the initial value of the Patterson function of x-ray crystallography ($W_3$, $\langle p^{-3}\rangle$), the total electron-electron repulsion energy ($\langle p^3\rangle$), etc. Moreover, the position and momentum moments can be experimentally extracted as discussed elsewhere [2, 4, 5, 12].

These ordinary and frequency moments play a relevant role in the analysis of the structure and dynamics of natural systems and phenomena, from atomic and molecular systems to systems with non-standard dimensionalities, as can be seen in the excellent monographs of Dong [14], Herschbach et al [15] and Sen [16].

This work deals with some generalized position-momentum uncertainty relations which go far beyond the familiar uncertainty relation based on the standard deviation. By now, it is well known that the standard deviation is not at all the best measure of uncertainty because at times it cannot capture the essence of the uncertainty principle. The standard deviation is a reasonable measure of the spread of a probability distribution with a single hump (e.g., the gaussian and quasi-gaussian distributions). However, when the probability distribution has more than one hump, the standard deviation loses some of its usefulness, especially in connection with the notion of uncertainty. This problem is caused by the fact that the standard deviation attributes an ever increasing weight to the tails of the probability distribution; thus, a very slight contribution to the probability density, provided that it is located very far from the center, may cause the standard distribution to blow up. These observations have been reiteratively pointed out by various authors (see e.g. [13, 71–74].

Accordingly, a variety of alternative formulations have been proposed which are based on other spreading measures of the probability distributions such as the ordinary moments of order higher orders and the frequency moments [6–10, 13, 16, 55]. Although endless variations on this theme can be given, let us just mention one practical application of these uncertainty inequalities: the problem of estimating the ground state energy for some given Hamiltonian. This technical problem has almost created an entire branch of mathematical physics, as can be seen in [23] and references therein. Needless to say, on the other hand, that lower and upper bounds for the products of moments in the two conjugate position and momentum spaces are very useful and relevant because, among many other things, they describe physical quantities which are experimentally accesible; in addition, the momentum-space quantities are not directly accessible, either in principle or due to experimental impediments.

Based on numerous semiclassical and Hartree-Fock-like ground-state calculations in atoms and diatomic molecules [4, 17–19], it has been found approximate relationships and semiclassical bounds connecting the momentum ordinary moments and position entropic moments of the form

$$\langle p^k\rangle \leq c_k W_{1+\frac{k}{3}}[\rho] \quad \text{for} \quad k=-2,-1 \tag{3}$$

and

$$\langle p^k\rangle \geq c_k W_{1+\frac{k}{3}}[\rho] \quad \text{for} \quad k=1,2,3,4 \tag{4}$$

with $c_k = 3(3\pi^2)^{k/3}(k+3)^{-1}$. Moreover the case $k=2$ was already conjectured by Lieb, and weaker versions of it have been rigorously proved, as discussed elsewhere [20]. These semiclassical bounds, which were found to be fulfilled by a large diversity of ground-state atoms and molecules [7, 8, 20], can be extended to $d$-dimensional systems of $N$ fermions with spin $s$ as

$$\langle p^k\rangle \geq K_d(k) q^{-\frac{k}{d}} W_{1+\frac{k}{d}}[\rho], \tag{5}$$

where $k>0$, $q=2s+1$ and

$$K_d(k) = \frac{d}{k+d}(2\pi)^k \frac{\left[\Gamma\left(1+\frac{d}{2}\right)\right]^{k/d}}{\pi^{k/2}}. \tag{6}$$

And for $k<0$ the sign of inequality (5) is inverted. Note that expression (5) simplifies to (3)-(4) for $d=3$ and $s=1/2$, since then $K_d(k) = 2^{\frac{k}{3}} c_k$. In fact, Eq. (5) with constant $K'_d(k) = K_d(k) \times B(d,k)$ with $B(d,k) = \left\{\Gamma\left(\frac{d}{k}\right) \inf_{a>0}\left[a^{-\frac{d}{k}}\left(\int_a^\infty du\, e^{-u}(u-a)u^{-1}\right)^{-1}\right]\right\}^{-\frac{k}{d}}$ has been rigorously proved by Daubechies [21]. Table I collects some values of the constant $B(d,k)$ in terms of $d$ and $k$.

| $B(d,k)$ | | | | |
|---|---|---|---|---|
| $k$ \ $d$ | 1 | 2 | 3 | 4 |
| 1 | 0.165728 | 0.405724 | 0.537513 | 0.618094 |
| 2 | 0.021331 | 0.165728 | 0.303977 | 0.405724 |
| 3 | 0.002056 | 0.061935 | 0.165728 | 0.262190 |
| 4 | 0.000158 | 0.021331 | 0.086812 | 0.165728 |

TABLE I: $B(d,k)$ for different values of $d$ and $k$.

As well, a number of authors have published some rigorous $d$-dimensional bounds of the same type [22, 23] with much less accuracy.

On the other hand, similar expressions have been found which depend not on any global spreading measure (like the moments $W_\alpha[\rho]$) but on measures of the position probability with a property of locality (because they depend on the gradient of $\rho$), like the *translationally or shift-invariant Fisher information* $I_d[\rho]$. Indeed, Zumbach [24] has found that

$$\langle p^2\rangle \leq \frac{1}{2}\left[1+C_d\left(\frac{N}{q}\right)^{2/3}\right] I_d[\rho], \tag{7}$$

where the non-optimal constant $C_d$ is given by

$$C_d = (4\pi)^2\frac{5d^2}{d+2}\left(\frac{2}{d+2}\right)^{2/d} \tag{8}$$

for $1 \leq d \leq 5$, and $I_d[\rho]$ denotes the shift-invariant Fisher information of the electron probability density for $d$-dimensional $N$-fermion systems defined [25] as

$$I_d[\rho] = \int_{\mathbb{R}_d} \frac{|\vec{\nabla}_d\sqrt{\rho(\vec{r})}|^2}{\rho(\vec{r})}\, d^d r = 4\int_{\mathbb{R}_d}\left(\vec{\nabla}_d\sqrt{\rho(\vec{r})}\right)^2 d^d r, \tag{9}$$

where $\vec{\nabla}_d$ denotes the $d$-dimensional gradient operator given by

$$\vec{\nabla}_d = \frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\sum_{i=1}^{d-2}\frac{1}{\prod_{k=1}^{i-1}\sin\theta_k}\frac{\partial}{\partial\theta_i}\hat{\theta}_i + \frac{1}{r\prod_{i=1}^{d-2}\sin\theta_i}\frac{\partial}{\partial\varphi}\hat{\varphi},$$

where the symbol $\hat{a}$ denotes the unit vector associated to the corresponding coordinate. Notice that for $d = 3$ the constant is $C_3 = 9(4\pi)^2\left(\frac{2}{5}\right)^{2/3}$, and the Fisher information $I_3[\rho] = 4\int_{\mathbb{R}_3}(\nabla\sqrt{\rho})^2\, d^3r$ denotes the standard Fisher information of real $N$-fermion systems [25].

The one-dimensional shift-invariant Fisher information is the translationally invariant version of the one-dimensional parametric Fisher information so much used to establish the ultimate bounds on sensitivity of measurements, which is a major goal of the parametric estimation theory. The latter quantity refers to the information about an unknown parameter in the probability distribution estimated from observed outcomes. Let us assume that we want to estimate a parameter $\theta$ doing $n$ measures in an experiment. These data, $\vec{y} \equiv \{y_i\}_{i=1}^n$, obey $y_i = \theta + x_i$ where $\vec{x} \equiv \{x_i\}_{i=1}^n$ are added noise values. The noise $\vec{x}$ is assumed to be intrinsic to the parameter $\theta$ under measurement ($\theta$ has a definite but unknown value). This system is specified by a conditional probability law $p_\theta(\vec{y}|\theta) = p(y_1, y_2, \cdots, y_n|\theta)$ and $\hat{\theta}(\vec{y}|\theta)$ is, on average, a better estimate of $\theta$ as compared to any of the data observables, $\hat{\theta}(\vec{y}) = \theta$. In this case, we can define the parametric Fisher information as

$$I \equiv \int \left[\frac{\partial \ln p_\theta(\vec{y})|\theta}{\partial\theta}\right]^2 p_\theta(\vec{y}|\theta)d\vec{y}, \tag{10}$$

which fulfils the known Crámer-Rao inequality $\sigma^2 \times I \geq 1$, where $\sigma^2$ is the mean-square error given by

$$\sigma^2 = \int \left[\hat{\theta}(\vec{y}) - \theta\right]^2 p_\theta(\vec{y})d\vec{y}. \tag{11}$$

Then, the parametric Fisher information measures the ability to estimate a parameter; that is, it gives the minimum error in estimating $\theta$ from the given probability density $p(\vec{y}\,|\theta\,)$. In the particular case of $n=1$, $p_\theta(\vec{y}|\theta)=p(y|\theta)$ and the fluctuations $x$ are invariant to the size of $\theta$, $p_\theta(y|\theta)=p_x(y-\theta)$ with $x=y-\theta$ (i.e. shift invariance); one has

$$I=\int\left[\frac{\partial\ln p(x)}{\partial x}\right]^2 p(x)dx=\int\frac{[p'(x)]^2}{p(x)}dx, \tag{12}$$

which is the one-dimensional *translationally-invariant Fisher information.* The extension to d dimensions is given by expression (9). This quantity is a measure of the gradient content of the density, so that it is very sensitive to the fluctuations of the density. Then, it quantifies the narrowness or localization of the density; so, it is a measure of the system disorder. See e.g., the monograph of Frieden [25] and references therein for further details.

Nowadays the notion of translationally-invariant Fisher information is playing an increasing role in numerous fields [25], in particular, for many-electron systems, partially because of its formal resemblance with kinetic [25–28] and Weiszäcker [1, 29] energies. The translationally-invariant Fisher information, contrary to the Shannon entropy, is a local measure of spreading of the density $\rho(\vec{r})$. The higher this quantity is, the more localized is the density, the smaller is the uncertainty and the higher is the accuracy in estimating the localization of the particle. However, it has an intrinsic connection with Shannon entropy via the de Bruijn inequality [30, 31] as well as a simple connection with the precision (variance $V\,[\rho]$) of the experiments by means of the celebrated Crámer-Rao inequality [30, 31], $I\,[\rho]\times V\,[\rho]\geq d^2$.

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 [33], the most distinctive nonlinear spectroscopic phenomena (avoided crossings) of atomic systems in strong external fields [32], the periodicity and shell structure in the periodic table of chemical elements [35] and the transition state and the bond breaking/forming regions of some specific chemical reactions [36], as well as to systematically investigate the origin of the internal rotation barrier between the eclipsed and staggered conformers of ethane [37] and the steric effect [38].

Recently, much effort is being devoted to build up a mathematical formulation of the quantum uncertainty principle based upon the Fisher-information measures evaluated on the conjugate position and momentum spaces. Nowadays it remains a strongly controversial problem [34, 39–44]. First, it was conjectured [40] in 2000 that the position-momentum Fisher information product had the lower bound $I_1(\rho)I_1(\gamma)\geq 4$ for one-dimensional quantum systems with the position and momentum densities $\rho(x)=|\Psi(x)|^2$ and $\gamma(p)=|\Phi(p)|^2$, being $\Phi(p)$ the Fourier transform of $\Psi(x)$. Later in 2006 it was proved [39] that this conjecture only holds for all real, even, one-dimensional wavefunctions $\Psi(x)$. Then, in 2011 this result was rigorously generalized [42] as $I_d(\rho)I_d(\gamma)\geq 4d^2$ for the $d$-dimensional systems provided that either the position wavefunction $\Psi(\vec{r})$ or the corresponding momentumspace wavefunction $\Phi(\vec{p})$ is real [42].

In addition, it has been found [34] that the uncertainty product $I_3(\rho)I_3(\gamma)$ can be explicitly expressed in terms of the Heisenberg product $\langle r^2\rangle\langle p^2\rangle$ for any three-dimensional central potential; even more, it is fulfilled that $I_3(\rho)I_3(\gamma)\geq f(l,m)$, where $f(l,m)$ is a known simple function of the orbital and magnetic quantum numbers, given by $l$ and $m$, respectiveley. Furthermore, let us also mention that the product of position and momentum Fisher information has been proposed [40] as a measure of joint classicality of quantum states, what has been recently used for wave packet and quantum revivals [53].

For completeness let us mention that a natural extension to the classical parametric Fisher information mentioned above, has been coined as (parametric) quantum Fisher information (see e.g., the monographs [45, 46]) and successfully applied to quantum statistical inference and estimation theory in various directions (see e.g. [47–52] and references therein).

In this work, we will use the $d$-dimensional Daubechies-Thakkar and Zumbach expressions, given by (5) and (7) respectively, to obtain novel (moment-based) Heisenberg-like and Fisher-information-based uncertainty-like relations for d-dimensional systems of $N$ fermions with spin $s$ in sections II and III, respectively. These relations extend and generalize previous general and specific uncertainty results of similar type. In addition, the accuracy of these results for a large variety of neutral and singly-ionized atoms and molecules is examined.

## II. HEISENBERG-LIKE UNCERTAINTY RELATIONS

Let us here obtain lower bounds on the Heisenberg-like uncertainty products $\langle r^\alpha\rangle\langle p^k\rangle$, with $\alpha\geq 0$ and $-2\leq k\leq 4$ for $d$-dimensional $N$-electron systems by taking into account both spatial and spin degrees of freedom. First we derive the bounds based on position and momentum expectation values with positive order, and then the corresponding ones involving momentum expectation values with a negative order. These results extend, generalize and/or improve similar results from various authors (see, e.g. [10, 12, 54, 56–61] and references therein).

### A. Uncertainty products $\langle r^\alpha\rangle\langle p^k\rangle$, with $\alpha \geq 0$ and $0 \leq k \leq 4$

We begin with the semiclassical lower bound on the momentum expectation value $\langle p^k\rangle$ given by Eqs. (5)-(6) in terms of the position entropy moments $W_{1+\frac{k}{d}}[\rho]$. Then, we apply the variational method of Lagrange's multipliers described in Refs. [62, 63] to bound the entropic moments $W_q[\rho]$. Indeed, let us minimize the quantity $\int[\rho(\vec{r})]^q\, d^dr$ subject to the constraints $\langle r^0\rangle \equiv \int \rho(\vec{r})\, d^dr = N$ and $\langle r^\alpha\rangle = \int r^\alpha \rho(\vec{r})\, d^dr$, $\alpha > 0$, by taking variations of the form

$$\delta\left\{\int[\rho(\vec{r})]^q\, d^dr - \lambda\int r^\alpha\rho(\vec{r})\, d^dr - \mu\int\rho(\vec{r})\, d^dr\right\} = 0,$$

where $\lambda$ and $\mu$ are Lagrange multipliers. One finds that the minimizer solution is given by the density

$$f(r) = \begin{cases} C(a^\alpha - r^\alpha)^{1/(q-1)}, & r \leq a, \\ 0, & r > a \end{cases}$$

where the values of the factor $C$ and the parameter $a$ are determined so that the two previous constraints are fulfilled. In fact, following the lines indicated in Refs. [62, 63, 70], one can show that the quantity

$$\int[f(r)]^q\, d^dr = F\ \langle r^\alpha\rangle^{-\frac{d}{\alpha}(q-1)} N^{\frac{d}{\alpha}(q-1)+q}$$

is a lower bound of the wanted entropic moment $W_q[\rho]$, where F is a known analytic function of the parameters $q, \alpha$ and $d$. Then, with $q = 1 + \frac{k}{d}$ one finally obtains the rigorous inequality

$$W_{1+\frac{k}{d}}[\rho] \geq F(d,\alpha,k)\langle r^\alpha\rangle^{-\frac{k}{\alpha}} N^{1+k\left(\frac{1}{\alpha}+\frac{1}{d}\right)}, \tag{13}$$

where

$$\begin{aligned} F(d,\alpha,k) &= \frac{\left(1+\frac{k}{d}\right)^{1+\frac{k}{d}}\alpha^{1+\frac{2k}{d}}}{\left[\Omega_d B\left(\frac{d}{\alpha}, 2+\frac{d}{k}\right)\right]^{\frac{k}{d}}} \\ &\times \left\{\frac{k^k}{\left[\left(1+\frac{k}{d}\right)\alpha + k\right]^{\left(1+\frac{k}{d}\right)\alpha+k}}\right\}^{\frac{1}{\alpha}}, \end{aligned} \tag{14}$$

where $\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the volume of the unit hypersphere.

Then, from Eqs. (5) and (13) we obtain the generalized Heisenberg-like uncertainty relation given by

$$\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq \mathcal{F}(d,\alpha,k)\, q^{-\frac{k}{d}} N^{1+k\left(\frac{1}{\alpha}+\frac{1}{d}\right)}, \tag{15}$$

where $\mathcal{F}(d,\alpha,k) = K_d(k)F(d,\alpha,k)$. From this general inequality of $N$-fermion systems with spatial dimensionality $d$ and spin dimensionality $q = 2s+1$, we can make numerous observations. First, the case $k = 2$ has been recently found [64] by means of the Lieb-Thirring inequality. Second, there exists a delicate balance between the contributions of the spatial and spin degrees of freedom making the relation more or less accurate than the corresponding spinless inequality for either small or large d, respectively. Third, for $d = 3$ and $q = 2$ we obtain

$$\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq \mathcal{F}(3,\alpha,k)\, 2^{-\frac{k}{3}} N^{\frac{k}{\alpha}+\frac{k+3}{3}}, \tag{16}$$

which holds for all N-electron systems. In particular, for $\alpha = k = 2$ one has $\langle r^2\rangle\langle p^2\rangle \geq 1.85733 \times q^{-\frac{2}{3}} N^{\frac{8}{3}} = 1.17005 N^{\frac{8}{3}}$. A number of other Heisenberg-like relations, which are also instances of this inequality, is explicitly given in Table II.

Let us now study the accuracy of the uncertainty relation (15) for some values of $\alpha$ and $k$ in a large set of $N$-electron systems of neutral and singly-ionized atoms as well as in a variety of molecules. This is done in Fig.1 and Fig.2 for the Heisenberg-like products $\langle r\rangle\langle p\rangle$ and $\langle r^2\rangle^{1/2}\langle p\rangle$, respectively, for all ground-state neutral atoms of the periodic table from Hydrogen ($N = 1$) to Lawrencium ($N = 103$) and their corresponding anions and cations, as well as for 87

| $\langle r^{\alpha}\rangle^{\frac{k}{\alpha}}\langle p^{k}\rangle \geq f(N)$ | | | | |
|---|---|---|---|---|
| $\alpha \setminus k$ | 1 | 2 | 3 | 4 |
| 1 | $\frac{9}{49}(45\pi)^{1/3}N^{7/3}$ | $\frac{243}{5324}(35\pi)^{2/3}N^{11/3}$ | $\frac{243}{625}\pi N^{5}$ | $\frac{841995}{39617584}(3465\pi^{4})^{1/3}N^{19/3}$ |
| 2 | $\frac{9}{22}\sqrt{\frac{3}{11}}(35\pi)^{1/3}N^{11/6}$ | $\frac{9}{16}3^{2/3}N^{8/3}$ | $\frac{135}{196}\sqrt{\frac{3}{7}}\pi N^{7/2}$ | $\frac{2268}{28561}\left(\frac{21}{13}\pi^{2}\right)^{1/3}\frac{\Gamma\left(\frac{17}{4}\right)}{\Gamma\left(\frac{11}{4}\right)}N^{13/3}$ |
| 3 | $\frac{3}{5}\left(\frac{9}{5}\pi\right)^{1/3}N^{5/3}$ | $3\left(\frac{45\pi}{196\sqrt{7}}\right)^{2/3}N^{7/3}$ | $\frac{1}{2}\pi N^{3}$ | $\frac{189}{484}\left(\frac{63}{44}\pi^{4}\right)^{1/3}N^{11/3}$ |
| 4 | $\frac{3}{38}\left(\frac{3}{19}\right)^{1/4}(3465\pi)^{1/3}N^{19/12}$ | $\frac{24\sqrt{3}}{169}\left(\frac{4\pi}{\sqrt{13}}\right)^{1/3}\left[\frac{\Gamma\left(\frac{17}{4}\right)}{\Gamma\left(\frac{3}{4}\right)}\right]^{2/3}N^{13/16}$ | $\frac{21}{4}\left(\frac{3}{11}\right)^{7/4}\pi N^{11/4}$ | $\frac{567}{3200}\left(\frac{63}{2}\right)^{1/3}\frac{\pi^{2}}{\left[\Gamma\left(\frac{3}{4}\right)\Gamma\left(\frac{11}{4}\right)\right]^{4/3}}N^{10/3}$ |

TABLE II: Some generalized Heisenberg-like uncertainty relations for $N$-electron systems, where both spatial and spin degrees of freedom are taking into account.

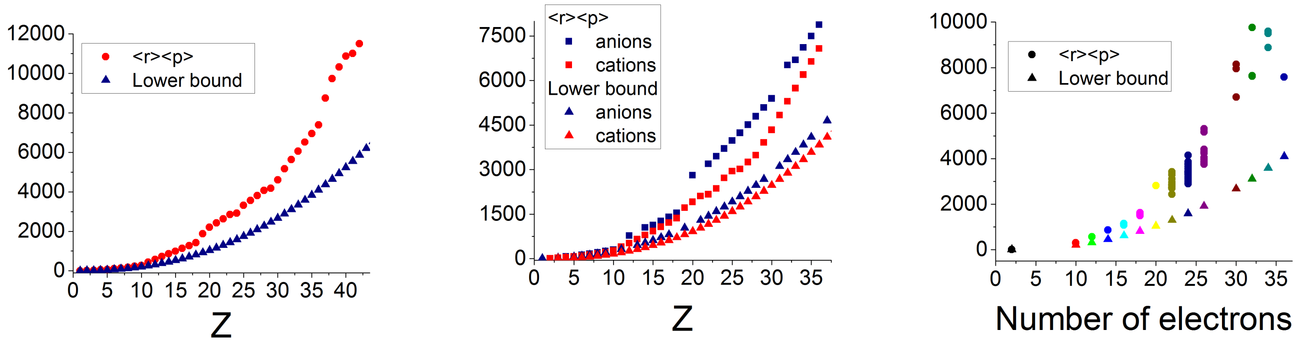

FIG. 1: (Color on line) Accuracy of $\langle r\rangle\langle p\rangle$ for all neutral atoms (left), all singly-ionized atoms (center) and 87 polyatomic molecules (right). The symbol Z denotes the nuclear charge for atoms and ions. The colors in the molecular graph on the right correspond to different isoelectronic groups as explained in Appendix.

polyatomic molecules (see Appendix). The molecular set chosen for the numerical study includes different types of chemical organic and inorganic systems (aliphatic and aromatic hydrocarbons, alcohols, ethers, ketones). It represents a variety of closed shell systems, radicals, isomers as well as molecules with heavy atoms such as sulphur, chlorine, magnesium and phosphorous. The symbol $Z$ in both figures denotes the nuclear charge for atoms and ions. The colors in the molecular graph on the right of the two figures correspond to different isoelectronic groups described in Appendix.

The accurate near-Hartree-Fock wavefunctions of Koga et al [65, 66] have been used to evaluate the atomic uncertainty products. In the molecular case we have used the Gaussian 03 suite of programs [67] at the $CISD/6-311++G(3df,2p)$ level of theory. For this set of molecules we have calculated position and momentum moments defined previously by employing software developed in our laboratory along with 3D numerical integration routines [68] and the DGRID suite of programs [69].

For each figure the numerical values of these uncertainty products and the corresponding bounds (as given by Table I) are represented in terms of the number of electrons of the system under consideration. We first observe that the Heisenberg-like relations are indeed fulfilled in all cases, what is a check of our theoretical results. Then, we notice that our bounds are quite accurate for light electronic systems. Moreover, their accuracy decreases as the number of electrons increases. So, there is still a lot of space for improvement in heavy N-electron systems.

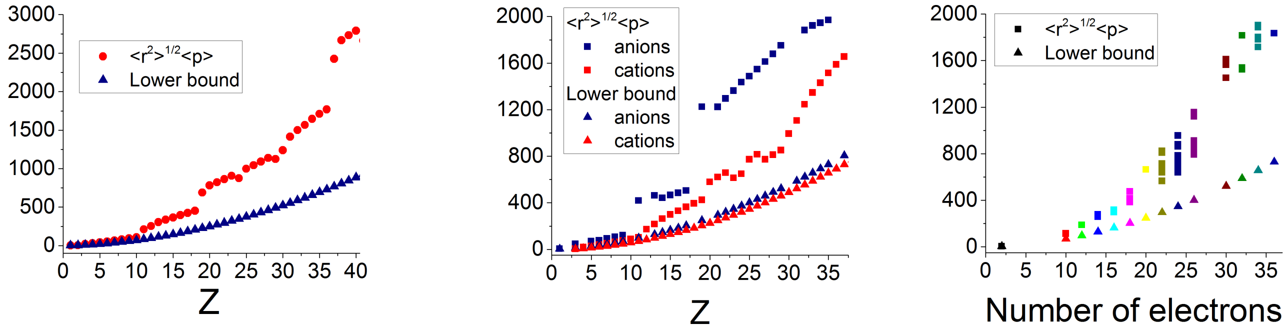

FIG. 2: (Color on line) Accuracy of $\langle r^2\rangle^{1/2}\langle p\rangle$ for all neutral atoms (left), all singly-ionized atoms (center) and 87 polyatomic molecules (right). The symbol Z denotes the nuclear charge for atoms and ions. The colors in the molecular graph on the right correspond to different isoelectronic groups as explained in Appendix.

### B. Uncertainty products $\langle r^\alpha\rangle\langle p^k\rangle$, with $\alpha \geq 0$ and $k \leq 0$

Here we start from the semiclassical lower bound on the momentum expectation value $\langle p^k\rangle$ given by Eqs. (5)-(6) duly inverted because now k is assumed to have negative values, so that we have the following upper bound

$$\langle p^k\rangle \leq K_d(k) q^{-\frac{k}{d}} W_{1+\frac{k}{d}}[\rho], \tag{17}$$

in terms of the position entropy moments $W_{1+\frac{k}{d}}[\rho]$. Now, we use the above-mentioned variational method of Lagrange's multipliers given in Refs. [62, 63, 70] to bound the entropic moments $W_{k'}[\rho]$ with the given constraints $\langle r^0\rangle = N$ and $\langle r^\alpha\rangle$, $\alpha < 0$, obtaining the rigorous inequality

$$W_{k'}[\rho] \leq G_d(\alpha, k')\langle r^\alpha\rangle^{-\frac{k'}{\alpha}} N^{1+k'\left(\frac{1}{\alpha}+\frac{1}{d}\right)}, \tag{18}$$

where $k' < 1$, $\alpha > \frac{d(1-k')}{k'}$, and

$$G_d(\alpha, k') = \alpha^{1+\frac{2k'}{d}}(-k')^{k'/\alpha}\left(\frac{1}{\alpha+\frac{\alpha k'}{d}+k'}\right)^{k'\left(\frac{1}{\alpha}+\frac{1}{d}\right)+1}$$
$$\times\left(\frac{k'}{d}+1\right)^{\frac{k'}{d}+1}\left(\Omega_d\, B\left(-1-\frac{d(k'+\alpha)}{k'\alpha}, \frac{d}{\alpha}\right)\right)^{-\frac{k'}{d}} \tag{19}$$

where again $\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$.

Finally, from Eqs. (18) and (17) we obtain in an algebraic manner the Heisenberg-like uncertainty relation

$$\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \leq \mathcal{G}_d(\alpha, k) q^{-k/d} N^{1+k\left(\frac{1}{\alpha}+\frac{1}{d}\right)}, \tag{20}$$

with $k < 0$, $\alpha > -\frac{3k}{k+d}$, and $\mathcal{G}_d(\alpha, k) = K_d(k)G_d(\alpha, k)$, for $d$-dimensional systems of $N$ fermions with spin $s$.

This fermionic inequality gives rise to the two following uncertainty relations

$$\langle r^\alpha\rangle^{-\frac{1}{\alpha}}\langle p^{-1}\rangle \leq \mathcal{G}_3(\alpha, -1)\, 2^{1/3} N^{\frac{2}{3}-\frac{1}{\alpha}}, \quad \alpha > \frac{3}{2}, \tag{21}$$

and

$$\langle r^\alpha\rangle^{-\frac{2}{\alpha}}\langle p^{-2}\rangle \leq \mathcal{G}_3(\alpha, -2)\, 2^{1/3} N^{1+k\left(\frac{1}{\alpha}+\frac{1}{d}\right)}, \quad \alpha > 6,$$

for real $N$-electron systems, since then we have $d = 3$ and $q = 2$ and the exact $\langle p^k\rangle$ which are finite require that $k \geq -2$. As particular cases we have the Heisenberg-like uncertainty relations

$$\langle r^2\rangle^{-\frac{1}{2}}\langle p^{-1}\rangle \;\leq\; 3^{\frac{1}{6}}2^{\frac{1}{3}}N^{\frac{1}{6}} \approx 1.51309N^{\frac{1}{6}}, \tag{22}$$

$$\langle r^3\rangle^{-\frac{1}{3}}\langle p^{-1}\rangle \;\leq\; \left(\frac{6}{\pi}\right)^{\frac{1}{3}} N^{\frac{1}{3}} \approx 1.2407N^{\frac{1}{3}}, \tag{23}$$

$$\langle r^4\rangle^{-\frac{1}{4}}\langle p^{-1}\rangle \;\leq\; 2^{\frac{1}{2}}\left(\frac{3}{5}\right)^{\frac{5}{12}} N^{\frac{5}{12}} \approx 1.14308\,N^{\frac{5}{12}} \tag{24}$$

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by making $\alpha = 2, 3$ and 4, respectively in Eq. (21).

## III. FISHER-INFORMATION-BASED UNCERTAINTY RELATION

In this section we first express the position-momentum Fisher information product $I_d(\rho)I_d(\gamma)$ in terms of the Heisenberg uncertainty product $\langle r^2\rangle\langle p^2\rangle$ for $N$-electron $d$-dimensional systems. Then we use some results of the previous section to obtain a mathematical formulation of the position-mometum uncertainty principle for these systems. The resulting expressions extend and generalize various similar conjectures and inequalities in the sense already discussed in the first section [34, 39–42].

We begin with Eq. (7) and, due to the reciprocity of the position and momentum spaces, its *conjugate* inequality given by

$$\langle r^2\rangle \leq \frac{1}{2}\left[1 + C_d\left(\frac{N}{q}\right)^{2/d}\right] I_d[\gamma], \tag{25}$$

which lead to

$$I_d[\rho]I_d[\gamma] \geq \frac{4}{\left[1 + C_d\left(\frac{N}{q}\right)^{2/d}\right]^2}\langle r^2\rangle\langle p^2\rangle, \tag{26}$$

This expression clearly manifests the uncertainty-like character of the product of the position Fisher information and momentum Fisher information for $N$-fermion systems. Moreover, let us now take into account Eq. (15) with $\alpha = k = 2$, which gives the $d$-dimensional Heisenberg product [64]

$$\langle r^2\rangle\langle p^2\rangle \geq A(2,d)q^{-2/d}N^{2+2/d}, \tag{27}$$

with

$$A(2,d) = \left\{\frac{d}{d+1}[\Gamma(d+1)]^{1/d}\right\}^2.$$

Then, the combination of Eqs. (7) and (27) leads to the following lower bound on the position-momentum Fisher-information product of $N$-fermion $d$-dimensional systems

$$I_d[\rho]I_d[\gamma] \geq 4A(2,d)\frac{N^{2/d+2}q^{-2/d}}{\left[1 + C_d\left(\frac{N}{q}\right)^{2/d}\right]^2}. \tag{28}$$

For electronic systems ($q = 2$) this position-momentum uncertainty relation has the form

$$I_d[\rho]I_d[\gamma] \geq \frac{N^{\frac{2}{d}+2}\,2^{2-\frac{2}{d}}}{\left[1 + N^{2/d}\,80\pi^2 d^2(d+2)^{-\frac{d+2}{d}}\right]^2}A(2,d). \tag{29}$$

Let us note here that for systems with a sufficiently large number of constituents N so that $1+C_d\left(\frac{N}{q}\right)^{2/d} \approx C_d\left(\frac{N}{q}\right)^{2/d}$ we obtain

$$I_d[\rho]I_d[\gamma] \geq N^{2-\frac{2}{d}}q^{\frac{2}{d}}\frac{(d+2)^{\frac{4}{d}+2}}{25\pi^4 4^{\frac{2}{d}+3}d^4}A(2,d) \tag{30}$$

for fermionic systems, and

$$I_d[\rho]I_d[\gamma] \geq N^{2-\frac{2}{d}}\frac{(d+2)^{\frac{4}{d}+2}}{25\pi^4 4^{\frac{1}{d}+3}d^4}A(2,d). \tag{31}$$

for electronic systems.

And for real (i.e., $d = 3$) $N$-electron systems we obtain from Eqs. (29) and (31) the uncertainty relation

$$I_3[\rho]I_3[\gamma] \geq \frac{N^{8/3}}{\left(N^{2/3}\frac{144\pi^2}{5^{2/3}}+1\right)^2}\frac{3^{8/3}}{4}, \tag{32}$$

which for large $N$ reduces as

$$I_3[\rho]I_3[\gamma] \geq N^{4/3}\frac{5}{3072\pi^4}\left(\frac{5}{3}\right)^{1/3}, \tag{33}$$

where $\frac{5}{3072\pi^4}\left(\frac{5}{3}\right)^{1/3} \approx 0.0000198107$.

## IV. CONCLUSIONS

The (variance-based) Heisenberg-Kennard relation is known to be a weak (and, at times, misleading) mathematical formulation of the quantum uncertainty relation [71, 72]. Stronger uncertainty-like relations based either on moments of order other than 2 [6, 9, 54] or on some information-theoretic quantities have been developed. Among the latter ones, the entropic uncertainty relations based on the Shannon entropy and on the Rényi entropy are well known [75–78]. However the Fisher-information-based uncertainty-like relation still represents a controversial problem [34, 39–44] since its conjecture in 2000 for one-dimensional systems.

In this paper we have first found a set of (moment-based) Heisenberg-like uncertainty relations which extend and generalize the previous similar encountered expressions by starting from the Daubechies-Thakkar relations, which were semiempirically found by Thakkar for (three-dimensional) atoms and molecules and rigorously proved by Daubechies for $d$-dimensional quantum systems. Hereafter we have studied its accuracy for a large set of quantum systems: all the neutral and singly-ionized atoms of the periodic table and a large diversity of polyatomic molecules. Later, we have shown the uncertainty character of the product of the position and momentum Fisher information of finite fermionic systems by expressing it in terms of the Heisenberg-Kennard position-momentum product by means of an inequality-type relationship. Moreover, we have found a lower bound on this product in terms of the number $N$ of its constituents. This result is not only relevant from a fundamental point of view, but also because of its physical implications on e.g., the determination of nonclassicality measures for quantum states as previously discussed. Finally, we should point out though that the latter bound can be certainly improved because the Zumbach constant $C_d$ is non optimal.

### Acknowledgments

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### Appendix A: Set of molecules used

The molecular set chosen for the study includes different types of chemical organic and inorganic systems (aliphatic compounds, hydrocarbons, aromatic, alcohols, ethers, ketones). The set represents a variety of closed shell systems, radicals, isomers as well as molecules with heavy atoms such as sulphur, chlorine, magnesium and phosphorous. The geometries needed for the single point energy calculations above referred were obtained from experimental data from standard databases [79]. The molecular set might be organized by isoelectronic groups as follows:
N-2: $H_2$ (hydrogen)
N-10: $NH_3$ (ammonia) , $CH_4$ (methane), $HF$ (fluoride hydride)
N-12: $LiOH$ (lithium hydroxide)
N-14: $HBO$ (boron hydride oxide), $Li_2O$ (dilithium oxide)
N-15: $HCO$ (formyl radical), $NO$ (nitric oxide)
N-16: $H_2CO$ (formaldehyde), $NHO$ (nitrosyl hydride), $O_2$ (oxygen)
N-17: $CH_3O$ (methoxy radical)
N-18: $CH_3NH_2$ (methyl amine), $CH_3OH$ (methyl alcohol), $H_2O_2$ (hydrogen peroxide), $NH_2OH$ (hydroxylamine)
N-20: $NaOH$ (sodium hydroxide)
N-21: $BO_2$ (boron dioxide), $C_3H_3$ (radical propargyl), $MgOH$ (magnesium hydroxide), $HCCO$ (ketenyl radical)

N-22: $C_3H_4$ (cyclopropene), $CH_2CCH_2$ (allene), $CH_3CCH$ (propyne), $CH_2NN$ (diazomethane), $CH_2CO$ (ketene), $CH_3CN$ (acetonitrile), $CH_3NC$ (methyl isocyanide), $CO_2$ (carbon dioxide), $FCN$ (cyanogen fluoride), $HBS$ (hydrogen boron sulfide), $HCCOH$ (ethynol), $HCNO$ (fulminic acid), $HN_3$ (hydrogen azide), $HNCO$ (isocyanic acid), $HOCN$ (cyanic acid), $N_2O$ (nitrous oxide), $NH_2CN$ (cyanamide)
N-23: $NO_2$ (nitrogen dioxide), $NS$ (mononitrogen monosulfide), $PO$ (phosphorus monoxide),$C_3H_5$ (allyl radical), $CH_3CO$ (acetyl radical)
N-24: $C_2H_4O$ (ethylene oxide), $C_2H_5N$ (aziridine), $C_3H_6$ (cyclopropane), $CF_2$ (difluoromethylene), $CH_2O_2$ (dioxirane), $CH_3CHO$ (acetaldehyde), $CHONH_2$ (formamide), $FNO$ (nitrosyl fluoride), $H_2CS$ (thioformaldehyde), $HCOOH$ (formic acid), $HNO_2$ (nitrous acid) $NHCHNH_2$ (aminomethanimine), $O_3$ (ozone), $SO$ (sulfur monoxide)
N-25: $CH_2CH_2CH_3$ (npropyl radical), $CH_3CHCH_3$ (isopropyl radical), $CH_3OO$ (methylperoxy radical), $FO_2$ (dioxygen monofluoride), $NF_2$ (difluoroamino radical), $CH_3CHOH$ (ethoxy radical),$CH_3S$ (thiomethoxy)
N-26: $C_3H_8$ (propane), $CH_3CH_2NH_2$ (ethylamine), $CH_3CH_2OH$ (ethanol), $CH_3NHCH_3$ (dimethylamine), $CH_3OCH_3$ (dimethyl ether), $CH_3OOH$ (methyl peroxide), $F_2O$ (difluorine monoxide)
N-30: $ClCN$ (chlorocyanogen), $OCS$ (carbonyl sulfide), $SiO_2$ (silicon dioxide)
N-31: $PO_2$ (phosphorus dioxide), $PS$ (phosphorus sulfide)
N-32: $ClNO$ (nitrosyl chloride), $S_2$ (sulfur diatomic), $SO_2$ (sulfur dioxide)
N-33: $ClO_2$ (chlorine dioxide), $OClO$ (chlorine dioxide)
N-34: $CH_3CH_2SH$ (ethanethiol), $CH_3SCH_3$ (dimethyl sulfide),$H_2S_2$ (hydrogen sulfide), $SF_2$ (sulfur difluoride)
N-36: $HBr$ (bromide hydride)

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## 3.3 Semiclassical Heisenberg-like uncertainty relations of multidimensional fermionic systems

In this section we develop a novel two-step approach to derive position-momentum Heisenberg-like uncertainty relations of the type $\langle r^{\alpha}\rangle^{\frac{k}{\alpha}}\langle p^{k}\rangle \geq f\left(k,\alpha,q,N\right), q=2s+1$, for $d$-dimensional systems of $N$ fermions with spin $s$ which have two relevant features:

- They take into account the contribution of both the spatial and spin degrees of freedom, and
- they allow one to often improve the corresponding relationships published in the literature.

Firstly, we use the semiclassical Daubechies-Thakkar uncertainty-like inequality which connects the radial momentum expectation values of order $k, k>0$, and the position entropic moments of order $1+\frac{k}{d}$. Then, the latter position density functionals are estimated by means of the corresponding functionals of the extremum-distribution density of the systems obtained via the extremization principle of various information-theoretic quantities (Shannon entropy, Fisher information and Tsallis entropy) subject to two constraints, the normalization of the single-particle density and a position radial expectation value of given order.

These results have been published in the article with coordinates: *I. V. Toranzo, S. Lopez-Rosa, R. O. Esquivel and J. S. Dehesa, Journal of Physics A: Mathematical and Theoretical **49**, 025301 (**2016**)*, which is attached in the following.

# Extremum-entropy-based Heisenberg-like uncertainty relations

**J. Phys. A: Math. Theor. 49, 025301 (2016)*

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In this work we use the extremization method of various information-theoretic measures (Fisher information, Shannon entropy, Tsallis entropy) for $d$-dimensional quantum systems, which complementary describe the spreading of the quantum states of natural systems. Under some given constraints, usually one or two radial expectation values, this variational method allows us to determine an extremum-entropy distribution, which is the *least-biased* one to characterize the state among all those compatible with the known data. Then we use it, together with the spin-dependent uncertainty-like relations of Daubechies-Thakkar type, as a tool to obtain relationships between the position and momentum radial expectation values of the type $\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq f(k,\alpha,q,N), q=2s+1$, for $d$-dimensional systems of $N$ fermions with spin $s$. The resulting uncertainty-like products, which take into account both spatial and spin degrees of freedom of the fermionic constituents of the system, are shown to often improve the best corresponding relationships existing in the literature.

## I. INTRODUCTION

Let us consider a $d$-dimensional system of $N$ fermions with spin $s$ characterized by the wavefunction $\psi(\vec{r_1},\ldots,\vec{r_N};\sigma_1,\ldots,\sigma_N)$, for $\vec{r_i}\in\mathbb{R}^d$ and $\sigma_i\in\{1,2,\ldots,q\equiv 2s+1\}$, being antisymmetric in the pairs $(\vec{r_i},\sigma_i)$ for all $i$. Then the norm $\langle\psi|\psi\rangle$ is

$$\langle\psi|\psi\rangle=\sum_{\sigma_i=1}^{q}\int|\psi(\vec{r_1},\ldots,\vec{r_N};\sigma_1,\ldots,\sigma_N)|^2\prod_{i=1}^{N}d^dr_i,\quad i=1,2,\ldots,N$$

and the position single-particle density associated to the antisymmetric N-particle state $\psi$ is defined by

$$\rho(\vec{r})=N\sum_{\sigma_i=1}^{q}\int|\psi(\vec{r},\ldots,\vec{r_N};\sigma_1,\ldots,\sigma_N)|^2\prod_{i=2}^{N}d^dr_i, \tag{1}$$

which is completely characterized by the knowledge of its radial expectation values $\langle r^k\rangle=\int_{\mathbb{R}_d}r^k\rho(\vec{r})\,d^dr$. A similar statement can be written in momentum space for the momentum (i.e., Fourier-transformed) wavefunction $\tilde{\psi}(\vec{p_1},\ldots,\vec{p_N};\sigma_1,\ldots,\sigma_N)$, the momentum single-particle density $\gamma(\vec{p})$ and the momentum moments $\langle p^k\rangle=$

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$\int_{\mathbb{R}_d} p^k\gamma(\vec{p})\, d^dp$. Moreover, the notation $r = |\vec{r}|$, $p = |\vec{p}|$, and atomic units ($e = m = \hbar = 1$) have been used throughout the paper.

The search for relationships (generally of inequality type) which interconnect properties of the position and momentum densities of quantum systems has been of permanent interest from the very beginning of quantum mechanics [1] up to now [2–11] for both fundamental (e.g., mathematical realizations of the Heisenberg uncertainty principle, stability of matter) and applied (e.g., electronic structure of natural systems) reasons. These single-particle densities are completely characterized by the knowledge of the radial expectation values in the two conjugate spaces which often describe (aside of a numerical factor) numerous fundamental quantities of the system (see e.g., [9, 12, 13]), for instance the magnetic susceptibility $\langle r^2\rangle$, the height peak of the Compton profile $\langle p^{-1}\rangle$ the kinetic energy $\langle p^2\rangle$, the relativistic Breit-Pauli energy $\langle p^4\rangle$, the total electron-electron repulsion energy $\langle p^3\rangle$, etc. Emphasis is usually centered about the inequality-type relations among the expectation values $\langle r^n\rangle$ of the position density $\rho(\vec{r})$ and the momentum radial expectation values $\langle p^n\rangle$ [11, 12, 14–18] not only in three dimensions but also for quantum systems of arbitrary dimensionality $d$ [19–22]. All these inequality-type relations rely on some mathematical constraints on the momentum density $\gamma(\vec{p})$.

In this work, we have employed a novel procedure to obtain direct links between the expectation values $\langle r^\alpha\rangle$ and the momentum expectation values $\langle p^k\rangle$ for $d$-dimensional quantum systems, which starts with the inequality-type relationships between the momentum radial expectation values $\langle p^k\rangle$ and the entropic moments of the position density, $W_n[\rho]$ defined as

$$W_n[\rho] = \int [\rho(\vec{r})]^n\, d^dr. \tag{2}$$

The position entropic moments $W_n[\rho]$ describe, and/or are closely related to, some fundamental and/or experimentally accesible quantities (see e.g., [9, 11]), such as e.g. Thomas-Fermi kinetic energy $W_{\frac{5}{3}}[\rho]$, the Dirac-Slater exchange energy $W_{\frac{4}{3}}[\rho]$, the Patterson function of x-ray crystallography $W_3[\rho]$, etc. In fact, the energetic quantities of the many-electron systems can be expressed in terms of these entropic moments as already pointed out [23, 24] in the framework of the density theory functional[7]

Recently, it has been argued that the the momentum expectation values and the position entropic moments for $d$-dimensional systems of $N$ fermions with spin $s$ fulfil the following semiclassical spin-dependent uncertainty-like relations of Daubechies-Thakkar type [9, 11, 25] (see also [26]):

$$\langle p^k\rangle \geq K_d(k) q^{-\frac{k}{d}} W_{1+\frac{k}{d}}[\rho], \tag{3}$$

where $k > 0$, and

$$K_d(k) = \frac{d}{k+d}(2\pi)^k \frac{\left[\Gamma\left(1+\frac{d}{2}\right)\right]^{k/d}}{\pi^{k/2}}. \tag{4}$$

Note that for $k < 0$, the sign of inequality (3) is inverted. Also note that these expressions simplify for three-dimensional systems as

$$\langle p^k\rangle \leq c_k W_{1+\frac{k}{3}}[\rho] \quad \text{for} \quad k = -2, -1 \tag{5}$$

and

$$\langle p^k\rangle \geq c_k W_{1+\frac{k}{3}}[\rho] \quad \text{for} \quad k = 1, 2, 3, 4 \tag{6}$$

with $c_k = 3(3\pi^2)^{k/3}(k+3)^{-1}$ (since $K_d(k) = 2^{\frac{k}{3}} c_k$ for $d = 3$ and $s = 1/2$) , which were previously found by means of numerous semiclassical and Hartree-Fock-like ground-state calculations in atoms and diatomic molecules [9, 11, 14, 27–29]. Moreover, the case $k = 2$ in Eq. (3) was previously conjectured by Lieb (see e.g. [2]) and weaker versions of it have been rigorously proved, as discussed elsewhere [11]. In fact, Eq. (3) with constant $K'_d(k) = K_d(k) \times B(d,k)$ with $B(d,k) = \left\{\Gamma\left(\frac{d}{k}\right)\inf_{a>0}\left[a^{-\frac{d}{k}}\left(\int_a^\infty du\, e^{-u}(u-a)u^{-1}\right)^{-1}\right]\right\}^{-\frac{k}{d}}$ has been rigorously proved by Daubechies [25]. Let us also mention that a number of authors have published some rigorous $d$-dimensional bounds of the same type [3, 30] with much less accuracy. Furthermore, let us point out that the inclusion of the spin $s$ in the lower bound (3) for the expected value of $\langle p^2\rangle$ was considered by Hundertmark [30] and applied to obtain uncertainty-like relations in [31]; the extension to $\langle p^k\rangle$ has been recently used [26] in a similar sense.

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The second step in our procedure is to invoke the information-theoretical grounds of Tao [15, 16, 32] and other authors [12, 20, 33–38] to estimate to a very good approximation the position entropic moments $W_n[\rho]$ by means of the bounds provided by the entropic moments of the extremum-entropy distribution obtained with the extremum-entropy principle of information theory. This principle provides an interesting constructive method which objectively estimates the unknown distribution when only partial information (e.g., some radial expectation values) is given about a probability distribution. This method gives rise to an extremum-entropy distribution which is the 'least-biased' (minimally prejudiced) one among all those compatible with the known data, which are the constraints to be imposed in the variational problem when solving it by determining the values of the associated Lagrange multipliers. Indeed, for a generic information-theoretic measure $Q[\rho]$ subject to the constraints $\langle r^0\rangle \equiv \int \rho(\vec{r})\, d^dr = N$ and $\langle r^\alpha\rangle = \int r^\alpha \rho(\vec{r})\, d^dr$, $\alpha > 0$, we extremize it by taking variations of the form

$$\delta\left\{Q[\rho] - \lambda \int r^\alpha \rho(\vec{r})\, d^dr - \mu \int \rho(\vec{r})\, d^dr\right\} = 0,$$

where $\lambda$ and $\mu$ are Lagrange multipliers (see e.g. [37, 38]). The best known and most useful information-theoretic quantities, which complementary describe the spreading properties of the probability distribution $\rho(\vec{r})$, being $\vec{r} = (x_1, x_2, \ldots, x_d)$, all over the space are the Shannon entropy $S[\rho]$ defined (see e.g. [39]) by

$$S[\rho] := -\int \rho(\vec{r}) \ln \rho(\vec{r})\, d^dr, \tag{7}$$

the Tsallis entropy $T_q[\rho]$ given [40] by

$$T_t[\rho] := \frac{1}{t-1}\left\{1 - \int [\rho(\vec{r})]^t\, d^dr\right\}\ ; \quad t > 0,\, t \neq 1. \tag{8}$$

and the Fisher information $I[\rho]$ of the density which is defined [41] by

$$I_\rho := \int \rho(\vec{r}) \left(\frac{|\vec{\nabla}_d \rho(\vec{r})|}{\rho(\vec{r})}\right)^2 d^dr\,, \tag{9}$$

(where $\vec{\nabla}_d$ denotes the $d$-dimensional gradient operator), respectively. Let us point out the well-known fact that for $t \to 1$ the Tsallis entropy $T_q$ is equal to the Shannon value $S_\rho$. The corresponding extremization problems associated to the Shannon and Tsallis entropies are the maximization entropy problems, briefly called as *MaxEnt* and *MaxTent* problems; and the one associated with the Fisher information is called by minimization Fisher problem (briefly, *MinInf* problem); see e.g. [37, 38]) and references therein for further details.

Hereafter we use this two-step method to obtain the lower bounds to the Heisenberg-like products $\langle r^\alpha\rangle \langle p^k\rangle$ of $N$-fermion systems by use of the analytical solutions of the MaxEnt (see Section II), MinInf (see Section III) and MaxTent (see Section IV) problems with the above mentioned constraints ($\langle r^0\rangle = N, \langle r^\alpha\rangle$). Some particular cases are numerically examined for a large set of neutral atoms and, moreover, they are compared with the corresponding ones obtained by other authors.

## II. MAXENT-BASED HEISENBERG-LIKE UNCERTAINTY RELATION

Here we will apply the methodology described in the previous section to find the Heisenberg-like uncertainty products $\langle r^\alpha\rangle \langle p^k\rangle$ of $d$-dimensional $N$-fermion systems by use of the analytical solution $\rho_S(r)$ of the MaxEnt problem with the constraints ($\langle r^0\rangle = N, \langle r^\alpha\rangle$). Then, we center around the corresponding products in the three-dimensional case, and finally we consider a few particular cases.

Following the lines described in [37, 38], the $d$-dimensional density which maximizes the Shannon entropy (7) when the constraints correspond to one radial expectation value $\langle r^\alpha\rangle$ in addition to the normalization to the number of particles $N$ is given by

$$\rho_S(r) = e^{-\lambda - \mu\, r^\alpha}; \quad \alpha > 0\,, \tag{10}$$

where the Lagrange multipliers have the form

$$\lambda = \log\left(\frac{2\pi^{d/2} d^{-\frac{d}{\alpha}} \alpha^{\frac{d}{\alpha}-1} \langle r^\alpha\rangle^{d/\alpha} \Gamma\left(\frac{d}{\alpha}\right)}{\Gamma\left(\frac{d}{2}\right)} N^{-\frac{d}{\alpha}-1}\right) \tag{11}$$

$$\mu = \frac{d\,N}{\alpha\langle r^\alpha\rangle}. \tag{12}$$

Now, we compute the entropic moments (2) of the maximizer solution (10) and insert them into the semiclassical position-momentum inequality (3). We have found the following set of $d$-dimensional uncertainty-like relations:

$$\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq 2^{\frac{(d-2)k}{d}} d^{\frac{(\alpha+d)(d+k)}{\alpha d}} (d+k)^{-\frac{\alpha+d}{\alpha}} \alpha^{k\left(\frac{1}{d}-\frac{1}{\alpha}\right)} q^{-\frac{k}{d}} \Gamma\left(\frac{d}{2}\right)^{\frac{d+k}{d}} \Gamma\left(\frac{d}{\alpha}\right)^{-\frac{k}{d}} N^{k\left(\frac{1}{\alpha}+\frac{1}{d}\right)+1}, \tag{13}$$

with $\alpha > 0$, $k > 0$ and $q = 2s+1$. It is straightforward to obtain that for real N-electron systems ($d = 3$ and $q = 2$), one has that the uncertainty-like relations simplify as

$$\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq \frac{2^{-\frac{2k}{3}} \pi^{\frac{k}{3}} 3^{\frac{(\alpha+3)(k+3)}{3\alpha}} \Gamma\left(\frac{3}{\alpha}\right)^{-\frac{k}{3}} \alpha^{k\frac{(\alpha-3)}{3\alpha}}}{(k+3)^{1+\frac{3}{\alpha}}} N^{k\left(\frac{1}{\alpha}+\frac{1}{3}\right)+1}. \tag{14}$$

Some particular cases of these inequalities are shown in the Table I. Finally, let us remark that these results coincide with the corresponding ones obtained by Tao et al [15, 16, 32] with a similar methodology in a few particular three-dimensional cases derived one by one by these authors for the lowest orders of the radial expectation values, which constitutes a test of our results.. For completeness, we give in Table II the approximate values for the lower bounds of a few Heisenberg-like products. The accuracy of these uncertainty-like relations has also been studied for almost all the neutral atoms [15] and numerous diatomic molecules [16].

| $\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq f(k,\alpha,N)$ | | | | |
|---|---|---|---|---|
| $k \backslash \alpha$ | 1 | 2 | 3 | 4 |
| 1 | $\frac{243}{512}(3\pi)^{1/3}N^{7/3}$ | $\frac{27\,3^{1/3}\pi^{1/6}}{32\sqrt{2}}N^{11/6}$ | $\frac{9}{16}\left(\frac{3}{2}\right)^{2/3}\pi^{1/3}N^{5/3}$ | $\frac{9}{16}\left(\frac{3\pi}{\Gamma(3/4)}\right)^{1/3}N^{19/12}$ |
| 2 | $\frac{729(3\pi)^{2/3}}{2500}N^{11/3}$ | $\frac{81\sqrt[6]{3}\sqrt[3]{\pi}}{50\sqrt{5}}N^{8/3}$ | $\frac{27}{50}\sqrt[3]{\frac{3}{2}}\pi^{2/3}N^{7/3}$ | $\frac{9\;3^{11/12}\pi^{2/3}}{10\;5^{3/4}\left[\Gamma\left(\frac{3}{4}\right)\right]^{2/3}}N^{13/6}$ |
| 3 | $\frac{81\pi}{128}N^5$ | $\frac{9}{16}\sqrt{3\pi}N^{7/2}$ | $\frac{9\pi}{16}N^3$ | $\frac{3\;3^{3/4}\pi}{8\sqrt[4]{2}\Gamma\left(\frac{3}{4}\right)}N^{11/4}$ |
| 4 | $\frac{19683\sqrt[3]{3}\pi^{4/3}}{38416}N^{19/3}$ | $\frac{243\;3^{5/6}\pi^{2/3}}{196\sqrt{7}}N^{13/3}$ | $\frac{81}{196}\left(\frac{3}{2}\right)^{2/3}\pi^{4/3}N^{11/3}$ | $\frac{81\sqrt[12]{3}\,\pi^{4/3}}{28\;7^{3/4}\left[\Gamma\left(\frac{3}{4}\right)\right]^{4/3}}N^{10/3}$ |

TABLE I: Some MaxEnt-based Heisenberg-like uncertainty relations for $N$-electron systems. The contribution of both spatial and spin degrees of freedom are taken into account.

| | | | | |
|---|---|---|---|---|
| $\langle r\rangle^3\langle p^3\rangle$ | $\langle r^2\rangle^{\frac{3}{2}}\langle p^3\rangle$ | $\langle r^3\rangle\langle p^3\rangle$ | $\langle r\rangle^2\langle p^2\rangle$ | $\langle r^2\rangle\langle p^2\rangle$ |
| $1.98804\,N^5$ | $1.72686\,N^{\frac{7}{2}}$ | $1.76715\,N^3$ | $1.30107\,N^{\frac{11}{3}}$ | $1.27429\,N^{\frac{8}{3}}$ |
| $\langle r^3\rangle^{\frac{2}{3}}\langle p^2\rangle$ | $\langle r\rangle\langle p\rangle$ | $\langle r^2\rangle^{\frac{1}{2}}\langle p\rangle$ | $\langle r^3\rangle^{\frac{1}{3}}\langle p\rangle$ | |
| $1.32594\,N^{\frac{7}{3}}$ | $1.00252\,N^{\frac{7}{3}}$ | $1.04135\,N^{\frac{11}{6}}$ | $1.07953\,N^{\frac{5}{3}}$ | |

TABLE II: Numerical values of the MaxEnt-based lower bounds for various Heisenberg-like uncertainty products $\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle$.

## III. MININF-BASED HEISENBERG-LIKE UNCERTAINTY RELATION

In this section we apply the methodology to obtain the Heisenberg-like uncertainty products $\langle r^{-1}\rangle\langle p^k\rangle$ of $d$-dimensional systems of $N$ fermions with spin $s$, by use of the analytical solution $\rho_{I,d}(r)$ of the MinInf problem (i.e., minimization of the Fisher information) with the constraints $(\langle r^0\rangle = N, \langle r^{-1}\rangle)$. Thereupon, the resulting expressions are applied to real systems of finite many-electron systems and, for illustrative purposes, the instance $\langle r^{-1}\rangle^{-2}\langle p^2\rangle$ is compared with the best corresponding result published in the literature.

According to the lines developed in [36] (see also [37, 38]) we have determined the following expression for the minimizer density

$$\rho_I(r) = \frac{2^{-d}\pi^{\frac{1-d}{2}}(d-1)^d}{\Gamma\left(\frac{d+1}{2}\right)} N^{1-d}\langle r^{-1}\rangle^d e^{-\frac{(d-1)\langle r^{-1}\rangle}{N}r}, \tag{15}$$

which simplifies for the three dimensional case as

$$\rho_{I,3}(r) = \frac{1}{\pi N^2}\langle r^{-1}\rangle^3 e^{-\frac{2\langle r^{-1}\rangle}{N} r}. \tag{16}$$

Then, the semiclassical position-momentum inequality (3) together with the entropic moments of the minimizer density $\rho_{I,d}(r)$ allow us to obtain the uncertainty-like products

$$\langle r^{-1}\rangle^{-k}\langle p^k\rangle \geq d^{d+1}(d-1)^k(d+k)^{-d-1}\pi^{\frac{k}{2d}}\left[\frac{\Gamma\left(\frac{d}{2}+1\right)}{\Gamma\left(\frac{d+1}{2}\right)}\right]^{k/d} q^{-\frac{k}{d}} N^{\left(\frac{1}{d}-1\right)k+1}, \tag{17}$$

with $k > 0$, and $q$ denotes the number of spin states of each constituent fermion as already mentioned. In the particular case where $d = 3$ and $s = 1/2$, this inequality reduces to the following uncertainty-like relation

$$\langle r^{-1}\rangle^{-k}\langle p^k\rangle \geq \frac{3^{\frac{k}{3}+4}\pi^{k/3}}{(k+3)^4} N^{1-\frac{2k}{3}}, \tag{18}$$

which is valid for all antisymmetric wavefunctions of $N$-electron systems.

In Table III a few particular cases of this Heisenberg-like relation are given for the lowest values of $k$.

| $\langle r^{-1}\rangle^{-k}\langle p^k\rangle \geq f\,(k,N)$ | | | | |
|---|---|---|---|---|
| $k$ | 1 | 2 | 3 | 4 |
| $f(N)$ | $\frac{81}{256}\sqrt[3]{3\pi}N^{1/3}$ | $\frac{81(3\pi)^{2/3}}{625}N^{-1/3}$ | $\frac{3\pi}{16}N^{-1}$ | $\frac{243\sqrt[3]{3}\pi^{4/3}}{2401}N^{-5/3}$ |

TABLE III: Some Heisenberg-like uncertainty relations for $N$-electron systems obtained by use of the MinInf density. The contributions of both spatial and spin degrees of freedom have been taken into account.

Let us now compare these lower bounds on the Heisenberg-like products $\langle r^{-1}\rangle\,\langle p^k\rangle$ (obtained here by use of the MinInf density) with the corresponding MaxEnt-based results obtained by Tao et al [15, 16], which seems to be the best one published in the literature, at least for the instance $\langle r^{-1}\rangle^{-2}\langle p^2\rangle$. In particular, in Table IV we can appreciate that the MinInf-based lower bound on the uncertainty-like product $\langle r^{-1}\rangle^{-2}\langle p^2\rangle$ is a factor 1.25 better than the corresponding MaxEnt-based one [15, 16].

| | MinInf-based bound | MaxEnt-based bound |
|---|---|---|
| $\langle r^{-1}\rangle^{-2}\langle p^2\rangle$ | $0.5783N^{-\frac{1}{3}}$ | $0.4615N^{-\frac{1}{3}}$ |

TABLE IV: Comparison of the MinInf-based lower bounds obtained in the present work and the MaxEnt-based [15, 16] ones.

Finally, we should point out that there exist other lower bounds on the Heisenberg-like products $\langle r^{-1}\rangle\,\langle p^k\rangle$, but they only take into account the proper contribution of the spatial degrees of freedom. In particular, an interesting Rényi-based bound on the product $\langle r^{-1}\rangle^{-2}\langle p^2\rangle$, has been recently published [42] , where the electron density has been averaged for spin and normalized to unity. Hence, proper care has to be taken in comparing this with our results. The proper consideration of the contribution of the spin degrees of freedom decreases the lower bound, thus worsening its accuracy.

## IV. MAXTENT-BASED HEISENBERG-LIKE UNCERTAINTY RELATION

Let us now use the previous methodology to determine the Heisenberg-like uncertainty products $\langle r^\alpha\rangle\,\langle p^k\rangle$ of three-dimensional $N$-fermion systems by use of the analytical solution $\rho_T(r)$ of the MaxTent problem (i.e., the maximization of the Tsallis entropy $T_t[\rho]$) with the constraints $(\langle r^0\rangle = N, \langle r^\alpha\rangle)$.
According to the lines given in [37, 38], we first determine the density $\rho_T(r)$ which maximizes the Tsallis entropy (8) when the constraints are $(N, \langle r^\alpha\rangle)$. There are two different cases:

- If $t > 1$ and $\alpha > 0$, the maximum entropy density only exists for a finite interval $r \in [0, a]$, where $a$ is a parameter to be determined within the framework of our variational procedure, as a function of the corresponding Lagrange multipliers.
- If $0 < t < 1$ and $\alpha > 3\frac{1-t}{t}$, the maximum entropy density exists for any value of $r$.

### A. Case $0 < t < 1$, $\alpha > 3\frac{1-t}{t}$ and $k < 0$

In this case the Tsallis maximizer density is

$$\rho_T(r) = C\left[\frac{1}{t}(a^\alpha + r^\alpha)\right]^{\frac{1}{t-1}}, \tag{19}$$

where

$$\begin{aligned} a &= \left[\frac{\langle r^\alpha\rangle \alpha\,\Gamma\left(\frac{1}{1-t} - \frac{3}{\alpha}\right)}{N3\,\Gamma\left(-\frac{t}{t-1} - \frac{3}{\alpha}\right)}\right]^{1/\alpha} \qquad (20)\\ C &= t^{\frac{1}{t-1}}3^{\frac{3}{\alpha}+\frac{1}{t-1}}\alpha^{-\frac{3}{\alpha}+\frac{1}{1-t}+1}\langle r^\alpha\rangle^{\frac{1}{1-t}-\frac{3}{\alpha}}N^{\frac{3}{\alpha}+\frac{1}{t-1}+1} \\ &\times \frac{\Gamma\left(\frac{1}{1-t}\right)\Gamma\left(\frac{1}{1-t}-\frac{3}{\alpha}\right)^{-\frac{3}{\alpha}-\frac{t}{t-1}}\Gamma\left(-\frac{t}{t-1}-\frac{3}{\alpha}\right)^{\frac{3}{\alpha}+\frac{1}{t-1}}}{4\pi\Gamma\left(\frac{3}{\alpha}\right)} \qquad (21) \end{aligned}$$

Now we compute the entropic moments (2) of the maximizer solution (19) and insert them into the semiclassical position-momentum inequality (3), obtaining the following set of uncertainty-like relations:

$$\begin{aligned} \langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle &\le 2^{-\frac{k}{3}}\pi^{\frac{k}{3}}3^{\left(\frac{1}{\alpha}+\frac{1}{3}\right)k+1}\alpha^{\frac{(\alpha-3)k}{3\alpha}}q^{-\frac{k}{3}}N^{\left(\frac{1}{\alpha}+\frac{1}{3}\right)k+1} \\ &\times \frac{\Gamma\left(\frac{3}{\alpha}\right)^{-\frac{k}{3}}\Gamma\left(\frac{1}{1-t}\right)^{\frac{k}{3}+1}\Gamma\left(\frac{k+3}{3(1-t)}-\frac{3}{\alpha}\right)\Gamma\left(\frac{1}{1-t}-\frac{3}{\alpha}\right)^{-\left(\frac{1}{\alpha}+\frac{1}{3}\right)k-1}\Gamma\left(\frac{t}{1-t}-\frac{3}{\alpha}\right)^{k/\alpha}}{(k+3)\Gamma\left(\frac{k+3}{3(1-t)}\right)}, \end{aligned} \tag{22}$$

with $\alpha > 3\frac{1-t}{t}$, $0 < t < 1$ and $k < 0$, which are valid for all antisymmetric states of real systems of $N$ fermions with spin $s$.
In the particular case where $k = -1$, $\alpha = 2$ and $s = 1/2$ one obtains with $t \ge 0.78$ the uncertainty-like product

$$\langle r^2\rangle\langle p^{-1}\rangle^{-2} \le \frac{2^2\pi^{\frac{1}{3}}3^{-\frac{1}{3}}(t-1)\Gamma\left(\frac{1}{1-t}-\frac{3}{2}\right)^{4/3}\Gamma\left(\frac{2}{3(1-t)}\right)^2}{(3-5t)\Gamma\left(\frac{2}{3(1-t)}-\frac{3}{2}\right)^2\Gamma\left(\frac{1}{1-t}\right)^{\frac{4}{3}}}N^{-\frac{1}{3}}, \tag{23}$$

which is valid for all antisymmetric states of N-electron systems. A similar expresssion can be derived for an upper bound on the product $\langle p^2\rangle\langle r^{-1}\rangle^{-2}$. Their interest lies in the fact that the former uncertainty product allows one to correlate the diamagnetic susceptibility and the peak of the Compton profile (which are equal, except for a factor, to $\langle r^2\rangle$ and $\langle p^{-1}\rangle$, respectively, as previously mentioned), whilst the latter involves the kinetic and electron-nucleus attraction energy (which, except for a factor, are equal to $\langle p^2\rangle$ and $\langle r^{-1}\rangle$, respectively, as already mentioned).
Moreover, we have

$$0.4368\,N^{-\frac{1}{3}} \le \langle r^2\rangle\langle p^{-1}\rangle^{-2} \le 0.4958\,N^{-\frac{1}{3}}, \tag{24}$$

where we have used the upper bound (23) with $t = 0.78$ and the lower bound $(12N)^{-\frac{1}{3}}$ recently obtained (see Eq. (22) of [26]). A similar chain of inequalities can be written for the product $\langle r^{-1}\rangle^{-2}\langle p^2\rangle$.

### B. Case $t > 1$, $\alpha > 0$ and $k > 0$

In this case the Tsallis maximizer density is

$$\rho_T(r) = C \left[ \frac{1}{t}(a^\alpha - r^\alpha) \right]^{\frac{1}{t-1}}, \tag{25}$$

where

$$a = \left( \frac{\langle r^\alpha \rangle (\alpha t + 3(t-1))}{N(3(t-1))} \right)^{1/\alpha} \tag{26}$$

$$C = \frac{\alpha\, t^{\frac{1}{t-1}} \left( \frac{\langle r^\alpha \rangle (\alpha t + 3(t-1))}{N(3(t-1))} \right)^{-\frac{3}{\alpha} - \frac{1}{t-1}}}{4\pi B\left(\frac{3}{\alpha}, \frac{t}{t-1}\right)}, \tag{27}$$

where $B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$. Then, the calculation of the entropic moments (2) of the maximizer solution (25) and the semiclassical position-momentum inequality (3) allows us to determine the following set of uncertainty-like relations:

$$\begin{aligned} \langle r^\alpha \rangle^{\frac{k}{\alpha}} \langle p^k \rangle \;\geq\; & q^{-\frac{k}{3}} N^{\left(\frac{1}{\alpha}+\frac{1}{3}\right)k+1} \left(\frac{\pi}{2}\right)^{k/3} 3^{\left(\frac{1}{\alpha}+\frac{1}{3}\right)k+1} \alpha^{k/3} \left( \frac{\alpha t}{t-1} + 3 \right)^{-\frac{k}{\alpha}} (k+3)^{-1} \\ & \times \frac{\Gamma\left(\frac{k+3t}{3(t-1)}\right) \Gamma\left(\frac{3}{\alpha}\right)}{\Gamma\left(\frac{k+3t}{3(t-1)} + \frac{3}{\alpha}\right) B\left(\frac{3}{\alpha}, \frac{t}{t-1}\right)^{1+\frac{k}{3}}}, \end{aligned} \tag{28}$$

with $\alpha > 0$, $k > 0$ and $t > 1$, which are valid for all antisymmetric states of real $N$ fermions with spin $s$. A few particular cases of this set obtained with $t = 2$ are given in Table V.

| $\langle r^\alpha \rangle^{\frac{k}{\alpha}} \langle p^k \rangle \geq f(k, \alpha, q, N)$ | | | |
|---|---|---|---|
| $k$ \ $\alpha$ | 1 | 2 | 3 |
| 1 | $1.22995 N^{7/3} q^{-\frac{1}{3}}$ | $1.30485 N^{11/6} q^{-\frac{1}{3}}$ | $1.35791 N^{5/3} q^{-\frac{1}{3}}$ |
| 2 | $1.67378 N^{11/3} q^{-2/3}$ | $1.8647 N^{8/3} q^{-2/3}$ | $2.00783 N^{7/3} q^{-2/3}$ |
| 3 | $2.4429 N^5 q^{-1}$ | $2.83315 N^{7/2} q^{-1}$ | $3.14159 N^3 q^{-1}$ |

TABLE V: Some MaxTent-based Heisenberg-like uncertainty relations for real systems of $N$-fermions, where the contribution of both spatial and spin degrees of freedom are taken into account.

To illustrate the accuracy and validity of these Heisenberg-like uncertainty relations the MaxTent-based lower bounds for two Heisenberg-like products are compared in Table VI with the corresponding MaxEnt-based ones of Tao et al [15, 16] (also obtained in Section II of this work in a generic and unified way) and the corresponding Hartree-Fock values (obtained by means of the accurate near-Hartree-Fock wavefunctions of Koga et al [43, 44]) for all neutral atoms from He to Xe. Remark that the MaxTent-based lower bounds obtained in the present work are systematically higher (that is, better) than the corresponding bounds of Tao et al. Moreover, we observe that there is still a large gap between our bounds and the Hartree-Fock values to be fulfilled. This gap clearly grows when the atomic number increases. Nevertheless we should keep in mind that the Hartree-Fock values of the Heisenberg-like products are atom dependent, while the corresponding uncertainty products provided by our two-step method have an universal character in the sense that they are valid for any N-fermion system with arbitrary spin.

| | | $\langle r\rangle\langle p\rangle$ | | | $\langle r^2\rangle^{\frac{1}{2}}\langle p\rangle$ | | |
|---|---|---|---|---|---|---|---|
| Atom | $N$ | Tao et al | Present work | Hartree-Fock | Tao et al | Present work | Hartree-Fock |
| He | 2 | 5.052 | 5.056 | 5.191 | 3.711 | 3.714 | 4.309 |
| Li | 3 | 13.013 | 13.022 | 24.626 | 7.804 | 7.811 | 21.175 |
| Be | 4 | 25.462 | 25.481 | 45.563 | 13.225 | 13.235 | 30.938 |
| B | 5 | 42.856 | 42.888 | 72.529 | 19.9010 | 19.925 | 42.399 |
| C | 6 | 65.580 | 65.629 | 103.326 | 27.812 | 27.834 | 53.709 |
| N | 7 | 93.968 | 94.038 | 138.645 | 36.895 | 36.924 | 65.568 |
| O | 8 | 128.320 | 128.415 | 180.515 | 47.128 | 47.165 | 79.275 |
| Ne | 10 | 215.982 | 216.143 | 277.741 | 70.950 | 71.006 | 107.750 |
| Na | 11 | 269.774 | 269.975 | 441.672 | 84.496 | 84.563 | 212.256 |
| Mg | 12 | 330.502 | 330.748 | 570.342 | 99.110 | 99.188 | 253.193 |
| Al | 13 | 398.369 | 398.665 | 723.183 | 114.775 | 114.865 | 305.055 |
| Si | 14 | 473.569 | 473.921 | 858.352 | 131.478 | 131.581 | 336.696 |
| P | 15 | 556.285 | 556.699 | 990.945 | 149.206 | 149.323 | 364.153 |
| S | 16 | 646.692 | 647.173 | 1135.067 | 167.946 | 168.079 | 396.063 |
| Cl | 17 | 744.958 | 745.512 | 1279.150 | 187.690 | 187.837 | 424.992 |
| Ar | 18 | 851.243 | 851.876 | 1425.453 | 208.425 | 208.589 | 452.573 |
| Ti | 22 | 1359.578 | 1360.589 | 2633.898 | 301.110 | 301.347 | 863.813 |
| Fe | 26 | 2007.654 | 2009.147 | 3557.697 | 409.011 | 409.333 | 1043.880 |
| Ni | 28 | 2386.637 | 2388.412 | 4067.283 | 468.533 | 468.902 | 1139.181 |
| Zn | 30 | 2803.501 | 2805.585 | 4606.755 | 531.708 | 532.126 | 1238.371 |
| Ge | 32 | 3259.125 | 3261.548 | 5628.555 | 598.493 | 598.964 | 1500.495 |
| Se | 34 | 3754.354 | 3757.146 | 6517.395 | 668.850 | 669.376 | 1646.220 |
| Kr | 36 | 4289.996 | 4293.186 | 7383.097 | 742.743 | 743.328 | 1769.071 |
| Xe | 54 | 11049.344 | 11057.561 | 21127.164 | 1561.970 | 1563.199 | 4281.013 |

TABLE VI: Comparison of the MaxTent-based lower bounds on two Heisenberg-like products obtained in the present work, the MaxEnt-based ones of Tao et al and the corresponding Hartree-Fock values. The former ones were calculated with the Tsallis optimal parameter $t = 3$ and 2.3 for the two uncertainty products considered in this Table, respectively.

## V. CONCLUSIONS

We have developed a two-step method to derive position-momentum Heisenberg-like uncertainty relations of the type $\langle r^\alpha\rangle^{\frac{k}{\alpha}}\langle p^k\rangle \geq f\left(k,\alpha,q,N\right), q = 2s+1$, for $d$-dimensional systems of $N$ fermions with spin $s$ which have two relevant features: they take into account the contribution of both the spatial and spin degrees of freedom, and they allow one to often improve the corresponding relationships published in the literature. First, the method makes use of the semiclassical Daubechies-Thakkar uncertainty-like inequality (3) which connects the radial momentum expectation values of order $k, k > 0$, and the position entropic moments of order $1 + \frac{k}{d}$. Then, the latter position density functionals are estimated by means of the corresponding functionals of the extremum-distribution density of the systems obtained via the extremization principle of various information-theoretic quantities (Shannon entropy, Fisher information, Tsallis entropy) subject to two constraints, the normalization of the single-particle density and a position radial expectation value of given order.

In summary, the resulting MaxEnt-based and MinInf-based uncertainty-like inequalities given by Eqs. (13) and

(17), respectively, not only extend to $d$-dimensional systems the corresponding ones previously obtained in the literature for three-dimensional systems by use of different methodologies, but they often improve them. Moreover, the MaxTent-based inequality-like relationships given by Eqs. (22) and (28), here obtained for three-dimensional systems, seem to have in general a better accuracy than the corresponding MaxEnt-based ones (which are the most accurate values reported so far), as it is numerically shown here for various particular cases applied to a large variety of neutral atoms from He to Xe for illustrative purposes.

Nevertheless, there is still large room for improving these inequalities. Much work along the lines of the present study is needed, not only because of the insufficient accuracy of these uncertainty-like relations but also because of the the correlation between fundamental and/or experimentally accessible quantities (e.g., the volume, the ionization energy, electronegativity, hardness and other atomic and molecular properties) is very relevant in the framework of the density functional theory, as already pointed out elsewhere [6, 9–11, 14, 16, 17, 45].

Finally, we are aware that there exist other information-theoretic approaches to the uncertainty principle such as for example the application of majorization theory [46–51], which relies on the partial order on probability vectors to characterize uncertainty. Majorization-based formulations of the uncertainty principle, although mathematically more complex, complement the entropic and variance-based formulations, leading to a deeper knowledge of the fundamental aspects of uncertainty and disorder in quantum theory. They have been developed for finite-dimensional quantum systems, showing a great interest in the theory of quantum information. However, its extension to infinite-dimensional Hilbert spaces is presently very challenging. We wonder whether our work might provide hints towards the generalization of the majorization-like ideas for continuous variables. This is an open problem which deserves to be separately considered.

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## 3.4 Heisenberg- and entropy-like uncertainty measures of high-dimensional hydrogenic systems

In this section we determine in an analytical way the Heisenberg-like uncertainty measures (i.e., the radial expectation values of arbitrary order) of the high-dimensional hydrogenic system in position and momentum spaces and their associated uncertainty relations, by means of a bunch of mathematical techniques which include the parametric asymptotics of generalized hypergeometric functions of the type ${}_{p+1}F_p$, the weak-* asymptotics of the Laguerre and Gegenbauer polynomials which control the position and momentum hydrogenic stationary states, and the great diversity of simple and non-trivial properties of some elementary special functions such as the Gamma function.

In addition, the following results have been achieved:

- Calculation of the expectation values for all quantum states of the $D$-dimensional hydrogenic system at the high $D$ limit,
- determination of the corresponding uncertainty equality-type relations which fulfill and saturate the known uncertainty relations for both general and central systems, and
- explicit derivation of the bounds for the entropic uncertainty measures of the Shannon, Rényi and Tsallis type at high $D$ in terms of the position and momentum radial expectation values.

These results have been published in the article with coordinates: *I. V. Toranzo, A. Martinez-Finkelshtein and J. S. Dehesa, Journal of Mathematical Physics* ***57**, 082109* *(**2017**)*, which is attached below.

# Heisenberg-like uncertainty measures for $D$-dimensional hydrogenic systems at large $D$

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The radial expectation values of the probability density of a quantum system in position and momentum spaces allow one to describe numerous physical quantities of the system as well as to find generalized Heisenberg-like uncertainty relations and to bound entropic uncertainty measures. It is known that the position and momentum expectation values of the main prototype of the $D$-dimensional Coulomb systems, the $D$-dimensional hydrogenic system, can be expressed in terms of some generalized hypergeometric functions of the type ${}_{p+1}F_p(z)$ evaluated at unity with $p = 2$ and $p = 3$, respectively. In this work we determine the position and momentum expectation values in the limit of large $D$ for all hydrogenic states from ground to very excited (Rydberg) ones in terms of the spatial dimensionality and the hyperquantum numbers of the state under consideration. This is done by means of two different approaches to calculate the leading term of the special functions ${}_3F_2\,(1)$ and ${}_5F_4\,(1)$ involved in the large $D$ limit of the position and momentum quantities. Then, these quantities are used to obtain the generalized Heisenberg-like and logarithmic uncertainty relations, and some upper and lower bounds to the entropic uncertainty measures (Shannon, Rényi, Tsallis) of the $D$-dimensional hydrogenic system.

## I. INTRODUCTION

The study of the behavior of the physical properties of a $D$-dimensional system in terms of $D$ has a rich history in quantum mechanics and quantum field theory [1–8] and, more recently, in quantum information [9–11]. It has been observed that the physical phenomena depend on the dimension in a delicate way. For instance, the Huygens principle of the wave propagation holds only when the spatial dimension is odd, while it is observed anomalous dispersion for any other real value of $D$ [12, 13, 15]. Moreover, it is often possible to approximate the solution of difficult physical problems at the standard dimensionality ($D = 3$) by means of a Taylor-series development of similar systems with a non-standard dimensionality in powers of $1/D$. This was motivated by the observation that physics is much simpler when $D \to \infty$. This is true for a large variety of quantum systems from the single-particle systems moving in a $D$-dimensional central potential to more complex systems and phenomena (e.g. Casimir effects, random walks, and certain quantum field models containing $SU(D)$ gauge fields [2, 14, 15]) as well as for quantum state tomography and some quantum codes and channels [11].

Most relevant for our purposes is the development of the dimensional scaling method [3, 4] in the theory of many-electron systems, which offer novel, powerful and useful computational strategies for treating non-separable problems involving strong dynamical interactions [6, 7, 16–18]. This method typically starts with the generalization of the standard (three-dimensional) problem to a $D$-dimensional one and the introduction of a suitably scaled space to remove the major, generic $D$-dependence of the quantity under consideration; then, the evaluation of the scaled quantity at a large $D$ value, such as the limit $D \to \infty$, is performed in a relatively “easy” way and finally one

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obtains an approximation for the standard value by relating it to this large-$D$-value by means of some interpolation or extrapolation procedure [3, 19]. In the *pseudoclassical* limit $D \to \infty$ of a many-electron system, which is tantamount to $h \to 0$ and/or $m_e \to \infty$ in the kinetic energy, the electrons assume fixed positions relative to the nuclei and each other in the $D$-scaled space [20]. 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. For $D$ finite but very large, the electrons are confined to harmonic oscillations about the fixed positions attained in the $D \to \infty$ limit. Briefly, 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, 18].

Despite all these efforts the large $D$ limit of the main prototype of the Coulomb systems, the $D$-dimensional hydrogenic system, poses some open problems which can be solved analytically. It is known that the introduction of a $D$-dependent length scale converts the large $D$ limit of the associated Schrödinger equation into Bohr's model [5]. On the other hand, we should keep in mind that the $D$-dimensional hydrogenic system (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) includes a wide variety of quantum systems, such as hydrogenic atoms and ions, exotic atoms, antimatter atoms, excitons, qubits, etc.

Moreover, the electronic distribution of the $D$-dimensional hydrogenic system is known (see next section) to have such a form that one can analytically determine its moments around the origin (radial expectation values) in both position [21–26] and momentum [27, 28] spaces as well as its entropic and complexity measures [29, 30]. These quantities describe and/or are closely related to various fundamental and/or experimentally accessible quantities (e.g., the diamagnetic susceptibility, the kinetic energy, the height peak of the Compton profile, the total electron-electron repulsion energy, etc.) and they characterize some position-momentum uncertainty-like relationships of Heisenberg [31, 32] and entropic [26] types (see also [30] and references therein).

Recently the radial expectation values of the $D$-dimensional hydrogenic states lying at the highest extreme region of the energy spectrum for a fixed $D$ were determined in both position and momentum spaces in terms of $D$ and the state's hyperquantum principal and orbital quantum numbers [33]. In this work we analytically determine these position and momentum quantities for all quantum hydrogenic states in the large dimensionality limit. First, in Section II the known physical solutions of the Schrödinger equation of the $D$-dimensional hydrogenic system are given in the two conjugated spaces, as well as the associated position and momentum probability densities and their corresponding radial expectation values in terms of the space dimensionality and of the hyperquantum numbers which characterize the system's states. We will see that the position and momentum expectation values are expressed in terms of some generalized hypergeometric functions [34] of the type ${}_{p+1}F_p\left(a_1, \ldots, a_{p+1}; b_1, \ldots, b_p; z\right)$ evaluated at $z = 1$, with $p = 2$ and $p = 3$, respectively Then, in Sections III and IV the position and momentum expectation values of the system are evaluated in the large dimensionality limit for the ground and excited states, respectively. Two different asymptotic approaches are developed to calculate the dominant term of the special functions ${}_3F_2\left(a_1, a_2, a_3; b_1, b_2; 1\right)$ and ${}_5F_4\left(a_1, a_2, a_3, a_4, a_5; b_1, b_2, b_3, b_4; 1\right)$ involved in the large $D$ limit of the position and momentum quantities under consideration. In Section V the position and momentum expectation values of the Rydberg (i.e., large $n$) hydrogenic states are calculated in the large $D$ limit. In Section VI, we give the uncertainty relations of Heisenberg and logarithmic types for all the stationary states of a $D$-dimensional hydrogenic system at the large-$D$ limit, and we show that they fulfill and saturate the general inequality-type uncertainty relations of all quantum systems. In Section VII, the position and momentum expectation values are shown to bound the Shannon and Rényi entropic uncertainty measures from above, and the Tsallis' uncertainty measure from below. Finally, some conclusions and open problems are given.

## II. THE $D$-DIMENSIONAL HYDROGENIC DENSITIES IN POSITION AND MOMENTUM SPACES

In this section we briefly describe the wavefunctions of the ground and excited states of the $D$-dimensional hydrogenic system and the associated electronic distribution densities in the two conjugated position and momentum spaces, as well as the exact, compact values of their radial and logarithmic expectation values.

### A. Position space

The time-independent Schrödinger equation of a $D$-dimensional ($D \geqslant 1$) 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

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

where $\vec{\nabla}_D$ denotes the $D$-dimensional gradient operator, $Z$ is the nuclear charge, and the electronic position vector is given in hyperspherical units as $\vec{r} = (r, \theta_1, \theta_2, \ldots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$, $\Omega_{D-1} \in S^{D-1}$, where $r \equiv |\vec{r}| \in [0\,;\,+\infty)$ and $\theta_i \in [0\,;\,\pi), i < D-1$, $\theta_{D-1} \equiv \phi \in [0\,;\,2\pi)$. It is assumed that the nucleus is located at the origin.
It is known [7, 30, 35, 36] that the energies belonging to the discrete spectrum are given by

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

and the associated eigenfunction can be expressed as

$$\Psi_{\eta,l,\{\mu\}}(\vec{r}) = \mathcal{R}_{\eta,l}(r)\ \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \tag{3}$$

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

$$\begin{aligned}\mathcal{R}_{n,l}(r) &= K_{n,l}\left(\frac{r}{\lambda}\right)^l e^{-\frac{r}{2\lambda}}\mathcal{L}_{n-l-1}^{(2l+D-2)}\left(\frac{r}{\lambda}\right) \\ &= K_{n,l}\left[\frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\right]^{1/2}\mathcal{L}_{\eta-L-1}^{(2L+1)}(\tilde{r}) \\ &= \left(\frac{\lambda^{-D}}{2\eta}\right)^{1/2}\left[\frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\right]^{1/2}\widehat{\mathcal{L}}_{\eta-L-1}^{(2L+1)}(\tilde{r}),\end{aligned} \tag{4}$$

where the "grand orbital angular momentum quantum number" $L$ and the adimensional parameter $\tilde{r}$ are

$$L = l + \frac{D-3}{2}, \qquad l = 0, 1, 2, \ldots \tag{5}$$

$$\tilde{r} = \frac{r}{\lambda}, \qquad \lambda = \frac{\eta}{2Z}, \tag{6}$$

and $\omega_\beta(x) = x^\beta e^{-x}$, $\beta = 2l + D - 2$, is the weight function of the Laguerre polynomials with parameter $\beta$. The symbols $\mathcal{L}_n^{(\beta)}(x)$ and $\widehat{\mathcal{L}}_n^{(\beta)}(x)$ denote the orthogonal and orthonormal, respectively, Laguerre polynomials with respect to the weight $\omega_\beta(x) = x^\beta e^{-x}$ on the interval $[0, \infty)$, so that

$$\widehat{\mathcal{L}}_m^{(\beta)}(x) = \left(\frac{m!}{\Gamma(m+\beta+1)}\right)^{1/2}\mathcal{L}_m^{(\beta)}(x), \tag{7}$$

and finally

$$K_{n,l} = \lambda^{-\frac{D}{2}}\left\{\frac{(\eta-L-1)!}{2\eta(\eta+L)!}\right\}^{\frac{1}{2}} = \left\{\left(\frac{2Z}{n+\frac{D-3}{2}}\right)^D \frac{(n-l-1)!}{2\left(n+\frac{D-3}{2}\right)(n+l+D-3)!}\right\}^{\frac{1}{2}} \tag{8}$$

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

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

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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 $\mathcal{C}_n^{(\lambda)}(t)$ denotes the Gegenbauer polynomial of degree $n$ and parameter $\lambda$, orthogonal on [-1,1] with respect to the weight function $w_\nu(t) = (1-t^2)^{\nu-1/2}$.

The quantum probability density of a $D$-dimensional hydrogenic stationary state $(n, l, \{\mu\})$ is the square of the absolute value of the position eigenfunction,

$$\rho_{n,l,\{\mu\}}(\vec{r}) = \rho_{n,l}(\tilde{r})\ |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2, \tag{9}$$

where the radial part of the density is the univariate function

$$\rho_{n,l}(\tilde{r}) \ = \ [\mathcal{R}_{n,l}(r)]^2 = \frac{\lambda^{-D}}{2\eta}\ \frac{\omega_{2L+1}(\tilde{r})}{\tilde{r}^{D-2}}\ [\widehat{\mathcal{L}}_{\eta-L-1}^{(2L+1)}(\tilde{r})]^2. \tag{10}$$

The moments (centered at the origin) of this density function are the radial expectation values in the position space, and can be expressed in the following compact form [23–25, 30]:

$$\begin{aligned} \langle r^\alpha \rangle &= \int r^\alpha \rho_{n,l,\{\mu\}}(\vec{r})\, d\vec{r} = \int_0^\infty r^{\alpha+D-1}\rho_{n,l}(\tilde{r})\, dr \\ &= \frac{1}{2\eta}\left(\frac{\eta}{2Z}\right)^\alpha \int_0^\infty \omega_{2l+D-2}(\tilde{r})[\widehat{\mathcal{L}}_{n-l-1}^{(2l+D-2)}(\tilde{r})]^2\, \tilde{r}^{\alpha+1}\, d\tilde{r} &(11)\\ &= \frac{\eta^{\alpha-1}}{2^{\alpha+1}Z^\alpha}\frac{\Gamma(2L+\alpha+3)}{\Gamma(2L+2)} \\ &\quad \times\, {}_3F_2(-\eta+L+1, -\alpha-1, \alpha+2; 2L+2, 1; 1), &(12)\end{aligned}$$

which holds for $\alpha > -D-2l$. Notice that these quantities are given in terms of $\eta, L$ and the nuclear charge $Z$. In particular, we have $\langle r^0\rangle = 1$, as well as the following values for the first few negative and positive expectation values:

$$\begin{aligned} \langle r^{-1}\rangle &= \frac{Z}{\eta^2}, \quad \langle r\rangle = \frac{1}{2Z}[3\eta^2 - L(L+1)], \quad \langle r^2\rangle = \frac{\eta^2}{2Z^2}[5\eta^2+1-3L(L+1)], \quad \langle r^{-2}\rangle = \frac{Z^2}{\eta^3}\frac{1}{L+\frac{1}{2}} \\ \langle r^{-3}\rangle &= \frac{Z^3}{\eta^3 L(L+\frac{1}{2})(L+1)}, \quad \langle r^{-4}\rangle = Z^4\frac{3\eta^2-L(L+1)}{2\eta^5(L-\frac{1}{2})L(L+\frac{1}{2})(L+1)(L+\frac{3}{2})}. \end{aligned} \tag{13}$$

Furthermore, the radial logarithmic values [30] are given by

$$\begin{aligned} \langle \log r\rangle &= \int (\log r)\rho_{n,l,\{\mu\}}(\vec{r})\, d\vec{r} \\ &= \log\left(n+\frac{D-3}{2}\right) + \frac{2n-2l-1}{2n+D-3} + \psi(n+l+D-2) - \log(2Z), \end{aligned} \tag{14}$$

where $\psi(x) \equiv \Gamma'(x)/\Gamma(x)$ is the digamma function [34].

Some relevant particular cases are:

- For the ground state $(n = 1, l = 0)$ we obtain the expressions

$$\langle r^\alpha\rangle \ = \ \left(\frac{D-1}{4Z}\right)^\alpha \frac{\Gamma(D+\alpha)}{\Gamma(D)}; \quad \alpha > -D \tag{15}$$

$$\langle \log r\rangle \ = \ \psi(D) + \log(D-1) - 2\log 2 - \log Z \tag{16}$$

  for the radial, both conventional and logarithmic, expectation values in position space, respectively.

- For Rydberg states $(n \gg 1)$, the radial expectation values have been recently shown [33] to be given as

$$\langle r^\alpha\rangle = \left(\frac{\eta^2}{Z}\right)^\alpha \frac{2^{\alpha+1}\,\Gamma(\alpha+\frac{3}{2})}{\sqrt{\pi}\,\Gamma(\alpha+2)}\,(1+o(1))\,, \quad n\to\infty \tag{17}$$

  with $(\alpha, l, D)$ uniformly bounded and $\alpha > -3/2$.

### B. Momentum space

In momentum space we can work out similarly the corresponding Schrödinger equation of our system to find [36–38] the following expression for the momentum wavefunction of the $D$-dimensional hydrogenic stationary state $(n, l, \{\mu\})$:

$$\tilde{\Psi}(\vec{p}) = \mathcal{M}_{n,l}(p)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \tag{18}$$

where the radial momentum wavefunction is

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

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

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

Then, the momentum probability density is

$$\begin{aligned}\gamma_{n,l,\{\mu\}}(\vec{p}) &= |\tilde{\Psi}_{n,l,\{\mu\}}(\vec{p})|^2 = \mathcal{M}^2_{n,l}(p)|\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &= K^2_{n,l}\frac{(\eta\tilde{p})^{2l}}{(1+\eta^2\tilde{p}^2)^{2L+4}}\left[\mathcal{C}^{(L+1)}_{\eta-L-1}\left(\frac{1-\eta^2\tilde{p}^2}{1+\eta^2\tilde{p}^2}\right)\right]^2|\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2. \end{aligned} \tag{21}$$

The moments centered at the origin of this density function are the radial expectation values in the momentum space, which can be expressed in the following compact form [27, 28]:

$$\begin{aligned}\langle p^\alpha\rangle &= \int p^\alpha\gamma_{n,l,\{\mu\}}(\vec{p})\,d\vec{p} = \int_0^\infty p^{\alpha+D-1}\mathcal{M}^2_{n,l}(p)\,dp \\ &= \left(\frac{Z}{\eta}\right)^\alpha\int_{-1}^{1} w_\nu(t)[\widehat{\mathcal{C}}^{(\nu)}_k(t)]^2(1-t)^{\frac{\alpha}{2}}(1+t)^{1-\frac{\alpha}{2}}\,dt \\ &= \left(\frac{Z}{\eta}\right)^\alpha\frac{2^{2\nu-1}k!(k+\nu)}{\pi\Gamma(k+2\nu)}[\Gamma(\nu)]^2\int_{-1}^{1} w_\nu(t)[\mathcal{C}^{(\nu)}_k(t)]^2(1-t)^{\frac{\alpha}{2}}(1+t)^{1-\frac{\alpha}{2}}\,dt \qquad (22) \\ &= \frac{2^{1-2\nu}Z^\alpha\sqrt{\pi}}{k!\,\eta^\alpha}\frac{(k+\nu)\Gamma(k+2\nu)\Gamma(\nu+\frac{\alpha+1}{2})\Gamma(\nu+\frac{3-\alpha}{2})}{\Gamma^2(\nu+\frac{1}{2})\Gamma(\nu+1)\Gamma(\nu+\frac{3}{2})} \\ &\quad\times\,{}_5F_4(-k,k+2\nu,\nu,\nu+\frac{\alpha+1}{2},\nu+\frac{3-\alpha}{2};2\nu,\nu+\frac{1}{2},\nu+1,\nu+\frac{3}{2};1), \qquad (23)\end{aligned}$$

which holds for $\alpha \in (-D-2l, D+2l+2)$. Here the notations $k = \eta+L+1 = n-l-1$ and $\nu = L+1 = l+(D-1)/2$ have been used. Moreover, the symbol $\widehat{\mathcal{C}}^{(\lambda)}_m(t)$ denotes the orthonormal Gegenbauer polynomials so that

$$\widehat{\mathcal{C}}^{(\lambda)}_m(t) = \frac{m!(m+\lambda)[\Gamma(\lambda)]^2}{\pi\,2^{1-2\lambda}\Gamma(m+2\lambda)}\,\mathcal{C}^{(\lambda)}_m(t). \tag{24}$$

Observe again that the momentum expectation values $\langle p^\alpha\rangle$ are given in terms of $\eta, L$ and the nuclear charge $Z$; or, equivalently, in terms of $n, l, D$ and $Z$. In particular, we have $\langle p^0\rangle = 1$, as well as the following expectation values with negative and positive even powers:

$$\begin{aligned}\langle p^{-2}\rangle &= \frac{Z^{-2}}{\eta^{-2}}\frac{8\eta-3(2L+1)}{2L+1}, \quad \langle p^2\rangle = \frac{Z^2}{\eta^2}, \quad \langle p^4\rangle = \frac{Z^4}{\eta^4}\frac{8\eta-3(2L+1)}{2L+1}. \\ \langle p^6\rangle &= \frac{Z^6}{\eta^6}\frac{(4k+2\nu+1)(16k^2+40\nu k-4k+4\nu^2+16\nu+15)}{(2L+3)(2L+1)(2L-1)}. \end{aligned} \tag{25}$$

Moreover,

$$\langle p^{-\beta}\rangle = \eta^{2\beta+2}\langle p^{\beta+2}\rangle, \quad \beta = 0, 1, 2, ... \tag{26}$$

Note that the expectation values with odd integer powers are not explicitly known, except possibly for the case $p = -1$, which has a somewhat complicated expression [39].

Furthermore, the logarithmic expectation values of the momentum density function are given by

$$\begin{aligned}\langle \log p\rangle &= \int (\log p)\gamma_{n,l,\{\mu\}}(\vec{p})\, d\vec{p} \\ &= -\log\left(n+\frac{D-3}{2}\right)+\frac{(2l+D-2)(2n+D-3)}{(2n+D-3)^2-1}-1+\log(Z).\end{aligned} \tag{27}$$

Some relevant particular cases:

- For the ground state one obtains

$$\langle p^\alpha\rangle = \left(\frac{2Z}{D-1}\right)^\alpha \frac{2\Gamma(\frac{D-\alpha}{2}+1)\Gamma(\frac{D+\alpha}{2})}{D\Gamma^2\left(\frac{D}{2}\right)}, \quad -D<\alpha<D+2 \tag{28}$$

$$\langle \log p\rangle = -\log(D-1)+\log 2-\frac{1}{D}+\log Z \tag{29}$$

  for the radial (conventional and logarithmic) values in momentum space, respectively.

- For Rydberg states ($n \gg 1$), it has been recently shown [33] that for $(l, D)$ uniformly bounded, the momentum expectation values satisfy

$$\langle p^\alpha\rangle \simeq \left(\frac{Z}{\eta}\right)^\alpha \begin{cases} \frac{\alpha-1}{\sin(\pi(\alpha-1)/2)}, & -1<\alpha<3, \quad \alpha\neq 1, \\ 2/\pi, & \alpha=1 \end{cases} \tag{30}$$

  understanding by $\simeq$ that the ratio of the left and right hand sides tends to 1 as $n\to\infty$. Moreover, for Rydberg states such that both $n$ and $l$ tend to infinity with the condition $n-l=$ constant, the radial momentum expectation values are given by

$$\langle p^\alpha\rangle \simeq \left(\frac{Z}{\eta}\right)^\alpha \frac{1}{2\pi}\int_{-1}^{1}\frac{(2-\sqrt{3}t)^{\frac{\alpha}{2}}(2+\sqrt{3}t)^{1-\frac{\alpha}{2}}}{\sqrt{1-t^2}}\, dt, \tag{31}$$

  provided that $D$ is bounded.

## III. POSITION EXPECTATION VALUES OF LARGE-$D$ HYDROGENIC SYSTEMS

In this section we calculate the position radial and logarithmic expectation values for an arbitrary (but fixed) state $(n, l, \{\mu\})$ of $D$-dimensional hydrogenic systems when $D\to\infty$. Let us first start with the radial expectation values $\langle r^\alpha\rangle$. We claim that these quantities have the following asymptotic expression:

$$\langle r^\alpha\rangle = \left(\frac{D^2}{4Z}\right)^\alpha\left(1+\frac{(\alpha+1)(\alpha+4l-2)}{2D}\right)\left(1+\frac{(\alpha+1)(\alpha+2)(n-l-1)}{D+2l-1}\right)\left(1+\mathcal{O}\left(\frac{1}{D^2}\right)\right) \tag{32}$$

as $D\to\infty$, which holds for $\alpha > -D-2l$. Notice that in such a limit one has that $\left(\frac{D^2}{4Z}\right)^{-\alpha}\langle r^\alpha\rangle \to 1$. Thus, our $D$-dimensional hydrogenic system has a characteristic length, $r_{char}=\frac{D^2}{4Z}$, which corresponds to the localization of the maximum of the ground-state probability density. Moreover, it is the radial distance at which the effective potential attains a minimum as $D\to\infty$. Therefore, the electron of the $D$-dimensional hydrogenic system behaves as it is moving in a circular orbit with radius $r_{char}$ and angular momentum $D/2$, experimenting quantum fluctuations from this orbit vanishing as $D^{-1/2}$, as it was previously noted by [22], since

$$\frac{\Delta r}{\langle r\rangle}=\frac{(\langle r^2\rangle-\langle r\rangle^2)^{1/2}}{\langle r\rangle}=\frac{1}{\sqrt{D}}.$$

For illustrative purposes, we show the rate of convergence of these large-$D$ values to the exact ones in Table I; see Appendix B.

Let us now prove the main result (32). We start from the general expression (11)-(12) for the radial expectation value of the $D$-hydrogenic state $(n, l, \{\mu\})$, which is given in terms of the generalized hypergeometric function ${}_3F_2$

evaluated at 1, and then we use the following asymptotic expression of ${}_{p+1}F_p$ for large parameters (see [40], [41, Eq. (7.3)] or [34, Eq. (16.11.10)]):

$$\begin{aligned} &{}_{p+1}F_p\left(a_1+r,\ldots,a_{k-1}+r,a_k,\ldots,a_{p+1};b_1+r,\ldots,b_k+r,b_{k+1},\ldots,b_p;z\right) = \\ &= \sum_{j=0}^{m-1}\frac{(a_1+r)_j\cdots(a_{k-1}+r)_j(a_k)_j\cdots(a_{p+1})_j}{(b_1+r)_j\cdots(b_k+r)_j(b_{k+1})_j\cdots(b_p)_j}\frac{z^j}{j!}+\mathcal{O}\left(\frac{1}{r^m}\right) \end{aligned} \tag{33}$$

as $r\to+\infty$, where $z$ is fixed, $|\arg(1-z)|<\pi$, $m\in\mathbb{Z}^+$, and $k$ can take any integer value from 1 to $p$. We have also used the Pochhammer symbol $(a)_j=\Gamma(a+j)/\Gamma(a)$. With $p=2$ and $k=1$ we obtain the following asymptotics for the ${}_3F_2$ hypergeometric function of our interest:

$${}_3F_2\left(a_1,a_2,a_3;b_1+r,b_2;z\right) = \sum_{j=0}^{m-1}\frac{(a_1)_j(a_2)_j(a_3)_j}{(b_1+r)_j(b_2)_j}\frac{z^j}{j!}+\mathcal{O}\left(\frac{1}{r^m}\right) \tag{34}$$

Applying this expression in (12) with $z=1$ and $r=D$, one has

$${}_3F_2\left(-n+l+1,-\alpha-1,\alpha+2;2l-1+D,1;1\right)=\sum_{j=0}^{m-1}\frac{(-n+l+1)_j(-\alpha-1)_j(\alpha+2)_j}{(2l-1+D)_j(1)_j}\frac{1}{j!}+\mathcal{O}\left(\frac{1}{D^m}\right), \tag{35}$$

which, when $D\to+\infty$, yields for $m=2$ the asymptotics

$${}_3F_2\left(-n+l+1,-\alpha-1,\alpha+2;2l-1+D,1;1\right)=1+\frac{(\alpha+1)(\alpha+2)(n-l-1)}{2l-1+D}+\mathcal{O}\left(\frac{1}{D^2}\right). \tag{36}$$

Now, by taking into account Eq. (12) together with (36) and the following asymptotics of the ratio (see e.g.,[34, Eq. (5.11.12)])

$$\frac{\Gamma(D+2l+\alpha)}{\Gamma(D+2l-1)}=D^{1+\alpha}\left(1+\frac{(\alpha+1)(\alpha+4l-2)}{2D}+\mathcal{O}\left(\frac{1}{D^2}\right)\right), \tag{37}$$

we have

$$\begin{aligned} \langle r^\alpha\rangle &= \left(\frac{D^2}{4Z}\right)^\alpha\left(1+\frac{(\alpha+1)(\alpha+4l-2)}{2D}\right)\left(1+\frac{(\alpha+1)(\alpha+2)(n-l-1)}{D+2l-1}\right)\left(1+\mathcal{O}\left(\frac{1}{D^2}\right)\right) \\ &= \left(\frac{D^2}{4Z}\right)^\alpha\left(1+\frac{(\alpha+1)(\alpha+4l-2)}{2D}\right)\left(1+\frac{(\alpha+1)(\alpha+2)(n-l-1)}{D}\right)\left(1+\mathcal{O}\left(\frac{1}{D^2}\right)\right), \end{aligned} \tag{38}$$

which gives the expression (32).

Now, let us explore the behavior of the logarithmic expectation value (14) of the $D$-dimensional hydrogenic system for large $D$. Taking into account that $\psi(z)=\log z-\frac{1}{2z}+\mathcal{O}\left(\frac{1}{z^2}\right)$ for $z\to\infty$ (see e.g., [34, Eq. (25.16.3)]) and $\log(a+bz)=\log(bz)+\frac{a}{bz}+\mathcal{O}\left(\frac{1}{z^2}\right)$ for $z\to\infty$, one has from (14) that

$$\langle\log r\rangle = 2\log D-\log(4Z)+\frac{5n-l-\frac{13}{2}}{D}+\mathcal{O}\left(\frac{1}{D^2}\right). \tag{39}$$

Finally, for circular states ($l=n-1$) one has that the position and logarithmic expectation values given by (32) and (39), respectively, reduce to

$$\langle r^\alpha\rangle_{cs}=\left(\frac{D^2}{4Z}\right)^\alpha\left[1+\frac{(\alpha+1)(4n+\alpha-6)}{2D}\right]\left(1+\mathcal{O}\left(\frac{1}{D^2}\right)\right) \tag{40}$$

and

$$\langle\log r\rangle_{cs}=\frac{4n-\frac{11}{2}}{D}+2\log D-\log(4Z)+\mathcal{O}\left(\frac{1}{D^2}\right), \tag{41}$$

respectively. Moreover, from these expressions we can easily obtain the position and logarithmic expectation values for the ground state ($n=1$) of the $D$-dimensional hydrogenic system at large $D$.

## IV. MOMENTUM EXPECTATION VALUES OF LARGE-$D$ HYDROGENIC SYSTEMS

In this section we calculate the momentum radial and logarithmic expectation values for an arbitrary (but fixed) state $(n, l, \{\mu\})$ of $D$-dimensional hydrogenic systems when $D \to \infty$. First, let us consider the momentum expectation values $\langle p^\alpha \rangle$. We claim that these quantities have the following asymptotic expression:

$$\begin{aligned}\langle p^\alpha \rangle &= \left(\frac{Z}{n+\frac{D-3}{2}}\right)^\alpha \left(1+\frac{\alpha(\alpha-2)(2n-2l-1)}{2D}+\mathcal{O}(D^{-2})\right)\\ &= \left(\frac{2Z}{D}\right)^\alpha \left(1+\frac{\alpha(\alpha-2)(2n-2l-1)}{2D}+\mathcal{O}(D^{-2})\right) \qquad (42)\end{aligned}$$

as $D \to \infty$, which holds for $\alpha \in (-D-2l, D+2l+2)$. Notice that in such limit one has that $\left(\frac{D^2}{4Z}\right)^{-\alpha} \langle p^\alpha \rangle \to 1$. Thus, our $D$-dimensional hydrogenic system has a characteristic momentum, $p_{char} = \frac{D^2}{4Z}$, which corresponds to the localization of the maximum of the ground-state probability density in momentum space. Moreover, it gives the velocity at which the electron of our system moves in the circular orbit defined in the previous section as $D \to \infty$. For illustrative purposes, we show the rate of convergence of these large-D values to the exact ones in Table I; see Appendix B.

Let us now prove the main result (42). We start from the general expression (22). Then, using the definition of the hypergeometric function and the duplication formula of the gamma function (see e.g., [34]), we can rewrite (22) as

$$\begin{aligned}\langle p^\alpha \rangle \frac{\eta^\alpha}{Z^\alpha} &= \frac{2}{k!}\frac{(k+\nu)\Gamma(k+2\nu)}{\Gamma(2\nu+1)}\frac{\Gamma(\nu+\frac{\alpha+1}{2})\Gamma(\nu+\frac{3-\alpha}{2})}{\Gamma(\nu+\frac{1}{2})\Gamma(\nu+\frac{3}{2})}\\ &\times \sum_{j=0}^{k}(-1)^j\binom{k}{j}\frac{(k+2\nu)_j(\nu)_j(\nu+\frac{\alpha+1}{2})_j(\nu+\frac{3-\alpha}{2})_j}{(2\nu)_j(\nu+1)_j(\nu+\frac{1}{2})_j(\nu+\frac{3}{2})_j} \qquad (43)\end{aligned}$$

We want to determine the asymptotics of this quantity in the $D \to \infty$ limit when $n$ and $l$ are fixed. Since $k = n-l-1$ and $\nu = l + (D-1)/2$, one realizes that we have to compute the asymptotics of (43) when $\nu \to \infty$ and $k$ is fixed. To begin with, we take into account the following identities for the Pochhammer symbols

$$\frac{(2\nu+k)_j}{(2\nu)_j} = \frac{(2\nu+j)_k}{(2\nu)_k}, \quad \frac{(\nu)_j}{(\nu+1)_j} = \frac{\nu}{\nu+j} \qquad (44)$$

in Eq. (43), so that we can rewrite it as follows

$$\langle p^\alpha \rangle \frac{\eta^\alpha}{Z^\alpha} = \frac{2}{k!}\frac{(k+\nu)\Gamma(k+2\nu)}{\Gamma(2\nu+1)}\frac{\Gamma(\nu+\frac{\alpha+1}{2})\Gamma(\nu+\frac{3-\alpha}{2})}{\Gamma(\nu+\frac{1}{2})\Gamma(\nu+\frac{3}{2})} f_k(\nu) \qquad (45)$$

with

$$f_k(\nu) = \frac{1}{(2\nu)_k}\sum_{j=0}^{k}(-1)^j\binom{k}{j}(2\nu+j)_k\, d_j, \qquad (46)$$

where

$$d_j \equiv d_j(\nu) = \frac{\nu}{\nu+j}\frac{(\nu+\frac{\alpha+1}{2})_j(\nu+\frac{3-\alpha}{2})_j}{(\nu+\frac{1}{2})_j(\nu+\frac{3}{2})_j}. \qquad (47)$$

In order to find the asymptotics of (45) we take into account that, as $\nu \to +\infty$,

$$2\frac{(k+\nu)\Gamma(k+2\nu)}{\Gamma(2\nu+1)} = (2\nu)^k\left(1+\frac{k(k+3)}{4\nu}+o(1/\nu)\right). \qquad (48)$$

and

$$\frac{\Gamma(\nu+\frac{\alpha+1}{2})\Gamma(\nu+\frac{3-\alpha}{2})}{\Gamma(\nu+\frac{1}{2})\Gamma(\nu+\frac{3}{2})} = 1+\frac{\alpha(\alpha-2)}{4\nu}+o(1/\nu), \qquad (49)$$

so that it only remains to obtain the asymptotics of $f_k(\nu)$ defined in (46). This is the most difficult issue, which is explicitly solved in Appendix A where we have found the first two terms of the asymptotics:

$$f_k(\nu) = \frac{k!}{(2\nu)^k}\left(1 - \frac{k(k+3+2\alpha(2-\alpha))}{4\nu} + \mathcal{O}\left(\frac{1}{\nu^2}\right)\right). \tag{50}$$

Then, inserting (48), (49) and (50) in (45) we get

$$\langle p^\alpha\rangle = \frac{Z^\alpha}{\eta^\alpha}\left(1 + \frac{\alpha(\alpha-2)(2k+1)}{4\nu} + o(1/\nu)\right), \quad \nu \to +\infty. \tag{51}$$

From this expression and taking into account that $\eta = n + \frac{D-3}{2}$ and $\nu = l + \frac{D-1}{2}$, one can obtain the asymptotics (42) at the limit $D \to \infty$ for the momentum expectation values of the $D$-dimensional hydrogenic system. It is worth mentioning that the method (see Appendix A) admits further refinement to obtain next terms of the asymptotic expansion of $\langle p^\alpha\rangle$.

Now let us consider the momentum logarithmic expectation value $\langle \log p\rangle$. From the general expression (27) one has this quantity in the large $D$ limit is given by

$$\langle \log p\rangle = -\frac{4n-2l-4}{D} - \log D + \log(2Z) + \mathcal{O}\left(\frac{1}{D^2}\right). \tag{52}$$

Finally, for the circular states ($l = n-1$) the general expressions (42) and (52) supply the following momentum radial and logarithmic expectation values

$$\langle p^\alpha\rangle_{cs} = \left(\frac{2Z}{D}\right)^\alpha\left(1 + \frac{\alpha(\alpha-2)}{2D} + \mathcal{O}(D^{-2})\right), \tag{53}$$

and

$$\langle \log p\rangle_{cs} = -\frac{1}{D} - \log\left(\frac{D}{2}\right) + \log(Z) + \mathcal{O}\left(\frac{1}{D^2}\right), \tag{54}$$

respectively. Moreover, from these expressions we can obtain the momentum and logarithmic expectation values for the ground state ($n = 1$) of the $D$-dimensional hydrogenic system at the $D \to \infty$ limit.

## V. EXPECTATION VALUES OF LARGE-$D$ FOR RYDBERG HYDROGENIC STATES

In this section we compute the radial expectation values in position and momentum spaces for D-dimensional Rydberg hydrogenic states $(n, l, \{\mu\})$ when $D \gg 1$ and $n \gg 1$, being $(l, \{\mu\})$ uniformly bounded. The final expressions are Eqs. (68) and (83) in the two reciprocal spaces, respectively.

### A. Position space

We begin with the expression (11) of the position expectation value of an arbitrary $D$-dimensional hydrogenic state characterized by the hyperquantum numbers $(n, l, \{\mu\})$,

$$2\eta\left(\frac{2Z}{\eta}\right)^\alpha \langle r^\alpha\rangle = \int_0^\infty \omega_\nu(t)[\widehat{\mathcal{L}}_k^{(\nu)}(t)]^2 t^{\alpha+1}\,dt, \tag{55}$$

with $k = n-l-1$ and $\nu = 2l+D-2$. This integral converges for all values of $\alpha > -2l-D$. For convenience we make the linear change $t = kx$, so that we can rewrite the previous expression as

$$2\eta\left(\frac{2Z}{\eta}\right)^\alpha \langle r^\alpha\rangle = k^{\alpha+1}\int_0^\infty x^\nu e^{-kx}[\hat{\mathcal{L}}_k^{(\nu)}(x)]^2 x^{\alpha+1}\,dx, \tag{56}$$

where the polynomial

$$\hat{\mathcal{L}}_k^{(\nu)}(x) \equiv k^{\frac{\nu+1}{2}}\,\widehat{\mathcal{L}}_k^{(\nu)}(kx) \tag{57}$$

is orthonormal on $[0,+\infty)$ with respect to the weight $x^\nu e^{-kx}$. We want to determine its asymptotics when $n$ and $D$ tend simultaneously to infinity and $l$ is uniformly bounded; that is, when both $k$ and $\nu$ tend to infinity simultaneously. So, $\lim_{n\to+\infty}\frac{l}{n}=0$ and we assume that

$$\lim_{k\to+\infty}\frac{\nu}{k}=\lambda\in(0+\infty). \tag{58}$$

In this situation, polynomials $\hat{\mathcal{L}}_k^{(\nu)}(x)$ given by (57) are orthogonal with respect to a varying weight, i.e. a weight which depends on the degree $k$ in the form

$$\omega_k(x)=x^{\alpha_k}e^{-\beta_k x}\quad\text{with}\quad \alpha_k=\nu\quad\text{and}\quad\beta_k=k. \tag{59}$$

It is a known fact (see [42, Chap. 7], also [33]) that the modified Laguerre function converges in the weak-* sense, as $k\to\infty$:

$$[\hat{\mathcal{L}}_{k,k}^{(\nu)}(x)]^2\omega_k(x)dx\to d\mu_1(x):=\frac{1}{\pi}\frac{\sqrt{(x-a)(b-x)}}{x}\,dx,\quad a<x<b, \tag{60}$$

where $\mu_1$ is the equilibrium measure on $\mathbb{R}_+$ in the external field

$$\phi(x)=-\frac{\lambda}{2}\log x+\frac{x}{2}; \tag{61}$$

it is supported on the interval $[a,b]$ given explicitly by

$$a=a_\lambda=\lambda+1-\sqrt{1+2\lambda},\quad b=b_\lambda=\lambda+1+\sqrt{1+2\lambda}. \tag{62}$$

Thus,

$$\lim_{k\to+\infty}\int_0^\infty x^\nu e^{-kx}[\hat{\mathcal{L}}_{k,k}^{(\nu)}(x)]^2x^{\alpha+1}\,dx=\frac{1}{\pi}\int_{a_\lambda}^{b_\lambda}x^\alpha\sqrt{(x-a_\lambda)(b_\lambda-x)}\,dx. \tag{63}$$

With the change of variable $z=\frac{x-a_\lambda}{b_\lambda-a_\lambda}$ we get

$$\begin{aligned}\lim_{k\to+\infty}\int_0^\infty x^\nu e^{-kx}[\hat{\mathcal{L}}_{k,k}^{(\nu)}(x)]^2x^{\alpha+1}\,dx &= \frac{a_\lambda^\alpha(b_\lambda-a_\lambda)^2}{\pi}\int_0^1\left(1+z\frac{b_\lambda-a_\lambda}{a_\lambda}\right)^\alpha z^{\frac12}(1-z)^{\frac12}\,dz\\ &= \frac{a_\lambda^\alpha(b_\lambda-a_\lambda)^2}{8}\,{}_2F_1\left(-\alpha,\frac{3}{2};3;\frac{a_\lambda-b_\lambda}{a_\lambda}\right),\end{aligned} \tag{64}$$

where we have used the integral representation of the ${}_2F_1$,

$${}_2F_1(a,b;c;z)=\frac{\Gamma(c)}{\Gamma(c-b)\Gamma(b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-zt)^{-a}\,dt. \tag{65}$$

by equation (56) we obtain

$$\lim_{k\to\infty}2\eta\left(\frac{2Z}{\eta}\right)\langle r^\alpha\rangle=\frac{k^{\alpha+1}a_\lambda^\alpha(b_\lambda-a_\lambda)^2}{8}\,{}_2F_1\left(-\alpha,\frac{3}{2};3;\frac{a_\lambda-b_\lambda}{a_\lambda}\right). \tag{66}$$

Then, for $k\to+\infty$ and $\nu\to+\infty$ satisfying (58) we finally get

$$\begin{aligned}\langle r^\alpha\rangle &= \frac{1}{2\eta}\left(\frac{\eta}{2Z}\right)^\alpha\frac{k^{\alpha+1}a_\lambda^\alpha(b_\lambda-a_\lambda)^2}{8}\,{}_2F_1\left(-\alpha,\frac{3}{2};3;\frac{a_\lambda-b_\lambda}{a_\lambda}\right)(1+o(1)) & (67)\\ &= \frac{(2n+D)^{\alpha-1}n^{\alpha+1}}{2^{2\alpha+3}Z^\alpha}a_\lambda^\alpha(b_\lambda-a_\lambda)^2\,{}_2F_1\left(-\alpha,\frac{3}{2};3;\frac{a_\lambda-b_\lambda}{a_\lambda}\right)(1+o(1)), & (68)\end{aligned}$$

where in the second equality we have considered the approximations $k=n-l-1\simeq n$ and $\eta=n+\frac{D-3}{2}\simeq n+\frac{D}{2}$.

### B. Momentum space

We turn to the general expression (22) of the momentum expectation values $\langle p^\alpha \rangle$ of a generic $D$-dimensional hydrogenic state. Our aim is to determine the asymptotics of $\langle p^\alpha \rangle$ when $n$ and $D$ tend simultaneously to infinity and for $l$ uniformly bounded; that is, when both $k$ and $\nu$ tend to infinity simultaneously and satisfy the condition (58).

For convenience we rewrite (22) as

$$\langle p^\alpha \rangle \;=\; Z^\alpha \left( \frac{2}{2n+D-3} \right)^\alpha \int_{-1}^{1} (1-t)^{\alpha/2} (1+t)^{1-\alpha/2} [G_k^{(\nu)}(t)]^2 c_\nu w^\nu(t)\, dt, \tag{69}$$

where the factor $c_\nu$ is given by

$$c_\nu = \frac{\Gamma(\nu+1)}{\sqrt{\pi}\,\Gamma(\nu+1/2)} \tag{70}$$

so that

$$\int_{-1}^{1} c_\nu w^\nu(t)\, dt = 1. \tag{71}$$

The appropriately normalized Gegenbauer polynomials,

$$G_k^{(\nu)}(x) = \left( \frac{k!(k+\nu)\Gamma(2\nu)}{\nu \Gamma(k+2\nu)} \right)^{1/2} \mathcal{C}_k^{(\nu)}(x), \tag{72}$$

are orthonormal with respect to the unit weight $c_\nu w^\nu(x)$, and exhibit the following weak-* asymptotics:

$$[G_k^{(\nu)}(x)]^2 c_\nu w^\nu(x)\, dx \longrightarrow \frac{1}{\pi} \frac{dx}{\sqrt{1-x^2}}, \quad k \to \infty. \tag{73}$$

Since $\nu, k \to +\infty$ with the condition (58) satisfied, and

$$\lim_{k \to +\infty} - \frac{\log(c_\nu w_\nu(x))}{2k} = \frac{\lambda}{2} \log \frac{1}{1-x^2}, \quad x \in (-1,1), \tag{74}$$

one has [33] that the weak-* asymptotics of the orthonormal Gegenbauer polynomials $G_k^{(\nu)}(x)$ is given by

$$[G_k^{(\nu)}(x)]^2 c_\nu w^\nu(x)\, dx \longrightarrow d\mu_2(x), \quad \nu, k \to \infty, \tag{75}$$

on $[-1,1]$, where $\mu_2$ is the probability equilibrium measure on $[-1,1]$ in the external field

$$\phi(x) = \frac{\lambda}{2} \log \frac{1}{1-x^2}, \quad x \in (-1,1), \tag{76}$$

created by two charges of size $\lambda/2$ fixed at $\pm 1$. The expression of $\mu_2$ is well-known (cf. [42], Examples IV.1.17 and IV.5.2). It is supported on $[-\xi_\lambda, \xi_\lambda]$, with

$$\xi_\lambda = \frac{\sqrt{\lambda + 1/4}}{\lambda + 1/2} > 0, \tag{77}$$

and

$$\mu_2'(x) = \begin{cases} \frac{1+2\lambda}{\pi} \frac{\sqrt{\xi_\lambda^2 - x^2}}{1-x^2} & \text{if } |x| \le \xi_\lambda, \\ 0 & \text{otherwise.} \end{cases} \tag{78}$$

Hence, we have

$$\begin{aligned} \lim_{k \to \infty} \int_{-1}^{1} (1-t)^{\alpha/2} (1+t)^{1-\alpha/2} [G_k^{(\nu)}(x)]^2 c_\nu w^\nu(t)\, dt \;&=\; \lim_{k \to \infty} \frac{\Gamma(\nu+1)}{\sqrt{\pi}\Gamma(\nu+1/2)} \frac{k!(k+\nu)\Gamma(2\nu)}{\nu\, \Gamma(k+2\nu)} \\ &\quad \times \int_{-1}^{1} (1-t)^{\alpha/2} (1+t)^{1-\alpha/2} [\mathcal{C}_k^{(\nu)}(x)]^2 w^\nu(t)\, dt \\ &=\; \frac{1+2\lambda}{\pi} \int_{-\xi_\lambda}^{\xi_\lambda} (1-t)^{-1+\alpha/2} (1+t)^{-\alpha/2} \sqrt{\xi_\lambda^2 - t^2}\, dt. \end{aligned} \tag{79}$$

From [34] we know that for $\mathrm{Re}(\lambda) > 0, \mathrm{Re}(\mu) > 0$, one has

$$\int_0^1 x^{\lambda-1}(1-x)^{\mu-1}(1-ux)^{-\rho}(1-vx)^{-\sigma}\,dx = B(\mu,\lambda)\,F_1(\lambda,\rho,\sigma,\lambda+\mu;u,v), \tag{80}$$

where $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Euler beta function, while the Appel's hypergeometric function $F_1(x,y)$ is defined for $|x| < 1$, $|y| < 1$ as

$$F_1(\alpha,\beta,\beta',\gamma;x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(\alpha)_{m+n}(\beta)_m(\beta')_n}{(\gamma)_{m+n}m!n!}\,x^m\,y^n, \tag{81}$$

and extended analytically elsewhere. Since $B(3/2,3/2) = \pi/8$,

$$\begin{aligned}\int_{-\xi_\lambda}^{\xi_\lambda} (1-t)^{-1+\alpha/2}(1+t)^{-\alpha/2}\sqrt{\xi_\lambda^2-t^2}\,dt = 4\xi_\lambda^2(1-\xi_\lambda)^{-1}&\\ \times\int_0^1\left(1-\frac{2\xi_\lambda}{1+\xi_\lambda}x\right)^{-1+\alpha/2}\left(1-\frac{-2\xi_\lambda}{1+\xi_\lambda}x\right)^{-\alpha/2} x^{1/2}\sqrt{1-x}\,dx&\\ =\frac{\pi}{8}\,F_1\left(\frac{3}{2},1-\frac{\alpha}{2},\frac{\alpha}{2},3;\frac{2\xi_\lambda}{1+\xi_\lambda},\frac{-2\xi_\lambda}{1+\xi_\lambda}\right).&\end{aligned} \tag{82}$$

Thus, from (69) *et sequel* we get that for $k \to +\infty$ and $\nu \to +\infty$ (i.e. when $n$ and $D$ tend to infinity) satisfying $\lim_{k\to+\infty}\frac{\nu}{k} = \lambda \in (0+\infty)$,

$$\begin{aligned}\langle p^\alpha\rangle =&Z^\alpha\left(\frac{2}{2n+D-3}\right)^\alpha\frac{1+2\lambda}{8}\,F_1\left(\frac{3}{2},1-\frac{\alpha}{2},\frac{\alpha}{2},3;\frac{2\xi_\lambda}{1+\xi_\lambda},\frac{-2\xi_\lambda}{1+\xi_\lambda}\right)\\ &\times\left(\frac{\Gamma(1+(D-1)/2)}{\Gamma(\nu)}\right)^2(1+o(1)),\end{aligned} \tag{83}$$

where $\nu = 2l + D - 2$.

## VI. UNCERTAINTY RELATIONS AT THE PSEUDOCLASSICAL LIMIT

In this section we study the uncertainty relations of Heisenberg and logarithmic types for the stationary states of a $D$-dimensional hydrogenic system at the pseudoclassical large-$D$ limit, and we illustrate that they fulfill the inequality-type uncertainty relations of both a general quantum system and a system with a central potential. Let us recall that the Heisenberg-like uncertainty relation [43]

$$\langle r^2\rangle\langle p^2\rangle \geq \frac{D^2}{4}, \tag{84}$$

and the logarithmic-type uncertainty relation [44]

$$\langle\log r\rangle + \langle\log p\rangle \geq \psi\left(\frac{D}{4}\right) + \log 2; \quad l = 0,1,2,\ldots \tag{85}$$

are fulfilled for all stationary states of general $D$-dimensional quantum systems. Moreover, when the quantum-mechanical potential of the system is spherically symmetric, these uncertainty relations can be refined [45] as

$$\langle r^2\rangle\langle p^2\rangle \geq \left(L+\frac{3}{2}\right)^2 = \left(\frac{D}{2}+l\right)^2 \tag{86}$$

and [44]

$$\langle\log r\rangle + \langle\log p\rangle \geq \psi\left(\frac{D+2l}{4}\right) + \log 2; \quad l = 0,1,2,\ldots \tag{87}$$

respectively.

### A. Heisenberg-like relations

Taking into account the results of Section I, we have that the generalized Heisenberg-like uncertainty product $\langle r^\alpha\rangle\langle p^\beta\rangle$ of the $D$-dimensional hydrogenic system is given by

$$\begin{aligned}
\langle r^\alpha\rangle\langle p^\beta\rangle &= \frac{2Z^k\eta^{\alpha-k-1}\Gamma\left(\frac{1}{2}(D-k+2)+l\right)\Gamma\left(\frac{D+k}{2}+l\right)\Gamma(D+2l+\alpha)\Gamma(D+l+n-2)}{\left[\Gamma\left(\frac{D}{2}+l\right)\right]^2\Gamma(D+2l-1)\Gamma(D+2l+1)\Gamma(n-l)} \\
&\times {}_3F_2(l-n+1,-\alpha-1,\alpha+2;1,D+2l-1;1) \\
&\times {}_5F_4\Bigg(\frac{D-1}{2}+l,\frac{1}{2}(D-k+2)+l,\frac{D+k}{2}+l,l-n+1,D+l+n-2 \\
&\qquad ;\frac{D}{2}+l,\frac{D+1}{2}+l,\frac{D}{2}+l+1,D+2l-1;1\Bigg), \qquad (88)
\end{aligned}$$

which holds for $\alpha > -D-2l$ and $\beta \in (-D-2l, D+2l+2)$. Here again the notations $k = \eta + L + 1 = n - l - 1$ and $\nu = L + 1 = l + (D-1)/2$ have been used. Note that for for $\alpha = \beta$, the corresponding generalized uncertainty product $\langle r^\alpha\rangle\langle p^\alpha\rangle$ can be simplified further and, moreover, it does not depend on the nuclear charge $Z$ as one would expect. For the particular case $\alpha = \beta = 2$ this expression provides the following Heisenberg uncertainty product

$$\langle r^2\rangle\langle p^2\rangle = \frac{D^2}{4}\left\{1+\frac{1}{D}(10n-6l-9)+\frac{1}{D^2}[10n(n-3)-6l(l-2)+20]\right\}, \qquad (89)$$

which fulfills not only the general uncertainty relation (84) but also the refined uncertainty relation (86), as it should. Note that for the ground state we have the exact uncertainty relationship

$$\langle r^2\rangle_{gs}\langle p^2\rangle_{gs} = \frac{D^2}{4}\left(1+\frac{1}{D}\right)$$

What happens at the pseudoclassical large-$D$ limit? Taking into account (32) and (42), one has the following expression for the generalized Heisenberg-like uncertainty product of a general hydrogenic state $(n, l, \{\mu\})$ at the large-$D$ limit:

$$\begin{aligned}
\langle r^\alpha\rangle\langle p^\beta\rangle &= \left(\frac{D^2}{4Z}\right)^\alpha\left(\frac{D}{2Z}\right)^{-\beta}\left(1+\frac{(\alpha+1)(\alpha+4l-2)}{2D}\right)\left(1+\frac{(\alpha+1)(\alpha+2)(n-l-1)}{D}\right) \\
&\times\left(1+\frac{(\beta-2)\beta(2n-2l-1)}{2D}\right)(1+o(1)), \qquad (90)
\end{aligned}$$

which holds for $\alpha > -D-2l$ and $\beta \in (-D-2l, D+2l+2)$.
Particular case: for circular hydrogenic states $(n, n-1, \{n-1\})$ one obtains

$$\langle r^\alpha\rangle_{cs}\langle p^\beta\rangle_{cs} = \left(\frac{D^2}{4Z}\right)^\alpha\left(\frac{D}{2Z}\right)^{-\beta}\left(1+\frac{(\alpha+1)(4n-6)}{2D}\right)\left(1+\frac{\beta(\beta-2)}{2D}\right)(1+o(1)), \qquad (91)$$

which for $\alpha = \beta = 2$ gives

$$\langle r^2\rangle_{cs}\langle p^2\rangle_{cs} = \frac{D^2}{4}\left[1+\frac{6(n-1)}{D}\right](1+o(1)). \qquad (92)$$

Then, for the ground state ($n = 1$) we have that $\langle r^2\rangle_{gs}\langle p^2\rangle_{gs} = \frac{D^2}{4}$, so obtaining the equality in the general Heisenberg lower bounds given by (84) and (86).

### B. Logarithmic relations

The logarithmic uncertainty relation of a $D$-dimensional hydrogenic system has the form

$$\langle\log r\rangle+\langle\log p\rangle = \frac{2n-2l-1}{2n+D-3}+\frac{(2n+D-3)(2l+D-2)}{(2n+D-3)^2-1}-\log 2-1+\psi(n+1+D-2),$$

where $k = n - l - 1$ and $\nu = L + 1 = l + \frac{D-1}{2}$. Note again that this uncertainty relation does not depend on the nuclear charge, as one would expect. Taking into account again that [34] $\psi(z) = \log z - \frac{1}{2z} + o(1/z)$ for $z \to \infty$, one finds that at the large-$D$ limit, this relation gets refined as

$$\langle \log r \rangle + \langle \log p \rangle = \log \frac{D}{2} + \frac{n + l - \frac{5}{2}}{D} + \mathcal{O}\left(\frac{1}{D^2}\right). \tag{93}$$

Particular case: for the circular hydrogenic states which have $l = n - 1$, one has that

$$\langle \log r \rangle_{cs} + \langle \log p \rangle_{cs} = \log \frac{D}{2} + \frac{2n - \frac{7}{2}}{D} + \mathcal{O}\left(\frac{1}{D^2}\right), \tag{94}$$

so that for the ground state ($n = 1$) one obtains

$$\langle \log r \rangle_{gs} + \langle \log p \rangle_{gs} = \log \frac{D}{2} - \frac{3}{2D} + \mathcal{O}\left(\frac{1}{D^2}\right),$$

which saturates the general uncertainty inequalities (85) and (87).
Let us finally highlight that the general uncertainty inequalities of the $D$-dimensional quantum systems (84)-(87) saturate, i.e. become uncertainty equalities, for the $D$-dimensional hydrogenic atom.

## VII. BOUNDS ON ENTROPIC UNCERTAINTY MEASURES AT LARGE $D$

The Shannon and Rényi entropies of general $D$-dimensional quantum systems not only describe numerous fundamental quantities of these systems but also characterize most appropriately uncertainty measures, both in position and momentum spaces. However, they cannot be computed in a closed form for the stationary states of the system, except for those lying at the two extremes of the associated energetic spectrum (particularly the ground state and the Rydberg states) of the hydrogenic [30, 36, 46, 47] and oscillator-like [48, 49] systems.

In this section we obtain upper bounds on the Shannon [50] and Rényi [51] entropies and lower bounds on the Tsallis entropy [52] of arbitrary stationary states of the $D$-dimensional hydrogenic states at the large $D$ limit in terms of $D$ and the states' hyperquantum numbers. The hydrogenic Shannon, Rényi and Tsallis entropies are defined by the following logarithmic and power functionals of the electron probability density $\rho(\vec{r}) \equiv \rho_{n,l,\{\mu\}}(\vec{r})$ :

$$S[\rho] := -\int_{R_D} \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r}, \tag{95}$$

$$R_q[\rho] := \frac{1}{1-q} \log W_q[\rho] = \frac{1}{1-q} \log \int_{R_D} [\rho(\vec{r})]^q \, d\vec{r}, \tag{96}$$

and

$$T_q[\rho] := \frac{1}{q-1} [1 - W_q[\rho]] = \frac{1}{q-1} \left\{ 1 - \int_{R_D} [\rho(\vec{r})]^q \, d\vec{r} \right\} \tag{97}$$

respectively, where $\rho(\vec{r})$ is given by (9) and $q > 0$, $q \neq 1$. Notice that when $q \to 1$, both Rényi and Tsallis entropies reduce to Shannon entropy.

### A. Upper bounds

It is known [53] that the the Shannon entropy of general quantum systems have the following upper bounds, valid for all $\alpha > 0$,

$$S[\rho] \leq A_0(\alpha, D) + \frac{D}{\alpha} \log \langle r^\alpha \rangle, \tag{98}$$

with

$$A_0(\alpha, D) = \frac{D}{\alpha} + \log\left[\frac{2\pi^{\frac{D}{2}}}{\alpha} \left(\frac{\alpha}{D}\right)^{\frac{D}{\alpha}} \frac{\Gamma(\frac{D}{\alpha})}{\Gamma(\frac{D}{2})}\right]. \tag{99}$$

The Rényi entropy $R_q[\rho]$ can be bounded from above in terms of $\langle r^\alpha\rangle$, with $\alpha \in \mathbb{N}$, by

$$R_q[\rho] \leq \frac{1}{1-q} \log \left\{ L_1(q,\alpha,D) \, \langle r^\alpha \rangle^{-\frac{D}{\alpha}(q-1)} \right\} \tag{100}$$

and in terms of $\langle r^{-\alpha}\rangle$, with $\alpha \in \mathbb{N}$, but subject to the condition $\alpha < \frac{D}{q}(q-1)$, by

$$R_q[\rho] \leq \frac{1}{1-q} \log \left\{ L_2(q,\alpha,D) \, \left\langle r^{-\alpha} \right\rangle^{-\frac{D}{\alpha}(q-1)} \right\}. \tag{101}$$

Functions $L_i\,(q,\alpha,D)$, $i=1,2$, have an explicit expression,

$$L_1\,(q,\alpha,D) = \frac{q\alpha}{D(q-1)+\alpha q} \left\{ \frac{\alpha\Gamma\,(D/2) \left[\frac{D(q-1)}{D(q-1)+\alpha q}\right]^{\frac{D}{\alpha}}}{2\pi^{\frac{D}{2}} B\left(\frac{q}{q-1}, \frac{D}{\alpha}\right)} \right\}^{q-1} \tag{102}$$

and

$$L_2\,(q,\alpha,D) = \frac{q\alpha}{D(q-1)-\alpha q} \left\{ \frac{\alpha\Gamma\,(D/2) \left[\frac{D(q-1)-\alpha q}{D(q-1)}\right]^{\frac{D}{\alpha}}}{2\pi^{\frac{D}{2}} B\left(\frac{D}{\alpha} - \frac{1}{q-1}, \frac{q}{q-1}\right)} \right\}^{q-1}. \tag{103}$$

To derive these upper bounds we have used the variational bounds [54] on the entropic moments $W_\alpha[\rho]$ with a single expectation value $\langle r^\alpha\rangle$ as constraint. At the pseudoclassical limit we have that

$$A_0(\alpha,D) = -\frac{D-1}{2}\log\frac{D}{2} + \log(\pi e)\frac{D}{2} - \frac{1}{2}\log\frac{D}{\alpha} + \log\frac{2}{\alpha} + o(1), \tag{104}$$

where we have used the asymptotic expansion [34] $\log\Gamma(z) = \left(z-\frac{1}{2}\right)\log z - z + \frac{1}{2}\log 2\pi + o(1)$ for $z \to \infty$, and

$$\frac{D}{\alpha}\log\langle r^\alpha\rangle \;\sim\; 2D\log\frac{D}{2} - D\log Z + \frac{D}{\alpha}A_1(\alpha,D), \tag{105}$$

where the term $A_1(\alpha,D)$ is given by

$$A_1(\alpha,D) = \log\left[\left(1 + \frac{(\alpha+1)(\alpha+4l-2)}{2D}\right)\left(1 + \frac{(\alpha+1)(\alpha+2)(n-l-1)}{D}\right)\right] \tag{106}$$

and tends to 0 as $D \to \infty$. These asymptotic approximations allow us to write the following inequalities for the radial Shannon entropy

$$S[\rho] \lesssim A_2(\alpha,D) + \frac{D}{\alpha}A_1(\alpha,D) - D\log Z + \log\frac{2}{\alpha}, \tag{107}$$

where

$$A_2(\alpha,D) \;=\; 3D\log D + \log\left(\frac{\pi e}{8}\right)\frac{D}{2} + \frac{1}{2}\log\frac{\alpha}{2}. \tag{108}$$

Rearranging all terms in (107) and (108) we can write the asymptotics of the upper bound for the Shannon entropy as

$$S[\rho] \lesssim 3D\log D + \left[\log\left(\frac{\pi e}{8}\right)^{\frac{1}{2}} - \log Z + \frac{1}{\alpha}A_1(\alpha,D)\right]D - \frac{1}{2}\log\frac{\alpha}{2}, \tag{109}$$

at the large $D$ limit. Operating in a similar way for the radial Rényi entropy at the large-$D$ limit we find from (100) that

$$\begin{aligned} R_q[\rho] \;&\lesssim\; \frac{1}{1-q}\log L_1(q,\alpha,D) + 2D\log\frac{D}{2} - D\log Z + \frac{D}{\alpha}A_1(\alpha,D) \\ &\lesssim\; \frac{3D-1}{2}\log D + \left[\log\left(\frac{\pi e}{8}\right)^{\frac{1}{2}} - \log Z + \frac{1}{\alpha}A_1(\alpha,D)\right]D + \frac{1}{1-q}A_3(q), \end{aligned} \tag{110}$$

where

$$A_3(q) = \log\frac{q}{q-1} + (1-q)\log\Gamma\left(\frac{q}{q-1}\right) + \frac{1-q}{2}\log\frac{2}{\pi}.$$

Since $\log L_1 = \log L_2$ as $D \to \infty$, we obtain a similar expression for the lower bound in (101) by just changing $A_1(\alpha,D)$ to $A_1(-\alpha,D)$.

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### B. Lower bounds

We know from [55, Eqs. (1.49) and (1.50)] that the following inequalities for the Tsallis entropy hold: in terms of $\langle r^{\alpha} \rangle$ with $\alpha \in \mathbb{N}$,

$$1 + (1-q)T_q\left[\rho\right] \geq L_1\left(q, \alpha, D\right) \langle r^{\alpha} \rangle^{-\frac{D}{\alpha}(q-1)} \tag{111}$$

and in terms of $\langle r^{-\alpha} \rangle$ with $\alpha \in \mathbb{N}$ and for $\alpha < \frac{-D(q-1)}{q}$,

$$1 + (1-q)T_q\left[\rho\right] \geq L_2\left(q, \alpha, D\right) \left\langle r^{-\alpha} \right\rangle^{-\frac{D}{\alpha}(q-1)}. \tag{112}$$

The functions $L_i\left(q, \alpha, D\right)$ are defined in Eqs. (102) and (103), respectively. Operating as in the previous subsection we find in the limit $D \to \infty$ the following asymptotic lower bounds:

$$1 + (1-q)T_p[\rho] \gtrsim A_5(\alpha, D)A_1(\alpha, D)^{-\frac{D}{\alpha}(q-1)} \tag{113}$$

and

$$1 + (1-q)T_p[\rho] \gtrsim A_5(\alpha, D)A_1(-\alpha, D)^{-\frac{D}{\alpha}(q-1)}, \tag{114}$$

where

$$A_5(\alpha, D) = \frac{q}{q-1}\left[\frac{D^{3D-1}}{2^{3D+2}\pi^{D+1}Z^{2D}}\right]^{\frac{1-q}{2}} \frac{e^{(1-q)\frac{D}{2}}}{\alpha^q}\Gamma\left(\frac{q}{q-1}\right)^{1-q}. \tag{115}$$

Finally, let us comment that expressions similar to the inequalities (98), (100), (101), (113) and (114) for the position Shannon, Rényi and Tsallis entropies given by (95)-(98) are also valid for the corresponding quantities in the momentum space.

## VIII. CONCLUSIONS

The main prototype of the $D$-dimensional Coulomb many-body systems, the $D$-dimensional hydrogenic system, is investigated by means of the radial expectation values in both position and momentum spaces. These expectation values, which characterize numerous fundamental and/or experimentally accessible quantities of the system (e.g., kinetic and repulsion energies, diamagnetic susceptibility, etc.) and describe generalized Heisenberg-like uncertainty measures, are calculated for all quantum states of the system at the (pseudoclassical) large $D$ limit. Then, the uncertainty equality-type relations associated to them are determined, and show that they fulfill and saturate the known uncertainty inequality-type relations for both general quantum systems and for those systems with a quantum-mechanical spherically symmetric potential. Moreover, the position and momentum expectation values are used to bound the entropic uncertainty measures of the Shannon, Rényi and Tsallis types at large $D$. Finally, let us point out an open problem which is important *per se*: the determination of these three entropies at this pseudoclassical limit for all quantum $D$-dimensional hydrogenic states, which is left for future work.

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## Appendix A: Asymptotics of $f_k(\nu)$

Here obtain in full detail the asymptotics of the quantities $f_k(\nu)$ defined in Eq. (46); that is,

$$f_k(\nu) = \frac{1}{(2\nu)_k}\sum_{j=0}^{k}(-1)^j\binom{k}{j}(2\nu+j)_k\, d_j \tag{A1}$$

where

$$\begin{aligned} d_j \equiv d_j(\nu) &= \frac{\nu}{\nu+j}\,\frac{(\nu+\frac{\alpha+1}{2})_j(\nu+\frac{3-\alpha}{2})_j}{(\nu+\frac{1}{2})_j(\nu+\frac{3}{2})_j} \\ &= \frac{\nu}{\nu+j}\prod_{i=1}^{j}\left(1-\frac{p}{(\nu+i+\frac{1}{2})(\nu+i-\frac{1}{2})}\right), \end{aligned} \tag{A2}$$

and $p \equiv p(\alpha) = \frac{1}{4}\alpha(\alpha-2)$. We first establish two technical results (Lemma 1 and Proposition 1), which allow us to express the quantities $f_k(\nu)$ in terms of the backward-difference operator $\nabla d_k = d_k - d_{k-1}$. Then, we derive the asymptotic expansions of $d_k$ and $\nabla^i d_k$ by means of Lemma 2 and Corollary 1, respectively. Finally, the Corollary 2 yields the wanted asymptotics of $f_k(\nu)$ at large $D$.

**Lemma 1**. For $0 \leq j \leq k$,

$$\frac{(a+j)_k}{(a)_k} = k!\sum_{i=0}^{j}\binom{j}{i}\frac{1}{(k-i)!(a)_i}.$$

**Proof**. Since

$$\frac{(a+j)_k}{(a)_k} = \frac{(a+k)_j}{(a)_j}, \tag{A3}$$

the Vandermonde-like identity [56**?** ]

$$(a+b)_k = \sum_{i=0}^{k}(-1)^i\binom{k}{i}(a+i)_{k-i}(-b)_i$$

yields

$$\frac{(a+k)_j}{(a)_j} = \sum_{i=0}^{j}\binom{j}{i}\frac{k!}{(k-i)!}\frac{(a+i)_{j-i}}{(a)_j} = k!\sum_{i=0}^{j}\binom{j}{i}\frac{1}{(k-i)!(a)_i},$$

where we have used that $(a+i)_{j-i} = \frac{(a)_j}{(a)_i}$. □

**Proposition 1**. For $f_k(\nu)$ given in (46) we have that it can be rewritten in the form

$$f_k(\nu) = (-1)^k k!\sum_{i=0}^{k}\binom{k}{i}\frac{\nabla^i d_k}{i!(2\nu)_{k-i}}, \tag{A4}$$

where $\nabla$ denotes the operator of backward difference, i.e.,

$$\nabla d_k = d_k - d_{k-1}, \quad \nabla^{n+1} d_k = \nabla(\nabla^n d_k).$$

**Proof**. By Lemma 1 we have

$$\begin{aligned}
f_k(\nu) &= \sum_{j=0}^{k}(-1)^j\binom{k}{j}d_j\frac{(2\nu+j)_k}{(2\nu)_k}\\
&= \sum_{j=0}^{k}(-1)^j\binom{k}{j}d_j\left(k!\sum_{i=0}^{j}\binom{j}{i}\frac{1}{(k-i)!(2\nu)_i}\right)\\
&= k!\sum_{j=0}^{k}\sum_{i=0}^{j}(-1)^j\binom{k}{j}\binom{j}{i}d_j\frac{1}{(k-i)!(2\nu)_i}\\
&= k!\sum_{i=0}^{k}\sum_{j=i}^{k}(-1)^j\binom{k}{j}\binom{j}{i}d_j\frac{1}{(k-i)!(2\nu)_i}\\
&= k!\sum_{i=0}^{k}\sum_{j=0}^{k-i}(-1)^{j+i}\binom{k}{j+i}\binom{j+i}{i}d_{j+i}\frac{1}{(k-i)!(2\nu)_i}.
\end{aligned}$$

Since

$$\binom{k}{j+i}\binom{j+i}{i}=\binom{k-i}{j}\binom{k}{i},$$

we obtain

$$f_k(\nu)=k!\sum_{i=0}^{k}\binom{k}{i}\frac{1}{(k-i)!(2\nu)_i}\left(\sum_{j=0}^{k-i}(-1)^j\binom{k-i}{j}d_{j+i}\right).$$

It remains to observe that

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}d_{k-j}=\nabla^n d_k,\quad n=0,\dots,k,$$

so that

$$\sum_{j=0}^{k-i}(-1)^j\binom{k-i}{j}d_{j+i}=(-1)^{k-i}\nabla^{k-i}d_k. \qquad \square$$

**Lemma 2**. The asymptotic expansion of $d_k=d_k(\nu)$ is given by

$$d_k=d_k(\nu)=\sum_{n=0}^{\infty}(-1)^n\frac{\beta_n(k)}{\nu^n},\quad \nu\to+\infty, \tag{A5}$$

where $\beta_n(k)$ are monic polynomials in $k$. Furthermore, $\beta_0(k)=1$ and for $n\geq 1$,

$$\beta_n(k)=k^n-(n-1)p(\alpha)k^{n-1}+\text{lower degree terms}. \tag{A6}$$

**Proof**. We prove the result by induction in $k$. Observe first that $d_0=1$ and for $k\geq 1$,

$$\begin{aligned}
\frac{d_k}{d_{k-1}} &= 1-\frac{4p+1}{k+\nu}+\frac{p}{\nu+k-1/2}+\frac{3p}{\nu+k+1/2}\\
&= 1+\sum_{n=1}^{\infty}(-1)^n\frac{(4p+1)k^{n-1}-p(k-1/2)^{n-1}-3p(k+1/2)^{n-1}}{\nu^n}\\
&= \sum_{n=0}^{\infty}(-1)^n\frac{\gamma_n(k)}{\nu^n},
\end{aligned}$$

where

$$\gamma_0(k) = 1 \quad \text{and} \quad \gamma_n(k) = k^{n-1} - p(n-1)k^{n-2} + \ldots \quad \text{for} \quad n \geq 1.$$

Therefore, by assumptions,

$$d_k = \left(\sum_{m=0}^{\infty}(-1)^m \frac{\beta_m(k-1)}{\nu^m}\right)\left(\sum_{n=0}^{\infty}(-1)^n \frac{\gamma_n(k)}{\nu^n}\right) = \sum_{r=0}^{\infty}(-1)^r \frac{\zeta_r(k)}{\nu^r},$$

where

$$\zeta_r(k) = \sum_{m+n=r} \beta_m(k-1)\gamma_n(k).$$

For $r \geq 1$ we have

$$\begin{aligned}
\zeta_r(k) &= \beta_r(k-1) + \gamma_r(k) + \sum_{\substack{m+n=r\\0<m,n<r}} \beta_m(k-1)\gamma_n(k) \\
&= k^r - (p+1)(r-1)k^{r-1} + \ldots \\
&\quad + \sum_{\substack{m+n=r\\0<m,n<r}} \{(k-1)^m - p(m-1)(k-1)^{m-1} + \ldots\}\{k^{n-1} - p(n-1)k^{n-2} + \ldots\} \\
&= \sum_{m+n=r} \{k^m - (pm - p + m)k^{m-1} + \ldots\}\{k^{n-1} - p(n-1)k^{n-2} + \ldots\} \\
&= k^r - (p+1)(r-1)k^{r-1} + \left(\sum_{\substack{m+n=r\\0<m,n<r}} k^{r-1}\right) + \text{lower degree terms} \\
&= k^r - (p+1)(r-1)k^{r-1} + (r-1)k^{r-1} + \text{lower degree terms} \\
&= k^r - p(r-1)k^{r-1} + \text{lower degree terms,}
\end{aligned}$$

and the assertion follows. □

**Corollary 1**: The asymptotic expansion of $\nabla^n d_k$ is given by

$$\nabla^n d_k = \frac{(-1)^n n!}{\nu^n}\left(1 + \frac{np - (n+1)(k - n/2)}{\nu} + \mathcal{O}(\nu^{-2})\right), \quad \nu \to +\infty, \tag{A7}$$

where $p \equiv p(\alpha) = \frac{1}{4}\alpha(\alpha - 2)$.
**Proof**. It is sufficient to observe that $\nabla^n k^r = 0$ for $r < n$,

$$\nabla^n k^n = (-1)^n n! \quad \text{and} \quad \nabla^n k^{n+1} = (-1)^n n!(k - n/2). \qquad \square$$

**Corollary 2**: The asymptotic expansion of $f_k(\nu)$ is given by

$$f_k(\nu) = \frac{k!}{(2\nu)^k}\left(1 - \frac{k(k + 3 + 2\alpha(2-\alpha))}{4\nu} + \mathcal{O}\left(\frac{1}{\nu^2}\right)\right). \tag{A8}$$

**Proof**. Just use Corollary 1 in (A4).

### Appendix B: Table of convergence of the asymptotics of $\langle r^\alpha \rangle$ and $\langle p^\alpha \rangle$

In this table we show the rate of convergence for the position and momentum expectation values of the $D$-dimensional hydrogen state $(n = 2, l = 0)$ at large $D$ to the known exact values given in (32), (42), (11) and (22), respectively.

| $D$ | $\alpha$ | $\langle r^\alpha \rangle_{\text{asymp}}$ | $\langle p^\alpha \rangle_{\text{asymp}}$ | $\langle r^\alpha \rangle_{\text{exact}}$ | $\langle p^\alpha \rangle_{\text{exact}}$ |
|---|---|---|---|---|---|
| 50 | 0 | 1.00199 | 1 | 1 | 1 |
| 250 |  | 1.00199 | 1 |  |  |
| 500 |  | 1.00199 | 1 |  |  |
| 50 | 1 | 686 | 0.0388 | 612.5 | 0.0380789 |
| 250 |  | 15936 | 0.007952 | 15562.5 | 0.00792065 |
| 500 |  | 63123.5 | 0.003988 | 62375. | 0.00398008 |
| 50 | 2 | 484375. | 0.0016 | 365766. | 0.00153787 |
| 250 |  | $2.55859 \cdot 10^8$ | 0.000064 | $2.41176 \cdot 10^8$ | 0.0000634911 |
| 500 |  | $4 \cdot 10^9$ | 0.000016 | $3.88267 \cdot 10^9$ | 0.0000159362 |
| 50 | -1 | 0.0016 | 27.25 | 0.00160064 | 27.7927 |
| 250 |  | 0.000064 | 127.25 | 0.000064001 | 127.758 |
| 500 |  | 0.000016 | 252.25 | 0.0000160001 | 252.754 |

TABLE I: Rate of convergence of the asymptotic expectation values in terms of $D$ for the hydrogen ($Z = 1$) state with $n = 2$ and $l = 0$.

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## 3.5 Monotonicity property of complexity measures

In this section, to better understand the conditions under which a given theoretic-informational quantity of a many-body system is a proper measure of its complexity, we have done the following:

- Introduce the mathematical notion of monotonicity of the complexity measure of a probability distribution patterned after the resource theory of quantum entanglement and coherence,
- explore whether this property is satisfied by the basic intrinsic measures of complexity (Crámer-Rao, Fisher-Shannon, LMC) and some of their generalizations, and
- find that the Crámer-Rao and Fisher-Shannon complexity measures as well as some particular cases of the LMC-Rényi measure fulfill the desired requirement.

These results have deserved the publication of the article with coordinates: *L. Rudnicki, I. V. Toranzo, P. Sánchez-Moreno and J. S. Dehesa, Physics Letters A* ***380****, 377-380* ***(2016)***, which is attached in the following.

# Monotone measures of statistical complexity

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We introduce and discuss the notion of monotonicity for the complexity measures of general probability distributions, patterned after the resource theory of quantum entanglement. Then, we explore whether this property is satisfied by the three main intrinsic measures of complexity (Crámer-Rao, Fisher-Shannon, LMC) and some of their generalizations.

## I. INTRODUCTION

On which grounds shall one build a sound description of complexity? Despite the great efforts done in many areas of science ranging from atomic, molecular an nuclear physics up to the adaptive complex systems and ultimately the living beings [1–11], this question does not have a definitive answer supported by a systematic treatment. 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, namely 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.

The complexity, however, behaves in a completely different manner. 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. A complexity quantifier applicable to physical systems with different degrees of order/disorder, the great majority of which lie down somewhere between the two extremes, shall take the above observation into account. In other words, a proper *measure of complexity* (with a suitably chosen, scenario-adapted notion of non-complexity) shall assume the minimal value for a non-complex input.

But the theory of quantum entanglement [12] together with recent developments made for quantum coherence [13], point out that being discriminative with respect to separable or incoherent states is not enough to be a faithful measure of the resource. The measure of entanglement (coherence) needs to be a monotone which does not increase under LOCC (incoherent) operations. This means, that one cannot generate entanglement or quantum coherence by performing only "classical" or "local" operations.

The aim of this contribution is to transfer the intuition related to quantification of entanglement and coherence, to the field of statistical complexity. If one wishes to quantify the complexity of a certain probability distribution, one shall take into account the fact that the distribution at hand can be smeared in a way that it becomes closer to the

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description of the non-complex system. A good measure of complexity shall then assign a lower value to such new, transformed distribution. Note that we do not mean here any possible smearing, but only transformations which lead to less complex distributions.

More formally, we say that a complexity measure $C[\rho]$ defined for a single-particle probability density $\rho(x)$ is a monotone in the following sense:

(i) There exists a family $\Xi$ of densities with minimal complexity, so that if $\rho \in \Xi$, then $C[\rho] \leq C[\rho']$ for any other density $\rho'$.

(ii) There exists a class of operations $\mathcal{G}$ that preserve $\Xi$, i.e. if $\rho \in \Xi$, then $\mathcal{G}[\rho] \in \Xi$.

(iii) The complexity measure $C$ is monotonic with respect to all operations from the class $\mathcal{G}$, what means that $C[\mathcal{G}[\rho]] \leq C[\rho]$ for any density $\rho$.

These three properties capture the idea of monotonicity as described above. Following the theory of quantum entanglement we shall now postulate that the proper measure of statistical complexity satisfies the monotonicity requirement. Note that the "axioms" (i–iii) provide only a general framework for studying measures of statistical complexity. Working with particular scenarios one always first needs to specify the notion of being non-complex and think of the operations which potentially only decrease the complexity. It shall turn out that various measures are monotones with respect to different couples $(\Xi, \mathcal{G})$, what physically implies that they are able to properly describe distinct emanations of complexity.

In the last few years various measures of the complexity of a finite many-particle system have been suggested in terms of two spreading measures (e.g., variance, Shannon entropy, Fisher information, disequilibrium) of a single-particle probability density. The most important examples are the complexity measures of Crámer-Rao [20, 22, 23], Fisher-Shannon [28–30] and LMC (López-ruiz, Mancini and Calvet)[5]. In Section 2 we briefly review the construction of these measures, while in Section 3 we use them to explain the idea behind the postulated monotonicity. In particular, we show that both Crámer-Rao and Fisher-Shannon measures are monotones with respect to a convolution with any Gaussian probability distribution, while the discrete LMC complexity measures are monotone with respect to all stochastic operations preserving the class containing the uniform distribution and the Kronecker delta distributions. Note that while the former case seems to be complete, the monotonicity of LMC complexity in the continuous scenario, even though very likely to occur, is left as an open question.

## II. BASIC COMPLEXITY MEASURES

Let us consider a general one-dimensional random variable $X$ characterized by the continuous probability distribution $\rho(x)$, $x \in \Lambda \subseteq \mathbb{R}$, which is assumed to be normalized so that $\int_\Lambda \rho(x)dx = 1$. The information theory provides various spreading measures of the distribution beyond the familiar variance $V[\rho]$, such as the well-known Shannon entropy [15]

$$S[\rho] = -\int_\Lambda \rho(x) \ln \rho(x) dx, \tag{1}$$

the Rényi entropy of order $\lambda$ [14] given by

$$R_\lambda[\rho] = \frac{1}{1-\lambda} \ln \int_\Lambda [\rho(x)]^\lambda dx, \quad \lambda \neq 1 \tag{2}$$

(whose limiting value $\lambda \to 1$ yields the Shannon entropy), and the Fisher information [16, 17]

$$F[\rho] = \int_\Lambda \frac{1}{\rho(x)} \left( \frac{d}{dx} \rho(x) \right)^2 dx, \tag{3}$$

which due to the involved derivative is a bit less global quantity. Opposite to the variance, these information-theoretic spreading measures do not depend on any particular point of the interval $\Lambda$ being the domain of $\rho$. Note that all these measures ($V[\rho]$, $S[\rho]$, $R_\lambda[\rho]$, $F[\rho]$) are complementary, since each of them grasps a single different facet of the probability density $\rho(x)$. Indeed, the variance measures the concentration of the density around the centroid while the Rényi and Shannon entropies are measures of the extent to which the density is in fact concentrated. The Fisher informations is a quantitative estimation of the oscillatory character of the density since it measures the pointwise concentration of the probability over its support interval $\Lambda$.

All measures of complexity mentioned in the Introduction (Crámer-Rao, Fisher-Shannon and LMC) are defined as the products of two of the previously listed spreading measures. Each of them thus estimates the combined balance of two different facets of the probability density. The Crámer-Rao complexity [20, 22, 23], which is defined as

$$C_{CR}\left[\rho\right] = F\left[\rho\right]\, V\left[\rho\right], \tag{4}$$

quantifies the gradient content of $\rho(x)$ jointly with the probability concentration around the centroid. The Fisher-Shannon complexity [28–30], which is given by

$$C_{FS}[\rho] = F[\rho] \times \frac{1}{2\pi e} e^{2S[\rho]}, \tag{5}$$

measures the gradient content of $\rho(x)$ together with its total extent in the support interval. Finally, the biparametric LMC complexity (or LMC-Rényi complexity) [24–27] is:

$$C_{\alpha,\beta}[\rho] = e^{R_\alpha[\rho]-R_\beta[\rho]}, \quad 0 < \alpha < \beta, \quad \alpha, \beta \neq 1. \tag{6}$$

Note that the case ($\alpha \to 1$, $\beta = 2$) corresponds to the plain LMC complexity measure [5] $C_{1,2}[\rho] = D[\rho] \times e^{S[\rho]}$, which measures the combined balance of the average height of $\rho(x)$ (also called disequilibrium $D[\rho] = e^{-R_2[\rho]}$), and its total extent.

These three complexity measures are known to be (a) dimensionless, (b) bounded from below by unity [20, 21], and (c) invariant under translation and scaling transformation [6, 7]. Moreover, the question whether the complexity measures are minimum for the two extreme (or *least complex*) distributions corresponding to perfect order and maximum disorder (associated to a extremely localized Dirac delta distribution and a highly flat distribution in the one dimensional case, respectively) is a long standing and controverted issue, not yet solved (see e.g. [10]).

## III. MONOTONICITY OF THE COMPLEXITY MEASURES

In this Section we investigate whether the complexity measures of Crámer-Rao, Fisher-Shannon, and LMC-Rényi types given by the expressions (4), (5) and (6), respectively, are complexity monotones.

### A. Fisher-Shannon complexity

Let us first prove that for $\rho(x)$ with unbounded support, the Fisher-Shannon complexity $C_{FS}[\rho]$ given by (5) is monotonic in the previously specified sense, with the family $\Xi$ of non-complex states formed by all the Gaussian densities (with arbitrary mean value and variance). The relevant operations $\mathcal{G}$ preserving $\Xi$ are in this case constructed in terms of the convolution of a given distribution with some (once more arbitrary) Gaussian density. As the convolution of two Gaussians is another Gaussian, the family $\Xi$ is properly preserved.

The required monotonicity means that

$$C_{FS}[\rho_\tau] \leq C_{FS}[\rho],$$

where $\rho_\tau = \mathcal{G}[\rho]$ is the convolution of $\rho$ with a Gaussian of variance $\tau$ (the mean value does not play any role). Taking into account the known properties of the Gaussian densities (convergence to the Dirac delta distribution) and the convolution, we have that

$$\rho = \lim_{\tau \to 0} \rho_\tau,$$

so that it is sufficient to show that $C_{FS}[\rho_\tau]$ is a decreasing function of $\tau$; that is,

$$\frac{d}{d\tau} C_{FS}[\rho_\tau] \leq 0. \tag{7}$$

To achieve that goal, we recall the de Bruijn identity [18]

$$\frac{d}{d\tau} S[\rho_\tau] = \frac{1}{2} F[\rho_\tau], \tag{8}$$

which implies that

$$C_{FS}[\rho_\tau] = \frac{d}{d\tau} N[\rho_\tau],$$

where $N[\rho] \equiv \frac{e^{2S[\rho]}}{2\pi e}$ denotes the entropy power of $\rho$. The desired inequality (7) follows from the concavity of the entropy power

$$\frac{d^2}{d\tau^2} N[\rho_\tau] \leq 0,$$

which was proved by Costa [19].

### B. Crámer-Rao complexity

Studying the second quantity, namely the Crámer-Rao complexity given by (4), we show that it is monotonic in the same sense as the Fisher-Shannon complexity measure. Analogously to the Fisher-Shannon case, we want to prove that

$$\frac{d}{d\tau} C_{CR}[\rho_\tau] \leq 0. \tag{9}$$

Using again the de Bruijn identity (8) together with the known relation

$$V[\rho_\tau] = V[\rho] + \tau,$$

we obtain

$$\frac{d}{d\tau} C_{CR}[\rho_\tau] = 2\frac{d}{d\tau} S[\rho_\tau] + 2(V[\rho] + \tau)\frac{d^2}{d\tau^2} S[\rho_\tau].$$

The concavity of the entropy power implies that:

$$\frac{d^2}{d\tau^2} N[\rho_\tau] = 2N[\rho_\tau]\left[2\left(\frac{d}{d\tau} S[\rho_\tau]\right)^2 + \frac{d^2}{d\tau^2} S[\rho_\tau]\right] \leq 0,$$

from which we get the inequality

$$\frac{d^2}{d\tau^2} S[\rho_\tau] \leq -2\left(\frac{d}{d\tau} S[\rho_\tau]\right)^2.$$

This inequality together with the de Bruijn identity (8) yield the relation

$$\frac{d}{d\tau} C_{CR}[\rho_\tau] \leq F[\rho_\tau] - (V[\rho] + \tau)(F[\rho_\tau])^2. \tag{10}$$

The right-hand side of (10) is a negative function of $F[\rho_\tau]$ provided that

$$F[\rho_\tau] \geq \frac{1}{2(V[\rho] + \tau)}.$$

But the last inequality is always satisfied due to the Crámer-Rao bound [20]

$$F[\rho_\tau] \geq \frac{1}{V[\rho_\tau]} = \frac{1}{V[\rho] + \tau}. \tag{11}$$

Moreover, if the Crámer-Rao bound becomes saturated, the right-hand side of (10) vanishes. Since the derivative of $C_{CR}[\rho_\tau]$ is upper-bounded by a decreasing function of $F[\rho_\tau]$ whose maximum value is equal to zero, the proposed inequality (9) is proved.

### C. LMC-Rényi complexity

In the last part we shall discuss the generalized LMC complexity measure $C_{\alpha,\beta}[\rho]$. This measure becomes relevant when the set $\Xi$ of non-complex states is assumed to contain all the uniform densities $\rho(x) = 1/L$ with bounded (not necessarily compact) support of length $L$. In the limit of a very narrow, compact support ($L \to 0$) the non-complex density becomes the Dirac delta distribution concentrated in the center of the support.

A more difficult question is about the complete family of operations $\mathcal{G}$ preserving the class $\Xi$. In order to better understand the non-complex landscape described by $\Xi$, we will study the simplest, discrete counterpart scenario in dimension two. In this case [instead of $\rho(x)$] one uses a collection of two probabilities $(p, 1-p)$, given in terms of a single number $0 \le p \le 1$. In this simplified situation there are three non-complex states given by the values $p \in \{0, 1/2, 1\}$.

We start by an assumption that any allowed operation performed on discrete probability distributions can be represented by a stochastic matrix. Thus, in the two-dimensional case every operation applicable to the probability vector is of the form

$$\begin{pmatrix} a & b \\ 1-a & 1-b \end{pmatrix}, \tag{12}$$

with $0 \le a, b \le 1$. There are only four matrices, different from the identity, which preserve the set of the three non-complex probability vectors:

$$\begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{13}$$

The first three operations simply output each of the non-complex vectors, independently of the input. The last one is the permutation.

While increasing the dimension (but staying on the discrete ground) the number of allowed operations also increases, but the qualitative description of the set $\mathcal{G}$ remains the same. In order to preserve the class of non-complex states one can either transform any probability vector to become the member of the class $\Xi$, or freely permute the probability components. At the end of the day, we are left with a conclusion that only the permutations provide non-trivial but allowed transformations of the set $\Xi$.

But the discrete counterpart $C_{\alpha,\beta}[q]$ of the generalized LMC complexity measure (given by discrete Rényi entropies of the probability vector $q$) is invariant with respect to permutations. This fact implies that in the discrete scenario the LMC measure somehow trivially satisfies the monotonicity requirement. For any probability vector $q$ either $C_{\alpha,\beta}[\mathcal{G}[q]] = C_{\alpha,\beta}[q]$ or $C_{\alpha,\beta}[\mathcal{G}[q]] = 1$.

The remaining question is if the discrete analysis discussed above can directly be transferred to the continuous scenario. It seems to be very likely that the measure $C_{\alpha,\beta}[\rho]$ is a monotone in the same sense as $C_{\alpha,\beta}[q]$. On the other hand, the fundamental entropic uncertainty relation [32] shows that the continuous limit does not need to be direct, since between the uniform and the peaked distribution there is room for the Gaussians. We shall thus leave the construction of the full class $\mathcal{G}$ in the continuous case, as well as the rigorous proof of the monotonicity for LMC, as two open questions for future research.

## IV. CONCLUSIONS

The purpose of this communication is to contribute to quantify how simple or how complex are the many-particle systems in terms of the one-particle probability density which, according to the density functional theory, characterize their physical and chemical properties. Since there does not exist a unique notion of complexity able to grasp our intuition in the appropriate manner it is important to better understand the conditions under which a given quantity is a proper measure of complexity. It is even more important as perhaps the most universal and appropriate descriptions of statistical complexity are not yet known.

To contribute to settle down this issue, we have introduced the mathematical notion of monotonicity of the complexity measure of a probability distribution patterned after the resource theory of quantum entanglement and coherence.

We have discussed under what conditions the basic complexity measures of physical systems satisfy this requirement. As the main aim of the letter was to provide a general framework, the studies of particular examples, with special emphasis on the LMC complexity measure, shall be continued in the future. The mathematical results collected during the investigation of Gaussian-based monotonicity might be useful for other research such as studies of pointer-based measurements [33].

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## 3.6 Monoparametric complexities for Coulomb systems

In this section we first explore the notion of a complexity quantifier for the finite quantum many-particle systems, the one-parameter Fisher-Rényi complexity, and also examine its main analytical properties. This notion extends all the previously known measures of complexity which are sensitive to the quantum fluctuations of the physical wavefunctions of the systems (Crámer-Rao, Fisher-Shannon, Fisher-Rényi-type) in the following sense:

- It does not depend on any specific point of the system's region (opposite to the Crámer-Rao measure), and
- it quantifies the combined balance of various aspects of the fluctuations of the single-particle density beyond the gradient content (opposite to the Fisher–Shannon complexity and the Fisher-Rényi product, which only take into account a single aspect given by the density gradient content) and different facets of the spreading of this density function.

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

These results have been published in the article with coordinates: *I. V. Toranzo, P. Sánchez-Moreno, L. Rudnicki and J. S. Dehesa, Entropy **19**, 16 (**2017**)*, which is attached below.

# One-parameter Fisher-Rényi complexity: Notion and hydrogenic applications

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

## I. INTRODUCTION

We all have an intuitive sense of what *complexity* means. In the last two decades an increasing number of efforts have been published [1–12] to refine our intuitions about complexity into precise, scientific concepts, pointing out a large amount of open problems. Nevertheless there is not a consensus for the term *complexity* nor whether there is a simple core to *complexity*. Contrary to the Boltzmann-Shannon entropy which is ever increasing according to the second law of thermodynamics, the complexity seems to behave very differently. Various precise, widely applicable, numerical and analytical proposals (see e.g., [13–30] and the monograph [8]) have been done but they are yet very far to appropriately formalize the intuitive notion of complexity [11, 29]. The latter suggests that complexity should be minimal at either end of the scale. However, a complexity quantifier to take into account the completely ordered and completely disordered limits (i.e., perfect order and maximal randomness, respectively) and to describe/explain the maximum between them is not known up until now.

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

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

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

## II. ONE-PARAMETER FISHER-RÉNYI COMPLEXITY MEASURE

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

### A. The notion

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

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

where $D_\lambda$ is the normalization factor given as

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

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

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

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

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

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

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

### B. The properties

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

1. **Lower bound.** The Fisher-Rényi complexity measure $C_{FR}^{(\lambda)}[\rho]$ fulfills the inequality

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

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

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

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

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

with

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

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

2. **Invariance under scaling and translation transformations**. The complexity measure $C_{FR}^{(\lambda)}(\rho)$ are scaling and translation invariant in the sense that

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

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

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

Note that in writing the first equality we have used that

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

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

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

In particular, we have

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

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

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

   Two of the main properties of rearrangements is that they preserve the $L^p$ norms, which implies that the rearrangements of a probability density give rise to another probability density, and that they make everything spherically symmetric. The second feature makes the rearrangement operation relevant for quantification of statistical complexity [11], since a spherically symmetric variant of a probability density can in an atomic context be viewed as less complex. Then, we introduce the definition of this operation as well as its effects over the entropic quantities that make up our complexity measure.

   Let $f$ be a real-valued function, $f:\mathbb{R}^n\to[0,\infty)$ and $A_t=\{x:f(x)\geq t\}$. The symmetric decreasing rearrangement of $f$ is defined as

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

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

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

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

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

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

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

   if both $S[\rho]$ and $S[\rho^*]$ are well defined, where $\lim_{p\to1}R_p[\rho]=S[\rho]$. The invariance of the Rényi entropy follows from the preservation of the $L^p$ norms via rearrangements and the proof of the invariance of the Shannon entropy is done in [37]. Moreover, Wang and Madiman [37] consider the Fisher information, finding that the standard Fisher information decreases monotonically under rearrangements, i.e.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

4. **Behavior under replications**. Let us now study the behavior of the Fisher-Rényi complexity $C^{(\lambda)}_{FR}(\rho)$ under $n$ replications. We have found that for one-dimensional densities $\rho(x)$, $x \in \mathbb{R}$ with bounded support, this complexity measure behaves as follows:

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

where the density $\tilde{\rho}$ representing $n$ replications of $\rho$ 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 disjoints. Then, the integrals

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

and

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

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

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

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

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

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

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

and

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

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

## III. THE HYDROGENIC APPLICATION

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

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

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

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

and

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

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

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

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

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

where $D_\lambda$ is the normalization constant given by (2) and the symbols $I_1$ and $I_2$ denote the integrals

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

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

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

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

1. Generalized Fisher-Rényi complexity of hydrogenic $(ns)$ states.

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

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

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

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

   with

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

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

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

where

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

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

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

which allows us to find the following value

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

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

2. Generalized Fisher-Rényi complexity of hydrogenic circular states.

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

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

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

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

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

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

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

$$\begin{aligned}
I_{1a}^{(ang)} &= 2\pi \left[\frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}\right]^{2\lambda-1} \int_0^{\pi} (\sin\theta)^{2(n-1)(2\lambda-1)} \sin\theta \, d\theta \\
&= 2^{2(1-\lambda)}\pi^{3(1-\lambda)} \left[\frac{\Gamma(n+1/2)}{\Gamma(n)}\right]^{2\lambda-1} \frac{\Gamma(2-n+2\lambda(n-1))}{\Gamma(5/2-n+2\lambda(n-1))}, \qquad (39)\\
I_{1b}^{(ang)} &= 2\pi \left[\frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}\right]^{2\lambda-1} \int_0^{\pi} (\sin\theta)^{2(n-1)(2\lambda-3)} \left[\frac{d}{d\theta}(\sin\theta)^{2(n-1)}\right]^2 \sin\theta \, d\theta \\
&= 2^{3-2\lambda}\pi^{3(1-\lambda)}(n-1)^2 \left[\frac{\Gamma\left(n+\frac{1}{2}\right)}{\Gamma(n)}\right]^{2\lambda-1} \frac{\Gamma[(2\lambda-1)(n-1)]}{\Gamma\left[2\lambda(n-1)-n+\frac{5}{2}\right]}, \qquad (40)\\
I_2^{(ang)} &= 2\pi \left[\frac{\Gamma(n+1/2)}{2\pi^{3/2}\Gamma(n)}\right]^{\lambda} \int_0^{\pi} (\sin\theta)^{2(n-1)\lambda} \sin\theta \, d\theta \\
&= 2^{1-\lambda}\pi^{\frac{3}{2}(1-\lambda)} \left[\frac{\Gamma(n+1/2)}{\Gamma(n)}\right]^{\lambda} \frac{\Gamma[1+\lambda(n-1)]}{\Gamma[\frac{3}{2}+\lambda(n-1)]}. \qquad (41)
\end{aligned}$$

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

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

for the one-parameter Fisher-Rényi complexity measure of the hydrogenic circular states. This expression gives for the ground state (which is also a particular circular state with $l = n-1 = 0$) the same previously obtained value (34), what is a further checking of our results.

## IV. CONCLUSIONS

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

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

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## Appendix A: Calculation of the Fisher and Rényi-like hydrogenic integrals

Let us here show the methodology to solve the integrals

$$\begin{aligned} I_1 &= \int |\,[\rho_{n,l,m}(\vec{r})]^{\lambda-2}\ \nabla\rho_{n,l,m}(\vec{r})|^2\,\rho_{n,l,m}(\vec{r})\,d\vec{r} = \int [\rho_{n,l,m}(\vec{r})]^{2\lambda-3}\ |\nabla\rho_{n,l,m}(\vec{r})|^2\,d\vec{r}, && \text{(A1)}\\ I_2 &= \int [\rho_{n,l,m}(\vec{r})]^{\lambda}\ d\vec{r} = I_2^{(rad)} \times I_2^{(ang)}, && \text{(A2)} \end{aligned}$$

with

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

and

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

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

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

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

$$\begin{aligned} I_{1a}^{(rad)} &= \int_0^\infty [\rho_{n,l}(\tilde{r})]^{2\lambda-3}\left[\frac{d}{dr}\rho_{n,l}(\tilde{r})\right]^2 r^2\, dr && \text{(A6)}\\ I_{1b}^{(rad)} &= \int_0^\infty [\rho_{n,l}(\tilde{r})]^{2\lambda-1}\ dr, && \text{(A7)} \end{aligned}$$

and

$$\begin{aligned} I_{1a}^{(ang)} &= \int_\Omega [\Theta_{l,m}(\theta,\phi)]^{2\lambda-1}\ d\Omega\ = I_2^{(ang)}(2\lambda-1) && \text{(A8)}\\ I_{1b}^{(ang)} &= \int_\Omega [\Theta_{l,m}(\theta,\phi)]^{2\lambda-3}\left[\frac{d}{d\theta}\Theta_{l,m}(\theta,\phi)\right]^2 d\Omega, && \text{(A9)} \end{aligned}$$

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

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

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

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

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

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

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where the $\Phi_k$-linearization coeffients are

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

with the Pochhammer symbol [39] $(a)_\mu$, the binomial number $\binom{a}{b}$, and the Lauricella hypergeometric function of $(r+1)$ variables $F_A^{r+1}$ [40, 41].
Then, we obtain the following analytical expressions for the radial integrals in terms of the parameters $\{Z,\lambda,n,l\}$ of the system:

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

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

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

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

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

where one should keep in mind that the $\Phi_0$ functions are given as in (A13).
Similarly we can obtain the angular integrals by means of linerization-like formulas of the Gegenbauer polynomials or the associated Legendre polynomials of the first kind.

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

Here we will determine the value of

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

where

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

and

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

since

$$\begin{aligned}
&\Phi_0\left(2,0,2(2\lambda-1),\{0,\ldots,0,-1\},\{1,\ldots,1,2\};\left\{\frac{1}{2\lambda-1},1\right\}\right) \\
&\qquad = (1)_0\begin{pmatrix}1\\0\end{pmatrix}^{2(2\lambda-1)-1}\begin{pmatrix}1\\-1\end{pmatrix}F_A^{2(2\lambda-1)+1}(\ldots) = 0.
\end{aligned}$$

Then, we obtain that

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

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## 3.7 Entropy and complexity properties of the $d$-dimensional blackbody radiation

In this section we investigate the entropy and complexity quantities of the $d$-dimensional blackbody radiation for standard ($d = 3$) and non-standard dimensionalities. We have calculated the main entropy and complexity measures of the corresponding spectral energy density in terms of the universe dimensionality $d$ and the temperature of the system $T$. Briefly, the main achievements are the following:

- We have determined the variance, the disequilibrium, the Shannon entropy and the Fisher information of the $d$-dimensional Planck density in an explicit way,
- besides the frequency $\nu_{max}$ at which the density is maximum, we have used these frequency-spreading measures to introduce three further characteristic frequencies of the spectrum, which have been referred as Heisenberg, Shannon and Fisher frequencies for obvious reasons,
- we have found that these new frequencies have a dependence on the temperature similar to the one given by the well-known Wien's law followed by $\nu_{max}$,
- the values of these charateristic frequencies for the cosmic microwave background (CMB) radiation have been given and physically discussed, suggesting the potential interest of the Fisher frequency to grasp the CMB anisotropy, and
- we have shown that the three main measures of complexity (i.e., Crámer-Rao, Fisher-Shannon and LMC) do not depend on the temperature, but only on the universe dimensionality. The corresponding values for the CMB radiation turns out to be dimensionless constants, noting that the Crámer-Rao complexity is bigger than the Fisher-Shannon and LMC quantities mainly because of the high smoothness and extent of the corresponding 3-dimensional Planck density.

On the other hand, given that for the analysis of the CMB anistropies it is probably most convenient and useful to set up a histogram from the CMB measured data, it would be interesting and complementary to estimate the Crámer-Rao and Fisher-Shannon complexities of the measured data because of the sensitivity of the Fisher-information component to the fluctuations of the associated non-smoothed Planck density due to (a) different physical processes such as the photon scattering by high-energy electrons (Sunyaev-Zel'dovich effect) or gravitational shift of photon energy caused by varying gravitational fields (Sachs-Wolfe effect), and (b) cavity finite-size corrections [70, 130]. The latter quantities would provide us with estimates of the CMB anisotropies as a whole.

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# Entropy and complexity properties of the $d$-dimensional blackbody radiation

*Eur. Phys. J. D 68, 316 (2014)*

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Space dimensionality is a crucial variable in the analysis of the structure and dynamics of natural systems and phenomena. The dimensionality effects of the blackbody radiation has been the subject of considerable research activity in recent years. These studies are still somewhat fragmentary, posing formidable qualitative and quantitative problems for various scientific and technological areas. In this work we carry out an information-theoretical analysis of the spectral energy density of a $d$-dimensional blackbody at temperature $T$ by means of various entropy-like quantities (disequilibrium, Shannon entropy, Fisher information) as well as by three (dimensionless) complexity measures (Crámer-Rao, Fisher-Shannon and LMC). All these frequency-functional quantities are calculated and discussed in terms of temperature and dimensionality. It is shown that all three measures of complexity have an universal character in the sense that they depend neither on temperature nor on the Planck and Boltzmann constants, but only on the the space dimensionality $d$. Moreover, they decrease when $d$ is increasing; in particular, the values 2.28415, 1.90979 and 1.17685 are found for the Crámer-Rao, Fisher-Shannon and LMC measures of complexity of the 3-dimensional blackbody radiation, respectively. In addition, beyond the frequency at which the spectral density is maximum (which follows the well-known Wien displacement law), three further characteristic frequencies are defined in terms of the previous entropy quantities; they are shown to obey Wien-like laws. The potential usefulness of these distinctive features of the blackbody spectrum is physically discussed.

## I. INTRODUCTION

Space dimensionality plays a very fundamental role in numerous scientific and technological areas, from field theory, string theory and quantum cosmology (see e.g., [1, 2]), to atomic and molecular physics (see e.g., [3]), quantum optics [4], condensed matter (see e.g., [5–7]) and quantum information and computation (see e.g.,[8, 9]). See also [10] for a recent summary. The idea that the universe is trapped on a membrane in some high-dimensional space-time may explain why gravity is so weak, and could be tested at high-energy particle accelerators [11, 12] in the ongoing LHC experiments with hadronic beams colliding at 7 to 14 TeV. On the other hand, many quantum systems and phenomena possess natural generalizations in which the number of degrees of freedom is a free parameter [14–17]. On the other hand, it is well-known that the dimensionality substantially modifies the physical solutions of the quantum wave equations of the systems, and thus all their properties (see e.g., [13, 17–19]).

In the last few years there has been a growing interest in the analysis of the influence of the space dimensionality in the blackbody radiation[20–27] from different standpoints. This is not surprising at all. Let us mention, for instance, that the cosmic microwave background radiation today is known to be the most perfect blackbody radiation ever observed in nature, with a temperature of about $2.725\,K$ [28].

Various research [20, 21] has shown that the spectral energy density of a d-dimensional ($d > 1$) blackbody at temperature $T$ (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 $T$) is given by the generalized Planck radiation law

$$\rho_T^{(d)}(\nu) = \frac{2(d-1)h\left(\frac{\sqrt{\pi}}{c}\right)^d}{\Gamma\left(\frac{d}{2}\right)} \frac{\nu^d}{e^{\frac{h\nu}{k_B T}} - 1}, \tag{1}$$

where $T$ denotes the blackbody temperature, $h$ and $k_B$ are the Planck and Boltzmann constants, respectively, and $\Gamma(x)$ denotes the gamma function of Euler [29].

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Up until now there is no information-theoretic analysis of this unimodal density in the literature, to the best of our knowledge. This is certainly striking not only from a mathematical standpoint, but mainly because of its physical relevance in so many areas of physics, chemistry and technology as briefly mentioned above. In this study we carry out such an analysis by means of the main entropy quantifiers (disequilibrium, Shannon entropy and Fisher information) and the following three complexity measures of intrinsic type: Crámer-Rao, Fisher-Shannon and Lopez-Ruiz-Mancini-Calvet (LMC in short).

The structure of the work is the following. In section II the basic spreading quantities (variance, entropy and complexity measures) of a general continuous one-dimensional probability distribution are defined, and their meanings and properties relevant to this effort are briefly given and discussed. In Section III the variance and the main entropy-based quantifiers (disequilibrium, Shannon entropy and Fisher information) of the d-dimensional blackbody spectrum are explicitly determined in terms of temperature and space dimensionality. Later, in section IV the subsequient results are used to define three new characteristic spectral frequencies besides the frequency $\nu_{max}$ at which the spectrum reaches its maximum, finding that they obey some displacement law similar to the well-known Wien law followed by $\nu_{max}$. Then, in section V the measures of complexity of the blackbody spectrum are examined, finding that they depend on the space dimensionality only; this dependence is numerically studied. Finally, some concluding remarks are given, and various open problems are pointed out.

## II. INFORMATION-THEORETIC MEASURES: BASICS

In this Section we briefly describe the definitions and meanings of the entropy and complexity measures of a probability distribution. 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 asumed that the density is normalized to unity, so that $\int_\Lambda \rho(x)dx = 1$. To quantify the spread of $X$ over the interval $\Lambda$ we usually employ the statistical root-mean-square or standard deviation (or even, Heisenberg length) $l_{Heis} \equiv \Delta x$, which is the square root of the variance

$$V[\rho] = \langle x^2 \rangle - \langle x \rangle^2, \tag{2}$$

where

$$\langle f(x) \rangle = \int_\Lambda f(x)\rho(x)dx.$$

The information theory provides other spreading measures such as the disequilibrium, the Shannon entropy and the Fisher information. The Shannon entropy $S[\rho]$ of $\rho(x)$ is defined [31] by

$$S[\rho] = -\int_\Lambda \rho(x) \ln \rho(x)dx. \tag{3}$$

The disequilibrium (also known as the Onicescu entropy) [30] is given by

$$D[\rho] = \langle \rho \rangle = \int_\Lambda \rho(x)^2\, dx \tag{4}$$

The Fisher information of $\rho(x)$ is defined [32, 33] as

$$F[\rho] = \int_\Lambda \frac{\left(\frac{d}{dx}\rho(x)\right)^2}{\rho(x)}\, dx. \tag{5}$$

It is worth remarking that: (a) these three information-theoretic spreading measures do not depend on any particular point of their interval $\Lambda$, contrary to the standard deviation, (b) the Fisher information has a locality property because it is a functional of the derivative of $\rho(x)$, and (c) the standard deviation and the disequilibrium and Shannon entropies are global properties because they are power and logarithmic functionals of $\rho(x)$, respectively. Moreover they have different units, so that they can not be compared each other. To overcome this difficulty, the following information-theoretic lengths have been introduced [34, 35]

$$l_{Shan} = \exp\left(S[\rho]\right), \quad \text{Shannon length}, \tag{6}$$

$$l_{Fish} = \frac{1}{\sqrt{F[\rho]}}, \qquad \text{Fisher length}. \tag{7}$$

It is straightforward to observe that these two lengths, as well as the standard deviation or Heisenberg length $l_{Heis} \equiv \Delta x$, have the same units of $X$. Moreover, all of them scale linearly with $X$, are invariant under translations of X, and vanish in the limit as $\rho(x)$ approaches a delta function.

Let us note that the quantities ($V[\rho]$, $S[\rho]$, $D[\rho]$, $F[\rho]$), and its related measures ($l_{Heis}$, $l_{Shan}$, $l_{Fish}$), are complementary since each of them grasps a different single facet of the probability density $\rho(x)$. So, the variance measures the concentration of the density around the centroid while the disequilibrium and the Shannon entropy are measures of the extent to which the density is in fact concentrated, and the Fisher information is a quantitative estimation of the oscillatory character of the density since it measures the pointwise concentration of the probability over its support interval $\Lambda$. The disequilibrium and the Shannon and Fisher quantities are considered to be quantitative measures of the departure from uniformity, total spreading and gradient content of the density, respectively.

Moreover, while the Heisenberg length is a measure of separation of the region(s) of the probability concentration with respect to a particular point of the density (namely, the mean value), both Shannon and Fisher lengths are measures of the extent to which the probability density is in fact concentrated. The Fisher length has two further distinctive features. First, it can be considered as a measure of the length scale over which $\rho(x)$ varies rapidly. Second, it depends on the derivative of the density, so that it vanishes for discontinuous distributions and it is very sensitive to fluctuations of the density. For completeness, let us also collect here that these three lengths satisfy the two following inequality-type relations:

$$l_{Fish} \leq l_{Heis}, \tag{8}$$

$$(2\pi e)^{1/2} l_{Fish} \leq l_{Shann} \leq (2\pi e)^{1/2} l_{Heis}, \tag{9}$$

where the equalities are reached for the Gaussian distribution.

Recently, composite density-dependent information-theoretic quantities have been introduced: the complexity measures of Crámer-Rao, Fisher-Shannon and López-Ruiz-Mancini-Calbet (LMC) types. They are given by the product of two of the previous single spreading measures as

$$C_{CR}[\rho] = F[\rho] \times l_{Heis}^2, \tag{10}$$

$$C_{FS}[\rho] = F[\rho] \times \frac{1}{2\pi e} e^{2S[\rho]} = \frac{1}{2\pi e} F[\rho] \times l_{Shan}^2, \tag{11}$$

$$C_{LMC}[\rho] = D[\rho] \times e^{S[\rho]} = \langle \rho \rangle \times l_{Shan}, \tag{12}$$

for the Crámer-Rao [36–38], Fisher-Shannon [39, 40] and LMC complexities [41], respectively. Each of them grasps the combined balance of two different facets of the probability density. The Crámer-Rao complexity quantifies the gradient content of $\rho(x)$ jointly with the probability spreading around the centroid. The Fisher-Shannon complexity measures the gradient content of $\rho(x)$ together with its total extent in the support interval. The LMC complexity measures the combined balance of the average height of $\rho(x)$ (as given by the disequilibrium $D[\rho]$), and its total extent (as given by the Shannon entropic power or Shannon length $l_{Shan} = e^{S[\rho]}$). Moreover, it may be observed that these three complexity measures are (a) dimensionless, (b) bounded from below by unity (when $\rho$ is a continuous density in $\mathbb{R}$ in the Crámer-Rao and Fisher-Shannon cases, and for any $\rho$ in the LMC case)[42], and (c) minimum for the two extreme (or least complex) distributions which correspond to perfect order (i.e. the extremely localized Dirac delta distribution) and maximum disorder (associated to a highly flat distribution). Finally, they fulfill invariance properties under replication, translation and scaling transformation [43, 44].

## III. ENTROPY MEASURES OF A D-DIMENSIONAL BLACKBODY

In this section we determine the main quantifiers of the frequency spreading of the spectral density of a multidimensional blackbody, $\rho_T^{(d)}(\nu), d > 1$, in terms of the space dimensionality d and temperature T; namely, variance, disequilibrium, Shannon entropy and Fisher information. According to the previous section, we first normalize to unity the blackbody density by finding that the associated normalization constant (which corresponds to the total energy). It turns out that the normalized $d$-dimensional Planck radiation formula is given by

$$\rho(\nu) \equiv \rho_T^{(d)}(\nu) = \frac{1}{\Gamma(d+1)\zeta(d+1)} \left(\frac{h}{k_B T}\right)^{d+1} \frac{\nu^d}{e^{\frac{h\nu}{k_B T}} - 1}, \tag{13}$$

where $\zeta(x)$ denotes the zeta function of Riemann [29].

### A. Variance

We have found that the variance of the d-dimensional blackbody radiation density $\rho(\nu)$ is

$$V(d,T) \equiv V^{(d)}[\rho] = \langle \nu^2 \rangle - \langle \nu \rangle^2 = C_1(d) \left( \frac{k_B T}{h} \right)^2 , \tag{14}$$

with

$$C_1(d) = \frac{(d+1)\left((d+2)\zeta(d+1)\zeta(d+3) - (d+1)\zeta(d+2)^2\right)}{\zeta(d+1)^2}.$$

In particular, for $d = 3$ one finds that the variance grows quadratically with temperature as $V(3,T) \simeq 4.11326 \left(\frac{k_B T}{h}\right)^2$.

### B. Disequilibrium

The disequilibrium of the $d$-dimensional blackbody radiation density $\rho(\nu)$ is, according to eq. (4),

$$D(d,T) \equiv D^{(d)}[\rho] = \langle \rho \rangle = \int_0^\infty \rho(\nu)^2 \, d\nu = C_2(d) \frac{h}{k_B T}, \tag{15}$$

where

$$C_2(d) = \frac{\Gamma(1+2d)}{\Gamma(1+d)^2 \zeta(1+d)^2} (\zeta(2d) - \zeta(2d+1)).$$

Then, the disequilibrium for 3-dimensional blackbody radiation turns out to be $D(3,T) \simeq 0.153553 \, \frac{h}{k_B T}$.

### C. Shannon entropy

The Shannon entropy of the d-dimensional blackbody radiation density $\rho(\nu)$ is, according to eq. (3),

$$S(d,T) \equiv S^{(d)}[\rho] \;=\; -\log \frac{h}{k_B T} + C_3(d) \tag{16}$$

where

$$C_3(d) = \log[\Gamma(1+d)\zeta(1+d)] - \frac{I(d)}{\Gamma(1+d)\zeta(1+d)}$$

where $I(d)$ denotes the function

$$\begin{aligned} I(d) \;&=\; \int_0^\infty \frac{x^d}{e^x - 1} \log\left( \frac{x^d}{e^x - 1} \right) dx \\ &= \; d\,\Gamma(1+d)(\psi^{(0)}(1+d)\zeta(1+d) + \zeta'(1+d)) \\ &\quad -\Gamma(2+d)\zeta(2+d) + \Gamma(1+d) \times \\ &\quad \left( \frac{d+1}{2} \zeta(d+2) - \sum_{k=1}^{d-1} \zeta(d+1-k)\zeta(1+k) \right), \end{aligned} \tag{17}$$

Then, the Shannon entropy of the 3-dimensional blackbody radiation is $S(3,T) \simeq 2.03655 - \log\left(\frac{h}{k_B T}\right)$.

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### D. Fisher information

The Fisher information of the $d$-dimensional blackbody radiation density $\rho(\nu)$ is, according to eq. (5),

$$F(d,T) \equiv F^{(d)}[\rho] = \int_0^\infty \frac{[\rho'(\nu)]^2}{\rho(\nu)}\, d\nu = C_4(d) \left(\frac{h}{k_B T}\right)^2 \tag{18}$$

with

$$\begin{aligned} C_4(d) &= \frac{\int_0^\infty x^{d-2} \frac{[d(1-\exp(x))+x\exp(x)]^2}{(\exp(x)-1)^3}}{\Gamma(d+1)\zeta(1+d)} \\ &= \frac{1}{\Gamma(d+1)\zeta(1+d)}[d^2\,\Gamma(d-1)\zeta_1(d-1,1) \\ &\quad -2d\,\Gamma(d)\zeta_2(d,1) + \Gamma(d+1)\zeta_3(d+1,1)], \\ &= \frac{1}{\Gamma(d+1)\zeta(1+d)}\, J(d), \end{aligned}$$

where $\zeta_n(z)$ represents the so-called "multiple" zeta function. Then, the Fisher information of the 3-dimensional blackbody radiation is $F(3,T) =\simeq 0.555313 \left(\frac{h}{k_B T}\right)^2$.

## IV. CHARACTERISTIC FREQUENCIES OF A $d$-DIMENSIONAL BLACKBODY

The most characteristic frequency of the Planck radiation spectrum in a $d$-dimensional universe is $\nu_{max}(d,T)$, the frequency where the density reaches the maximum. It is well known that this frequency, according to the generalised Wien displacement law [20, 21], is proportional to temperature as

$$\nu_{max}(d,T) = C_0(d)\,\frac{k_B T}{h}, \tag{19}$$

with the constant $C_0(d) = d + W(-de^{-d})$, where the Lambert function $W(z)$ is defined [29] as $W(z) + e^{W(z)} = z$. Then, taking into account the properties of this function, the constant $C_0(d)$ can be shown to increase as the dimensionality is increasing. Let us also collect here that for $d = 3$, the constant $C_0(3) \simeq 2.82144$.

Here, following the indications given in section II, we introduce for the first time to the best of our knowledge three new characteristic frequencies of the d-dimensional Planck spectrum based on the spreading measures of the Planck density discussed in the previous section; namely, the variance, the Shannon entropy and the Fisher information. They are referred as Heisenberg, Shannon and Fisher frequencies, respectively, for obvious reasons.

The Heisenberg, Shannon and Fisher frequencies of the $d$-dimensional Planck frequency density are given, according to the corresponding notions defined in section II and eqs. (2), (3) and (5), by

$$\nu_{Heis}(d,T) \;=\; \sqrt{V(d,T)} = \sqrt{C_1(d)}\,\frac{k_B T}{h}, \tag{20}$$

$$\nu_{Shan}(d,T) \;=\; \exp\left(S(d,T)\right) = \exp\left(C_3(d)\right)\frac{k_B T}{h} \tag{21}$$

$$\nu_{Fish}(d,T) \;=\; \frac{1}{\sqrt{F(d,T)}} = \frac{1}{\sqrt{C_4(d)}}\,\frac{k_B T}{h}, \tag{22}$$

respectively. Note that these three frequencies follow a displacement law similar to the generalised Wien law (**??**) fulfilled by the frequency $\nu_{max}(d,T)$ where the spectrum is maximum. Indeed they do depend linearly on the temperature, and the proportionality constant only depends on the universe dimensionality. The relative comparison among these four Wien-like laws is done in Figure 1, where the dimensionless quantity

$$x_i = \frac{h}{k_B T}\nu_i, \quad \text{for i = max, Heis, Shan, Fish,} \tag{23}$$

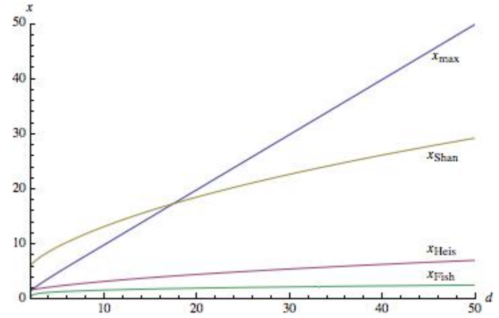

FIG. 1: Wien-like laws of the characteristic frequencies $x_i(d)$ for the $d$-dimensional blackbody radiation

has been plotted as a function of the dimensionality $d$.

We observe the following relative behaviour among the four characteristics frequencies of the $d$-dimensional blackbody spectrum:

$$\begin{aligned} x_{Fish} < x_{max} < x_{Heis} < x_{Shan} \quad &, \quad d \simeq 2 \\ x_{Fish} < x_{Heis} < x_{max} < x_{Shan} \quad &, \quad 3 \lesssim d \lesssim 17 \\ x_{Fish} < x_{Heis} < x_{Shan} < x_{max} \quad &, \quad 18 \lesssim d \end{aligned}$$

It is worth noting that this behaviour is universally valid in the sense that it holds for any value of the absolute temperature of the system. Let us also mention that for $d \gtrsim 13$, $x_{max}$ grows linearly with $d$. Moreover, it is trivial to show that $(2\pi e)^{1/2}\, x_{Fish} < x_{Shan} < (2\pi e)^{1/2}\, x_{max}$ so that the general inequality (8) is fulfilled, what is a further checking of our results.

On the other hand, for $d = 3$ one has that the variance-based Heisenberg frequency and the entropy-based Shannon and Fisher frequencies of the 3-dimensional blackbody radiation are given by $\nu_{Heis}(3,T) \simeq 2.02812\, \frac{k_B T}{h}$, $\nu_{Shan}(3,T) \simeq 7.66411 \frac{k_B T}{h}$, and $\nu_{Fish}(3,T) \simeq 1.34193\, \frac{k_B T}{h}$, respectively. Then, in particular, for the temperature $T = 2.725$K one finds that $\nu_{max}(cmb) = 1.60201 \cdot 10^{11}$Hz and the following values

$$\begin{aligned} \nu_{Fish}(cmb) &\simeq 6.57748 \cdot 10^{10}\,\text{Hz}, \\ \nu_{Heis}(cmb) &\simeq 1.15156 \cdot 10^{11}\text{Hz}, \\ \nu_{Shan}(cmb) &\simeq 4.35167 \cdot 10^{11}\,\text{Hz}, \end{aligned}$$

for the Heisenberg, Shannon and Fisher frequencies of the 3-dimensional cosmic microwave background (cmb, in short) radiation. It is interesting to realise that the Fisher frequency has the lowest value among all the four characteristic spectral frequencies, partially reflecting the high degree of smoothness of the cosmic microwave spectrum. Since tiny fluctuations of $\rho(\nu)$ can cause huge changes in the Fisher frequency but hardly alter the other three characteristic frequencies of the spectrum, this quantity might be paradoxically the most important frequency to detect the small deviations of the Planck radiation formula which have been observed [47] in the cosmic microwave radiation. These deviations have been argued to be due to the interaction between photons and other microscopic particles and/or to the nonextensive statistics environment which is presumably associated to the long-range interactions; much work along these lines are being done in the last few years [26, 48–50]. Then, we are led to conjecture that the Fisher frequency is an appropriate quantifier of the anisotropies of the cosmic microwave radiation that should be calculated in the framework of the nonlinear models [26] and non-extensive theories [45] of the cosmic background radiation recently proposed, and it might be experimentally determined.

## V. COMPLEXITY MEASURES OF A $d$-DIMENSIONAL BLACKBODY

In this section we calculate the three main intrinsic complexity measures of the energy density of the $d$-dimensional blackbody radiation; namely, the Crámer-Rao, Fisher-Shannon and LMC quantities. The Crámer-Rao measure quantifies the frequency-gradient content of the spectrum distribution jointly with the frequency concentration around its mean value, while the Fisher-Shannon complexity measures the frequency-gradient content together with its spreading. On the other hand, the LMC complexity measures the combined balance of the average height of the spectrum and its effective extent.

Taking into account the corresponding notions defined in section II and eqs. (2), (4), (3) and (5), the Crámer-Rao, Fisher-Shannon and LMC complexity measures of the $d$-dimensional Planck frequency density are given by

$$\begin{aligned} C_{CR}(V,T) &= F(d,T)\cdot V(d,T) = C_4(d)\,C_1(d) && (24)\\ C_{LMC}(d,T) &= D(d,T)\; e^{S(d,T)} = C_2(d)\,e^{C_3(d)}, && (25)\\ C_{FS}(d,T) &= F(d,T)\cdot \frac{1}{2\pi\,e} e^{2\,S(d,T)} = C_4(d)\frac{1}{2\pi\,e}e^{2C_3(d)}, && (26)\end{aligned}$$

respectively. Moreover, taking into account the dimensionless constants $C_i$, with $i = 1, 2, 3$ and 4, given in the previous section, one finds the following values

$$\begin{aligned} C_{CR}(d,T) &= \frac{J(d)}{\zeta(d+1)^3\Gamma(d+1)}\times \\ & \quad (d+1)[(d+2)\zeta(d+1)\zeta(d+3) \\ & \quad -(d+1)\zeta(d+2)^2], && (27)\\ C_{LMC}(d,T) &= \frac{\Gamma(1+2d)(\zeta(2d)-\zeta(2d+1))}{\Gamma(1+d)\zeta(1+d)} \\ & \quad \times\ \exp\left(-\frac{I(d)}{\Gamma(1+d)\zeta(1+d)}\right), && (28)\\ C_{FS}(d,T) &= \frac{1}{2\pi e}\Gamma(d+1)\zeta(1+d)\,J(d) \\ & \quad \times\ \exp\left(-\frac{2\,I(d)}{\Gamma(1+d)\zeta(1+d)}\right) && (29)\end{aligned}$$

for the Crámer-Rao, Fisher-Shannon and LMC complexity measures of the $d$-dimensional blackbody radiation, respectively.

Interestingly, we notice that all three complexities of the $d$-dimensional blackbody radiation depend neither on temperature nor on the Planck and Boltzmann constants, but they only depend on dimensionality. The former result indicates that these three measures of complexity have an universal character for any $d$-dimensional blackbody; at least in principle, that is without taking into account possible physical processes which might slightly modify the blackbody spectrum, such as the photon scattering by high-energy electrons, quantum gravity effects and non-extensivity effects of the medium, among others. The dimensionality dependence of the complexity measures is shown in Figure 2.

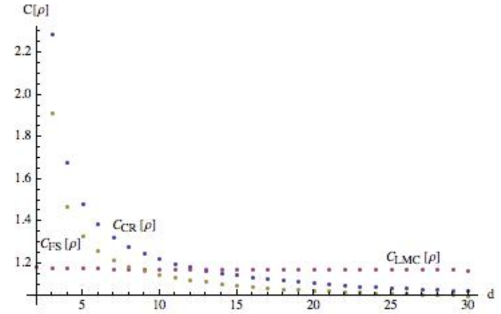

FIG. 2: The Crámer-Rao, Fisher-Shannon and LMC complexity measures of the $d$-dimensional blackbody radiation in terms of $d$.

Therein we observe that the three measures of complexity monotonically decrease with different slopes when the dimensionality is increasing. The LMC complexity is almost constant when $d \geq 2$. The other two measures of complexity clearly decrease, mainly because of the Fisher component included in both quantities. The Fisher-Shannon measure decreases faster than the Crámer-Rao one, basically because the Shannon component included in the former measure is bigger than the variance component of the latter complexity. This is the same phenomenon which explains that the Shannon frequency is always bigger than the Heisenberg frequency, as discussed in the previous section. On the other hand, let us highlight that the Fisher-Shannon and Crámer-Rao measures of complexity can be used as quantifiers of the space dimensionality as grasped by the blackbody spectrum. Moreover, they drastically vary even with small dimensional oscillations of the spectrum because of the huge variations of their Fisher ingredient, as already mentioned. From this point of view, these two measures of complexity could be eventually used to detect dimensional anisotropies of the spectrum. Let us finally note that for $d = 3$ one finds the values 1.17685, 1.90979, 2.28415 for the LMC, Fisher-Shannon and Crámer-Rao measures of complexity of the 3-dimensional blackbody radiation.

## VI. CONCLUSIONS

In this paper we have investigated the entropy and complexity quantities of the d-dimensional blackbody radiation for standard ($d = 3$) and non-standard dimensionalities. We have calculated the main entropy and complexity measures of the corresponding spectral energy density in terms of dimensionality $d$ and temperature $T$. First, we have determined the variance, the disequilibrium, the Shannon entropy and the Fisher information of the d-dimensional Planck density in an explicit way. Then, besides the frequency $\nu_{max}$ at which the density is maximum, we have used these frequency-spreading measures to introduce three further characteristic frequencies of the spectrum, which have been referred as Heisenberg, Shannon and Fisher frequencies for obvious reasons. We have found that these new frequencies have a dependence on the temperature similar to the one given by the well-known Wien's law followed by $\nu_{max}$. The values of these charateristic frequencies for the cosmic microwave background radiation have been given and physically discussed, suggesting the potential interest of the Fisher frequency to grasp the CMB anisotropy.

Second, we have shown that the three main measures of complexity (i.e., Crámer-Rao, Fisher-Shannon and LMC) do not depend on the temperature, but only on the universe dimensionality. The corresponding values for the cosmic microwave radiation turns out to be dimensionless constants, noting that the Crámer-Rao complexity is bigger than the Fisher-Shannon and LMC quantities mainly because of the high smoothness and extent of the corresponding 3-dimensional Planck density. On the other hand, it is worth remarking the potential quality of these complexities (mainly the Crámer-Rao and Fisher-Shannon) as identifiers of CMB anisotropies because of the sensitivity of the Fisher-information component to the fluctuations of the associated non-smoothed Planck density due to (a) different physical processes such as the photon scattering by high-energy electrons (Sunyaev-Zel'dovich effect) or gravitational shift of photon energy caused by varying gravitational fields (Sachs-Wolfe effect), and (b) cavity finite-size corrections [27, 46].

A possible extension of this work is the inclusion of quantum gravity effects, which will certainly modify the black body spectrum and might open new windows to know deeper the quantum gravitational features of the early universe through study of CMB spectrum. This could be done by taking into account the quantum gravity effects encoded in modified dispersion relations [25].

Finally, let us point out that this entropy and complexity analysis should be extended as well to the nonlinear blackbody radiation laws [26, 45], which presumably takes into account the small deviations from the Planck radiation formula that have been detected [47] in the cosmic microwave radiation. The origin of these deviations has been argued to be due both to the interaction between photons and other microcosmic particles [26] and the nonextensive statistics environment [45] which is associated with the long-range interactions. The last approach has received much attention (see e.g., [48–50] and references therein).

### Acknowledgments

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***Eur. Phys. J. D 68, 316 (2014)***

## 3.8 Rényi entropies of the highly-excited states of multidimensional harmonic oscillators

In 2012 the Shannon entropy, which corresponds to the limiting case $p \to 1$ of the Rényi entropy, was determined for the highest-lying (Rydberg) states of the one-dimensional harmonic oscillator [11], whose position-space wavefunctions are controlled by Hermite polynomials. In this section we extend this result in a two-fold way. Firstly, we develop a method to analytically calculate the leading term of the asymptotics of the associated Laguerre norms when the polynomial degree is very high. Then, we determine in an analytical way the Rényi entropies of all orders for the Rydberg states of a $D$-dimensional harmonic oscillator in position space, whose wavefunctions are known to be controlled by Laguerre polynomials.

Moreover, we have found the following physical results:

- For a given Rydberg state the Rényi entropy has a very fast decreasing behavior as the parameter order is increasing, indicating that the Rényi entropies with lowest orders are most significant,
- we study in detail the second-order Rényi entropy (i.e., the disequilibrium) of the system, which quantifies the separation of the electron distribution from equiprobability. It is found that it has a quasi-Gaussian behavior in terms of $D$, its maximum being located at $D = 12$ which is the universe dimensionality predicted by certain string theories [22], and
- the disequilibrium of the Rydberg ($ns$)-states of $D$-dimensional oscillator decreases (increases) as a function of the principal hyperquantum number $n$ when the dimensionlity $D$ is less (bigger) than 4, and it becomes constant when $D = 4$.

These results have been published in the article with coordinates: *A. I. Aptekarev, D. N. Tulyakov, I. V. Toranzo and J. S. Dehesa, The European Physical Journal B: Condensed Matter and Complex Systems **89**, 85 (**2016**)*, which is attached below.

# Rényi entropies of the highly-excited states of multidimensional harmonic oscillators by use of strong Laguerre asymptotics

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The Rényi entropies $R_p[\rho]$, $p > 0, \neq 1$ of the highly-excited quantum states of the $D$-dimensional isotropic harmonic oscillator are analytically determined by use of the strong asymptotics of the orthogonal polynomials which control the wavefunctions of these states, the Laguerre polynomials. This Rydberg energetic region is where the transition from classical to quantum correspondence takes place. We first realize that these entropies are closely connected to the entropic moments of the quantum-mechanical probability $\rho_n(\vec{r})$ density of the Rydberg wavefunctions $\Psi_{n,l,\{\mu\}}(\vec{r})$; so, to the $\mathcal{L}_p$-norms of the associated Laguerre polynomials. Then, we determine the asymptotics $n \to \infty$ of these norms by use of modern techniques of approximation theory based on the strong Laguerre asymptotics. Finally, we determine the dominant term of the Rényi entropies of the Rydberg states explicitly in terms of the hyperquantum numbers $(n, l)$, the parameter order $p$ and the universe dimensionality $D$ for all possible cases $D \geq 1$. We find that (a) the Rényi entropy power decreases monotonically as the order $p$ is increasing and (b) the disequilibrium (closely related to the second order Rényi entropy), which quantifies the separation of the electron distribution from equiprobability, has a quasi-Gaussian behavior in terms of $D$.

## I. INTRODUCTION

Harmonicity is one of the most frequent and useful approximations to simplify and solve the Schrödinger equation of the physical many-body systems. It often provides a deeper quantitative insight into the physical system under investigation, and in many cases allows for the conceptual understanding of physics in a straightforward and intuitive way. Moreover, the solutions of the wave equations of complex physical systems within this approximation are very valuable tools for checking and improving complicated numerical methods used to study such systems.

The one-dimensional isotropic harmonic oscillator first and then the $D$-dimensional ($D > 1$) oscillator, have been widely used through the history of physics since the 1926-dated seminal paper of Heisenberg [1]. Indeed they have been used in a great diversity of fields from fractional and quantum statistics [2, 3] up to quantum many-body physics [4–12] and black-holes thermodynamics [13, 14], and they have been applied to gain insight into numerous quantum phenomena and systems ranging from heat transport [15] and entanglement [16, 17] to Keppler systems [18], quantum dots [6, 19, 20], neural networks [21], cold atomic gases [22, 23] and systems with ontological states [24]. Let us also remark that the oscillator wavefunctions saturate the various mathematical realizations of the quantum uncertainty principle of Heisenberg and entropic types, which are based on the variance and its moment generalizations (Heisenberg-like uncertainty relations) [25, 26] and the Shannon entropy [27, 28], Rényi entropy [29, 30] and the Fisher information [25, 31] (entropic uncertainty relations), respectively.

The spatial extension or spreading of the position probability densities $\rho(\vec{r})$ of a $D$-dimensional isotropic harmonic oscillator, which control all its fundamental properties, has been examined by means of their central moments, particularly the second one (i.e., the variance) [26]. It can be complementarily described in the framework of Information Theory by use of the entropic moments of these densities and some related entropic measures [32–37], what is much more adequate because they do not depend on any specific point of their domain of definition, contrary to what

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happens with the moments about the origin and the central moments. The entropic moments of $\rho(\vec{r})$ are defined as

$$W_p[\rho] = \int_{\mathbb{R}^D} [\rho(\vec{r})]^p \, d\vec{r} = \|\rho\|_p^p; \quad p \geq 0, \tag{1}$$

where the position $\vec{r} = (x_1, \dots, x_D)$ 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 $\theta_i \in [0\,;\,\pi), i < D-1$, $\theta_{d-1} \equiv \phi \in [0\,;\,2\pi)$. By convention $\theta_D = 0$ and the empty product is the unity. And the volume element is naturally

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

with $2\alpha_j = D - j - 1$. The symbol $\|\cdot\|_p$ denotes the $L_p$ norm for functions: $\|\Phi\|_p = \left(\int_{\mathbb{R}^D} |\Phi(\vec{r})|^p d\vec{r}\right)^{1/p}$. The knowledge of the entropic moments or their closely connected quantities, the *Rényi entropies* $R_p[\rho]$ (also called by *information generating functionals* in other contexts [**?** ]), completely characterize the density $\rho(\vec{r})$. They are defined [**?** ] as

$$R_p[\rho] = \frac{1}{1-p} \ln W_p[\rho];\ 0 < p < \infty,\ p \neq 1. \tag{2}$$

Note that these quantities include the Shannon entropy (which measures the total extent of the density), $S[\rho] = \lim_{p\to 1} R_p[\rho]$, and the disequilibrium (which quantifies the separation of the density with respect to equiprobability), $\langle\rho\rangle = \exp(R_2[\rho])$, as two important particular cases. For a revision of their properties see [38–44] and the reviews [45, 46]. 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 [29, 44–46], ranging from the quantum-classical correspondence [47] and quantum entanglement [48] to pattern formation and Brown processes [49, 50], fractality and chaotic systems [51, 52], quantum phase transition [53] and disordered systems [54]. Moreover, the knowledge of these quantities allows us to reconstruct the corresponding probability density under certain conditions [41, 55].

In this work we will investigate the Rényi entropies of the quantum $D$-dimensional oscillator states of the potential $V_D(r) = \frac{1}{2}\lambda^2 r^2$, which are known to be described in position space [33, 56] by the eigenfunctions

$$\begin{aligned}\Psi_{n,l,\{\mu\}}(\vec{r}) &= \left[\frac{2n!\lambda^{l+\frac{D}{2}}}{\Gamma(n+l+\frac{D}{2})}\right]^{\frac{1}{2}} r^l e^{-\frac{\lambda r^2}{2}} L_n^{l+D/2-1}(\lambda r^2) \\ &\quad \times \mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}),\end{aligned} \tag{3}$$

and the corresponding energetic eigenvalues

$$E_{n,l} = \lambda\left(2n + l + \frac{D}{2}\right), \tag{4}$$

where $n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$. The symbol $L_n^{\alpha}(t)$ denotes the Laguerre polynomial of paramater $\alpha$ and degree $n$ (see definition in Eq. (18) below), and $\mathcal{Y}_{l,\{\mu\}}(\Omega_D)$ represents the hyperspherical harmonics defined by

$$\begin{aligned}\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) &= \mathcal{N}_{l,\{\mu\}} e^{im\phi} \\ &\quad \times \prod_{j=1}^{D-2} C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}}\end{aligned} \tag{5}$$

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 orbital quantum number $l$ and the magnetic quantum numbers $\{\mu\}$ are integers satisfying

$$l \geq \mu_1 \geq \mu_2 \geq \dots \geq |\mu_{D-1}| \equiv |m|,$$

and the symbol $C_n^{\lambda}(t)$ denotes the Gegenbauer polynomial of degree $n$ and parameter $\lambda$. Atomic units are used throughout the paper.

Then, the position probability density of the $D$-dimensional isotropic harmonic oscillator is given by the the squared modulus of the position eigenfunction as follows

$$\begin{aligned}\rho(\vec{r}) &= |\Psi_{n,l,\{\mu\}}(\vec{r})|^2 \\ &= \frac{2n!\lambda^{l+\frac{D}{2}}}{\Gamma(n+l+\frac{D}{2})} r^{2l} e^{-\lambda r^2}\left[L_n^{(l+D/2-1)}(\lambda r^2)\right]^2 \\ &\quad \times |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &= \frac{2n!\lambda^{\frac{D}{2}}}{\Gamma(n+l+\frac{D}{2})} x^{1-\frac{D}{2}} \omega_{l+\frac{D}{2}-1}(x)\left[L_n^{(l+D/2-1)}(x)\right]^2 \\ &\quad \times |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \\ &= 2\,\lambda^{\frac{D}{2}} x^{1-\frac{D}{2}} \omega_{l+\frac{D}{2}-1}(x)[\widehat{L}_n^{(l+D/2-1)}(x)]^2 \\ &\quad \times |\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})|^2 \end{aligned} \tag{6}$$

where $x = \lambda\, r^2$ and

$$\omega_\alpha(x) = x^\alpha e^{-x},\ \alpha = l + \frac{D}{2} - 1, \tag{7}$$

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 [33] that the probability density in momentum space (i.e., the squared modulus of the Fourier transform of the position eigenfunction) is given by $\gamma(\vec{p}) = \frac{1}{\lambda^D}\rho\left(\frac{\vec{p}}{\lambda}\right)$.

Then, by keeping in mind Eqs. (1) - (2), the main problem in this work is to calculate the quantities

$$\begin{aligned} W_p[\rho] &= \int_{\mathbb{R}^D} [\rho(\vec{r})]^p \, d\vec{r} \\ &= \int_0^\infty [\rho_{n,l}(r)]^p \, r^{D-1} dr \end{aligned} \tag{8}$$

where we have used the unity normalization of the hyperspherical harmonics

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

and the radial density function $\rho_{n,l}(r)$

$$\rho_{n,l}(X) = 2\,\lambda^{\frac{D}{2}} x^{1-\frac{D}{2}} \omega_{l+\frac{D}{2}-1}(x)[\widehat{L}_n^{(l+D/2-1)}(x)]^2 \tag{9}$$

For the low-energy quantum oscillator states (i.e., for low values of the principal quantum number $n$), the analytical expressions of the associated Laguerre polynomials are tractable and the corresponding entropic moments $W_p[\rho_{n,l}]$ can be numerically calculated by various accesible quadrature formulas in an effective and sufficiently accurate way. Then, it remains the truly dificult problem: the evaluation of the asymptotics of the quantities

$$\int_0^\infty \rho_{n,l}^p(r)\, r^{D-1} dr\,, \quad n \to \infty\,, \tag{10}$$

which represent the entropic moments of the Rydberg (high-energy) oscillator states. This is the purpose of the present work: to solve this problem in a fully analytical way. Thus, by looking at the expressions (9) and (10), this problem converts into an important issue, not yet solved, of the modern Approximation Theory: to study the asymptotics ($n \to \infty$) of the $L_p$-norm of the Laguerre polynomials

$$N_{n,l}(D,p) = \int_0^\infty \left(\left[\widehat{L}_n^{(\alpha)}(x)\right]^2 \omega_\alpha(x)\right)^p x^\beta \, dx\,, \quad p > 0\,, \tag{11}$$

where

$$\alpha = l + \frac{D}{2} - 1\,,\; l = 0, 1, 2, \ldots, \quad \text{and} \quad \beta = (p-1)(1 - D/2)\,. \tag{12}$$

We note that (7) and (12) guarantee the convergence of integral (11) at zero; i.e. the condition

$$\beta + p\alpha = pl + \frac{D}{2} - 1 > -1\,,$$

is always satisfied for physically meaningfull values of the parameters (12).

## II. ASYMPTOTICS OF $\mathcal{L}_p$ NORMS OF LAGUERRE POLYNOMIALS

In this section we will determine the asymptotics ($n \to \infty$) of the integral functionals $N_{n,l}(D,p)$ of the (orthonormal) Laguerre polynomials $\widehat{L}_n^{(\alpha)}(x)$ defined by Eq. (11). It essentially depends on the values of the parameters $D$ and $p$ (i.e. $\alpha, \beta$ and $p$) given by Eq.(12).

First of all we will make some general comments about the different regions of integration, pointing out the various asymptotical regimes of the Laguerre polynomials and the corresponding dominant contribution. Then, we give the asymptotical results of $N_{n,l}(D,p)$ for all the possible pairs $(D,p)$ in the form of three theorems. Finally we give a detailed proof of these theorems.

In fact, to make the $(0,\infty)$-integration in (11) for the different values (12) of the parameters we have various regions where the Laguerre polynomials have a precise asymptotical representation. First, in the neighborhood of zero (i.e. the left end point of the interval of orthogonality) the Laguerre polynomials can asymptotically be represented by means of Bessel functions as it is pointed out below. Then, to the right, in the bulk region of zeros location, the oscillatory behavior of the polynomials is modelled asymptotically by means of the trigonometric functions; and at the neighborhood of the extreme right zeros, asymptotics of the polynomials is given by Airy functions. Finally in the neighborhood of the infinity point, the polynomials has growing asymptotics. Moreover there are regions where these asymptotics match each other. Namely, asymptotics of the Bessel functions for large arguments match the trigonometric function, as well as asymptotics of the Airy functions do the same. Altogether there are five asymptotical regimes which can give (depending on $D$ and $p$) the dominant contribution in the asymptotics of $N_{n,l}(D,p)$ . Three of them exhibit the growth of $N_{n,l}(D,p)$ with $n$ by following a power law with an exponent which depends on $D$ and $p$. We call these regimes as Bessel, Airy and cosine (or oscillatory) regimes. Associated to each of these regimes, there is a characteristic constant whose value (as shown below) is

$$C_B(\alpha,\beta,p) := 2\int\limits_0^\infty t^{2\beta+1} |J_\alpha(2t)|^{2p}\, dt\,. \tag{13}$$

for the Bessel regime,

$$C_A(p) := \int_{-\infty}^{+\infty} \left[\frac{2\pi}{\sqrt[3]{2}}\,\mathrm{Ai}^2\left(-\frac{t\sqrt[3]{2}}{2}\right)\right]^p dt\,. \tag{14}$$

for the Airy regime, and

$$C(\beta,p) := \frac{2^{\beta+1}}{\pi^{p+1/2}}\,\frac{\Gamma(\beta+1-p/2)\,\Gamma(1-p/2)\,\Gamma(p+1/2)}{\Gamma(\beta+2-p)\,\Gamma(1+p)}\,. \tag{15}$$

for the cosine regime. The symbols $J_\alpha(z)$ and $\mathrm{Ai}(-z)$ denote the known Bessel and Airy functions [57], respectively, defined below; see Eqs. (20), (25) and (26).
In addition, there are two asymptotical regimes corresponding to the transition regions, cosine-Bessel and cosine-Airy. If these regimes dominate in integral (11), then the asymptotics of $N_n(D,p)$ has a factor $\ln n$ besides the power law in $n$. It is also curious to mention that if these regimes dominate then gamma factors in constant $C(\beta,p)$ in (15) for the oscillatory cosine regime explode. For the cosine-Bessel regime it happens for $\beta + 1 - p/2 = 0$, and for the cosine-Airy regime it happens for $1 - p/2 = 0$.

### A. Asymptotics of the Laguerre polynomials

Let us now give the asymptotical representation for the Laguerre polynomials $L_n^{(\alpha)}(x)$ defined by

$$L_n^{(\alpha)}(x) = \sum_{\nu=0}^{n} \tbinom{n+\alpha}{n-\nu} \frac{(-x)^\nu}{\nu!} \tag{16}$$

with the norm

$$\|L_n^{(\alpha)}\|^2 = \Gamma(\alpha+1)\, \tbinom{n+\alpha}{n} \ . \tag{17}$$

For the distinct scales of the variable $x$ with respect to $n$ the Laguerre polynomials have different asymptotics as indicated above.

For the Bessel regime (i.e. when $x$ is small with respect to $n$) there is Hilb asymptotics (see [58] , eq.(8.22.4)):

$$e^{-\frac{x}{2}} x^{\alpha/2} L_n^{(\alpha)}(x) = \tfrac{(n+\alpha)!}{n!}\, (N\,x)^{-\alpha/2} J_\alpha(2\sqrt{N\,x}) + \varepsilon(x,n) \ , \tag{18}$$

where

$$N = n + \tfrac{\alpha+1}{2} \ , \qquad \varepsilon(x,n) = \begin{cases} x^{\alpha/2+2}\, \underline{\underline{O}}(n^\alpha)\, , & 0 < x < \frac{c}{n} \\ x^{5/4}\, \underline{\underline{O}}(n^{\alpha/2-3/4})\, , & \frac{c}{n} < x < C \end{cases} \ , \tag{19}$$

and the Bessel function is defined by

$$J_\alpha(z) = \sum_{\nu=0}^{\infty} \frac{(-1)^\nu}{\nu!\,\Gamma(\nu+\alpha+1)} \left(\frac{z}{2}\right)^{\alpha+2\nu} \ . \tag{20}$$

For the transition region between Bessel regime and oscillatory regime we use the asymptotics of the Bessel function [57]:

$$J_\alpha(z) = \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{\alpha\pi}{2} - \frac{\pi}{4}\right) + e^{|\mathrm{Im}\, z|} \underline{\underline{O}}\left(\frac{1}{z}\right) \ , \quad |\arg z| < \pi \ . \tag{21}$$

The regimes of oscillatory, growing and Airy types are described by the Plancherel-Rotach asymptotics [58–60]:

- For $x = (4n + 2\alpha + 2)\, \cos^2\varphi$, $\varepsilon \leqslant \varphi \leqslant \dfrac{\pi}{2} - \varepsilon n^{-1/2}$

$$\begin{aligned} e^{-x/2}\, L_n^{(\alpha)}(x) = (-1)^n\, (\pi \sin\varphi)^{-1/2}\, x^{-\alpha/2-1/4} \times \\ \times n^{\alpha/2-1/4} \Big\{ \sin\left[\left(n + \tfrac{\alpha+1}{2}\right)\, (\sin 2\varphi - 2\varphi) + \tfrac{3\pi}{4}\right] \\ + (nx)^{-1/2}\, O(1) \Big\} \end{aligned} \tag{22}$$

- For $x = (4n + 2\alpha + 2)\, \mathrm{ch}^2\varphi$, $\varepsilon \leqslant \varphi \leqslant \omega$

$$\begin{aligned} e^{-x/2}\, L_n^{(\alpha)}(x) = \tfrac{1}{2}(-1)^n\, (\pi\, \mathrm{sinh}\varphi)^{-1/2}\, x^{-\alpha/2-1/4} \times \\ \times n^{\alpha/2-1/4} \exp\left[\left(n + \tfrac{\alpha+1}{2}\right)\, (2\varphi - \, \mathrm{sinh}2\varphi)\right]\, [1 + O(n^{-1})] \end{aligned} \tag{23}$$

- And for $x = 4n + 2\alpha + 2 - 2\left(\frac{2n}{3}\right)^{1/3} t\,$, $|t| < const$

$$\begin{aligned} e^{-x/2}\, L_n^{(\alpha)}(x) = (-1)^n\, \pi^{-1}\, 2^{-\alpha-1/3}\, 3^{1/3} \times \\ \times n^{-1/3} \{A(t) + O(n^{-2/3})\} \end{aligned} \tag{24}$$

  where the Airy function $A(t)$

$$A(t) = \frac{\pi}{3} \left(\frac{t}{3}\right)^{1/2} \left[J_{-1/3}\left(2\left(\frac{t}{3}\right)^{\frac{3}{2}}\right) + J_{1/3}\left(2\left(\frac{t}{3}\right)^{\frac{3}{2}}\right)\right] \tag{25}$$

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is the solution of the equation

$$\frac{d^2}{dt^2}y + \frac{1}{3}\,t\,y = 0\ ,$$

bounded when $t \to \infty$. In (14) we use normalization for the Airy function as

$$A(t) = \frac{\pi}{\sqrt[3]{3}}\,\mathrm{Ai}\left(-t/3\sqrt{3}\right)\ . \qquad (26)$$

During the last two decades there was an essential progress in proving global asymptotical representations for orthogonal polynomials (see Deift et al [61–63], Wong et al [64, 65] and others [60, 66]). In practice it means that classical asymptotics formulas (like Hilb and Plancherel-Rotach) hold true in wider domains providing matching of the asymptotics in the transition zones (for example, see in [60] for Hermite polynomials). In our paper we assume that matching of the classical asymptotics holds true for Laguerre polynomials as well.

### B. Main results

Now we are going to state our main asymptotics results. We split them in three theorems.

**Theorem 1** *Let* $D \in (2, \infty)$. *The weigthed* $\mathcal{L}_p$*-norms of Laguerre polynomials* $N_{n,l}(D,p)$, *given by (11), have the following asymptotical* ($n \to \infty$) *values:*

$$N_{n,l}(D,p) = \begin{cases} C(\beta,p)\,(2n)^{(1-p)\,D/2}\,(1+\bar{\bar{o}}(1)), & p \in (0,p^*) \\[2ex] \dfrac{2}{\pi^{p+1/2}n^{p/2}}\,\dfrac{\Gamma(p+1/2)}{\Gamma(p+1)}\,(\ln n + \underline{\underline{O}}(1))\,, & p = p^* \\[2ex] C_B(\alpha,\beta,p)\,n^{(p-1)D/2-p}\,(1+\bar{\bar{o}}(1)), & p > p^* \end{cases}\ , \qquad (27)$$

*where* $p^* := \frac{D}{D-1}$, *the constants* $C$ *and* $C_B$ *are defined in (15), (13) respectively, and the parameters* $\alpha \equiv \alpha(l,D)$ *and* $\beta \equiv \beta(p,D)$ *are given by (12).*

*Comments*: Let us note that

$$\beta(p^*,D) - \tfrac{p^*}{2} = (p^*-1)\left(1-\tfrac{D}{2}\right) - \tfrac{p^*}{2} = \tfrac{1}{D-1}\left(1-\tfrac{D}{2}-\tfrac{D}{2}\right) = -1\,,$$

so that from (15) we have $C(\beta,p) = \infty$. Thus, when $D > 2$ we have: 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 (11). For $p = p^*$ the transition cosine-Bessel regime determines the asymptotics of $N_{n,l}(D,p^*)$, and for $p > p^*$ the Bessel regime plays the main role.

Let us also highlight that the $\mathcal{L}_p$-norm is constant (i.e., independent of $n$) and equal to $C_B(\alpha,\beta,p)$, only when $(p-1)D/2 - p = 0$. This means that the constancy occurs either when $D = \frac{2p}{p-1}$ or $p = \frac{D}{D-2}$.

The next result is

**Theorem 2** *Let* $D = 2$. *The weigthed* $\mathcal{L}_p$*-norms of Laguerre polynomials* $N_{n,l}(D,p)$, *given by (11), have the following asymptotical* ($n \to \infty$) *values:*

$$N_{n,l}(D,p) = \begin{cases} C(0,p)\,(2n)^{(1-p)}\,(1+\bar{\bar{o}}(1))\ , & p \in (0,2) \\[2ex] \dfrac{\ln n + \underline{\underline{O}}(1)}{\pi^2 n}\ , & p = 2 \\[2ex] \dfrac{C_B(\alpha,0,p)}{n}\,(1+\bar{\bar{o}}(1))\ , & p > 2 \end{cases}\ . \qquad (28)$$

*where the constants* $C$ *and* $C_B$ *are defined in (15), (13) respectively, and the parameter* $\alpha \equiv \alpha(l,D)$ *is given by (12).*

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*Comments*: A peculiarity of the case $D = 2$ is the following. We have from Theorems 1 and 2

$$\lim_{D\to 2+} N_n(D,p) = N_n(2,p)\ , \quad p \in (0,2) \cup (2,\infty)\ .$$

However, from Theorem 1 we have

$$\lim_{D\to 2+} N_n(D,2) = \frac{3(\ln n + \underline{\underline{O}}(1))}{4\pi^2 n}\ . \tag{29}$$

On the other hand, Theorem 2 states:

$$N_n(2,2) = \frac{\ln n + \underline{\underline{O}}(1)}{\pi^2 n}\ .$$

Indeed, as we shall prove it below, the magnitude of integral $N_n(2,2)$ is performed mainly by two regions of $\mathbb{R}_+$ (with the same order of contribution). The first one is at the origin (Bessel-cosine regime), and the second one is around the right-extreme zeros of the Laguerre polynomials (Airy-cosine regime). The first region gives the contribution in $N_n(2,2)$ as in (29). The second one gives the rest of the contribution

$$\frac{\ln n + \underline{\underline{O}}(1)}{4\pi^2 n}\ . \tag{30}$$

Thus for $D = 2$ and $p = 2$ we have the competition of two transition regimes, namely the Bessel-cosine and Airy-cosine regimes.
Let us also highlight that the $\mathcal{L}_p$-norm is constant when $p = 1$, being its value $C(0,p) = 1$.

The third, final, result on asymptotics of $N_n(D,p)$ (we recall $\beta$ is defined in (12)) is the following.

**Theorem 3** *Let $D \in [0,2)$. The weigthed $\mathcal{L}_p$-norms of Laguerre polynomials $N_{n,l}(D,p)$, given by (11), have the following asymptotical ($n \to \infty$) values:*

- *For $p \in (0,2]$,*

$$N_n(D,p) = \begin{cases} C(\beta,p)\,(2n)^{(1-p)\frac{D}{2}}\,(1+\bar{\bar{o}}(1))\ , & p \in (0,2) \\ \dfrac{\ln n + \underline{\underline{O}}(1)}{\pi^2 (4n)^{1-\beta}}\ , & p = 2 \end{cases}\ . \tag{31}$$

- *For $p > 2$ and $4/3 < D < 2$,*

$$N_{n,l}(D,p) = \begin{cases} \dfrac{C_A(p)}{\pi^p}\,(4n)^{(\frac{1-2p}{3}+\beta)}(1+\bar{\bar{o}}(1))\,, & p \in (2,\widetilde{p}) \\ \left(\dfrac{C_A(p)}{\pi^p}\,4^{(\frac{1-2p}{3}+\beta)} + C_B(\alpha,\beta,p)\right)\,n^{-\beta-1}\ , & p = \widetilde{p} \\ C_B(\alpha,\beta,p)\,n^{-\beta-1}\ , & p \in (\widetilde{p},\infty) \end{cases}\ , \tag{32}$$

  *where $\widetilde{p} := \dfrac{-2+3D}{-4+3D}$, and*

- *For $p > 2$ and $D \leqslant 4/3$,*

$$N_n(D,p) = \tfrac{C_A(p)}{\pi^p}\,(4n)^{(\frac{1-2p}{3}+\beta)}(1+\bar{\bar{o}}(1))\,, \qquad p \in (2,\infty)\ . \tag{33}$$

*where the constants $C$, $C_A$ and $C_B$ are defined in (15), (14) and (13) respectively, and the parameters $\alpha \equiv \alpha(l,D)$ and $\beta \equiv \beta(p,D)$ are given by (12).*

*Comment*: Here we see, that the oscillatory regime in (31) for $p \in (0,2)$ matches the same regime in (27) and (28) for $p < p^*$. But for $p = 2$ the Airy-cosine regime wins versus Bessel-cosine regime and we have only contribution of (28) in $N_n(D,p)$. For $p \geq 2$ we get a new phenomena: the role of the oscillatory regime disappears and for the first time the Airy and Bessel regimes becomes competitive.

Here, the limits as $n \to \infty$ of the $\mathcal{L}_p$-norm is constant when $p = 1$, $\beta = -\frac{1-2p}{3}$ (i.e. when $p = 1 + \frac{2}{2-3D}$ or $D = \frac{2}{3}\frac{p-2}{p-1}$), and $\beta = -1$ (i.e. when $p = \frac{D}{D-2}$ or $D = \frac{2p}{p-1}$).

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## C. Proofs

For all three theorems we use the unified approach. We split the domain of integration $\mathbb{R}_+$ of (11) into nine intervals as

$$\begin{aligned} N_{n,l}(D,p) &= \frac{\int\limits_0^\infty ((L_n^{(\alpha)}(x))^2\, w(x))^p\, x^\beta\, dx}{\|L_n^{(\alpha)}\|^{2p}} \\ &= n^{-p\alpha}\left(\sum_{j=1}^{9} I_j\right), \end{aligned} \tag{34}$$

where

$$I_j := \int\limits_{\triangle_j} ((L_n^{(\alpha)}(x))^2\, w(x)^p\, x^\beta\, dx\ , \tag{35}$$

and

$$\begin{array}{lll} \Delta_1 = [0, M/n]\,; & \Delta_2 = [M/n, 1]\,; & \Delta_3 = [1, (4-\varepsilon)n]\,; \\ \Delta_4 = [(4-\varepsilon)n, 4n - n^{\frac{1}{3}+\theta}]\,; & & \Delta_5 = [4n - n^{\frac{1}{3}+\theta}, 4n - Mn^{\frac{1}{3}}]; \\ \Delta_6 = [4n - Mn^{\frac{1}{3}}, 4n]\,; & & \Delta_7 = [4n, 4n + Mn^{\frac{1}{3}}]\,; \\ \Delta_8 = [4n + Mn^{\frac{1}{3}}, 4n + n^{\frac{1}{3}+\theta}]\,; & & \Delta_9 = [4n + n^{\frac{1}{3}+\theta}, \infty]\,, \end{array} \tag{36}$$

for some big $M > 0$, small $\varepsilon > 0$ and $\theta > 0$. Then we replace $L_n^{(\alpha)}\, w$ in (35) by their asymptotics. For $j = 1$ we use Hilb asymptotics (18)-(19); for $j = 2$ we use Hilb asymptotics (18)-(19) and Bessel function asymptotics (21); for $j = 3, 4$ we use oscillatory asymptotics of Plancherel-Rotach (22); for $j = 5, 6, 7, 8$ we use Airy asymptotics of Plancherel-Rotach (24); and for $j = 9$ we use growing asymptotics of Plancherel-Rotach (23).

Eventually we estimate the contribution of each integral from $\{I_j\}_{j=1}^9$ finding the dominating terms.

## D. Proof of Theorem 1

Here we have $D > 2$ and $p^* = \frac{D}{D-1}$.

Let us start with the case $p > p^*$. Then in the representation (35)-(36) for $N_{n,l}(D,p)$ by the sum of integrals $\sum\limits_{j=1}^{9} I_j$, the main contribution for this case is given by $I_1$. We have

$$\begin{aligned} I_1 &= \int\limits_0^{M/n} (w^{1/2}(x)\, \widehat{L}_n^{(\alpha)}(x))^{2p}\, x^\beta\, dx \\ &= \int\limits_0^{M/n} \Bigg[ \left(\frac{(n+\alpha)!}{n!}\right)^2 (Nx)^{-\alpha} J_\alpha^2(2\sqrt{Nx}) \\ &\quad + O\left(x^{\alpha/2+2} n^\alpha\right)\Bigg]^p x^{p\,\alpha+\beta}\, dx. \end{aligned} \tag{37}$$

Making the change of the variable $t := \sqrt{Nx}$, we continue

$$\begin{aligned} I_1 &\simeq n^{2p\,\alpha} \cdot N^{-p\,\alpha-\beta-1} \int\limits_0^{\sqrt{\frac{MN}{n}}} 2t^{2p\,\alpha+2\beta+1} t^{-2p\,\alpha} |J_\alpha^{2p}|\,(2t)\, dt \simeq \\ &\simeq n^{p\,\alpha-\beta-1} \int\limits_0^{\sqrt{M}} 2t^{2\beta+1} |J_\alpha^{2p}|\,(2t)\, dt\ . \end{aligned} \tag{38}$$

The last integral converges at zero. Indeed, the integrand has there the order of singularity $2p\,\alpha + 2\beta + 1 > -1$ due to (12). The order of singularity of the integrand at infinity is $2\beta + 1 - p < -1$ due to $p > p^*$. Since the parameter $M$ is arbitrary in our partition of $\mathbb{R}_+$ in (36)), we take $M \to \infty$ and obtain

$$n^{-p\,\alpha} I_1 \simeq n^{-\beta-1} \int\limits_0^\infty 2t^{2\beta+1} |J_\alpha|^{2p}(2t)\, dt \, . \tag{39}$$

In fact, the contribution in $N_{n,l}$ of the remaining integrals $I_j$, $j = 2, \ldots, 9$ for $D > 2$, $p > p^*$ is less (we will see it latter). Thus, due to (12) and (13), asymptotics (39) is the same as in (27) for $p > p^*$.

Now, let us consider the case $p = p^*$. Then, the dominant behavior is coming from the two integrals $I_2$ and $I_3$. Indeed, we have from (38) that

$$n^{-p\,\alpha} I_1 = O\left(\frac{M^{p\,\alpha+\beta+1}}{n^{\beta+1}}\right) + \delta_n \, , \quad \delta_n = \frac{M^{p\,\alpha+\beta+3}}{n^{\beta+3}} \, . \tag{40}$$

We note that from (12) we have

$$\beta - \frac{p^*}{2} = (p^* - 1)\left(1 - \frac{D}{2}\right) - \frac{p^*}{2} = -1 \, . \tag{41}$$

Taking into account the asymptotics of the Bessel function (21), we have the following estimation or $I_2$:

$$\begin{aligned} n^{-p\,\alpha} I_2 \;&=\; \int\limits_{M/n}^{1} J_\alpha^{2p}(2\sqrt{Nx})\, x^\beta \, dx + \tilde{\delta}_n \\ &=\; \int\limits_{M/n}^{1} \frac{1}{\pi^p (Nx)^{p/2}} \Bigg\{ \cos\left(2\sqrt{Nx} - (2\alpha+1)\cdot\frac{\pi}{4}\right) \\ &\qquad + \underline{\underline{O}}\left(\frac{1}{\sqrt{N}}\right) \Bigg\}^{2p} x^\beta \, dx + \tilde{\delta}_n \, . \end{aligned} \tag{42}$$

Using ([67], Lemma 2.1) we can continue for $n \to \infty$ as

$$n^{-p\,\alpha} I_2 = \frac{1}{\pi} \int\limits_0^\pi |\cos\theta|^{2p}\, d\theta \int\limits_{M/n}^{1} \frac{x^{-p/2+\beta}\, dx}{\pi^p\, N^{p/2}} \,(1 + \bar{\bar{o}}(1)) \, .$$

The first integral is

$$\int\limits_0^\pi |\cos\theta|^{2p}\, d\theta = \frac{\sqrt{\pi}\,\Gamma(p+1/2)}{\Gamma(p+1)} \, .$$

Computing the second integral for $p = p^*$ (see (41)), we obtain

$$n^{-p^*\alpha} I_2 = \frac{\Gamma(p^*+1/2)\,(\ln n + \underline{\underline{O}}(1))}{\pi^{p^*+1/2}\,\Gamma(p^*+1)\, N^{p/2}} \, . \tag{43}$$

The Plancherel-Rotach asymptotics (22) for $\varphi = \arccos\sqrt{\frac{x}{4N}}$ can be transformed to

$$\tfrac{x^\alpha}{n^\alpha}\left(e^{x/2} L_n^\alpha(x)\right)^2 = \frac{2\sin^2\left[\frac{1}{2}\sqrt{x(4N-x)} - 2N \arccos\sqrt{\frac{x}{4N}} + \frac{3\pi}{4}\right] + O\left(\frac{1}{\sqrt{nx}}\right)}{\pi\sqrt{x(4N-x)}} \, . \tag{44}$$

Substituting it in $I_3$ and using ([67], Lemma 2.1) we have for $I_3$, as $n \to \infty$

$$n^{-p^*\alpha} I_3 = \int\limits_1^{(4-\varepsilon)n} \frac{x^{\alpha p^*}}{n^{\alpha p^*}} \left(e^{x/2} L_n^{(\alpha)}(x)\right)^{2p^*} x^\beta dx =$$

$$= \left(\frac{2}{\pi\sqrt{4n}}\right)^{p^*} \frac{1}{\pi}\int\limits_0^{\pi} |\sin\theta|^{2p^*} d\theta \cdot \int\limits_1^{(4-\varepsilon)n} x^{\beta - p^*/2} dx \, .$$

Thus, $I_3$ gives the same contribution in $N_{n,l}(D, p^*$ as $I_2$ in (43)

$$n^{-p^*\alpha} I_3 = \frac{\Gamma(p^* + 1/2)\,(\ln n + \underline{\underline{O}}(1))}{\pi^{p^*+1/2}\,\Gamma(p^*+1)\,N^{p/2}} \, . \tag{45}$$

We see from (40) that for $p = p^*$ the contribution from $I_1$ in $N_{n,l}(D, p^*)$ is less than that from $I_2$ and $I_3$. The same can be shown for the contribution of other integrals. Thus, summing up (43) and (45) we arrive at (27) for $p = p^*$.

It remains to consider the case $p \in (0, p^*)$. The dominant contribution here is given by $I_3$. Substituting asymptotics (44) in $I_3$, making the change of variable $t := \sqrt{\frac{x}{4n}}$ and using ([67], Lemma 2.1) we arrive to

$$N^{-p\,\alpha} I_3 = \left(\tfrac{2}{\pi 4n}\right)^p \, (2\sqrt{n})^{2\beta+2} \, \tfrac{1}{\pi} \int\limits_0^{\pi} |\sin\theta|^{2p} d\theta \cdot \int\limits_0^1 \tfrac{t^{2\beta+1}\,dt}{t^p(1-t^2)^{p/2}} \, (1 + \bar{\bar{o}}(1)) \, .$$

The last integral can be evaluated explicitly as

$$\int\limits_0^1 \frac{t^{2\beta+1}\,dt}{t^p(1-t^2)^{p/2}} = \frac{1}{2}\,\frac{\Gamma(\beta+1-p/2)\,\Gamma(1-p/2)}{\Gamma(\beta+2-p)} \, .$$

Thus, we obtain

$$n^{-p^*\alpha} I_3 = \tfrac{2^{\beta+1}}{\pi^{p+1}} \, \tfrac{\Gamma(\beta+1-p/2)\,\Gamma(1-p/2)\,\Gamma(1+p/2)}{\Gamma(\beta+2-p)\,\Gamma(1+p)} \, (2n)^{1-p+\beta} \, (1 + \bar{\bar{o}}(1)) \, . \tag{46}$$

It is clear that the contributions of $I_1$ and $I_2$ are less than $I_3$. The same can be shown for the contribution of other integrals. Theorem is proved.

### E. Proof of Theorem 2

Here we have $D = 2$. Then, $\beta \equiv 0$ and $p^* = 2$.

Let us start with the case $p > 2$. As for the case ($D > 2$, $p > p^*$), according to (35) – (36) we can see that the dominant contribution in $N_{n,l}(D, p)$ is given by $I_1$. Indeed, we have

$$\int\limits_0^{M/n} \left(w^{1/2}(x)\,\widehat{L}_n^{(\alpha)}(x)\right)^{2p} dx =$$

$$= \int\limits_0^{M/n} \left[\frac{n!}{(n+\alpha)!}\left(\frac{(n+\alpha)!}{n!}\right)^2 (Nx)^{-\alpha} J_\alpha^2(2\sqrt{Nx}) + x^{\alpha+4} O(n^\alpha)\right]^p x^{p\,\alpha}\,dx$$

$$= \frac{1}{n}\left(\int\limits_0^{\sqrt{M}} 2t\,|J_\alpha|^{2p}(2t)\,dt + \bar{\bar{o}}(1)\right) \, .$$

Since $M$ is an arbitrary constant, we let $M \to \infty$. At the same time, we see that the sum $J_6 + J_7$ also gives a perceptible contribution

$$\int\limits_{4N-Mn^{1/3}}^{4N+Mn^{1/3}} \left(w^{1/2}(x)\,\widehat{L}_n^{(\alpha)}(x)\right)^{2p} dx = \int\limits_{-M}^{M} \left[(2n)^{-2/3} A_i^2\left(-\tfrac{t}{2^{4/3}}\right)\right]^p n^{1/3}\,dt\,(1 + \bar{\bar{o}}(1) \, . \tag{47}$$

However, for $p > 2$

$$1/3 - p\,2/3 < -1 \, . \tag{48}$$

Thus the only contribution of $I_1$ plays the role, and we obtain (28) for $p > 2$.

Let us now consider the case $p = 2$. In comparison with the case ($D > 2$, $p = p^*$), not only the transition zone for the Bessel-cosine regimes (i.e. integrals $I_2$ and $I_3$) plays the role, but the transition zone for the cosine-Airy regimes (i.e. integrals $I_4$ and $I_5$) plays the role too.

For $I_2$ and $I_3$, substituting $p^* = 2$ in (43) and (45), we get

$$n^{-2\alpha}(I_2 + I_3) = \frac{3\ln n + \underline{\underline{O}}(1)}{4\pi^2 n} \,. \tag{49}$$

The second transition zone is $\left[(4-\varepsilon)n, 4n - n^{1/3+\theta}\right] \cup \left[4n - n^{1/3+\theta}, 4n - M \cdot n^{1/3}\right]$. For the oscillatory Plancherel-Rotach asymptotics (22) we have

$$\begin{aligned} &\int\limits_{(4-\varepsilon)N}^{4N-n^{1/3+\theta}} \left[\frac{2\sin^2\left(\frac{1}{2}\sqrt{x(4N-x)} - 2N\arccos\sqrt{\frac{x}{4N}} + \frac{3\pi}{4}\right) + O\left(\frac{1}{\sqrt{Nx}}\right)}{\pi\sqrt{x(4N-x)}}\right]^2 dx = \\ &= \frac{1}{\pi}\int\limits_0^{\pi} \sin^4\varphi \, d\varphi \cdot \int\limits_{4N}^{4N-n^{1/3+\theta}} \frac{4\,dx}{\pi x(4N-x)} = \frac{3}{8\pi^2 n}\left(\left(\tfrac{2}{3} - \theta\right)\ln n + \underline{\underline{O}}(1)\right) \,. \end{aligned} \tag{50}$$

For $I_5$ using (24) and asymptotics for the Airy function (see in [63])

$$A_i^4\left(-\frac{t}{2^{4/3}}\right) \simeq \frac{(1+\sin(t^{3/2}/3))^2}{4\pi^2(t/2^{4/3})} \,, \quad t \to \infty \,,$$

we obtain

$$\begin{aligned} &\int\limits_{4N-n^{(1/3+\theta)}}^{4n-Mn^{1/3}} (w^{1/2}(x)\widehat{L}_n^{(\alpha)}(x))^2 dx \simeq \int\limits_M^{n^\theta} \left[(2n)^{-2/3} A_i^2\left(-\tfrac{t}{2^{4/3}}\right)\right]^2 n^{1/3} dt \simeq \\ &\simeq \frac{1}{4\pi^2 n}\int\limits_0^{\pi}(1+\sin\varphi)^2 d\varphi \int\limits_M^{n^\theta} \frac{dt}{t} = \frac{3(\theta\ln n + \underline{\underline{O}}(1))}{8\pi^2 n} \,. \end{aligned} \tag{51}$$

Summing (50), (51) and (49), we obtain (28) for $p = 2$.

The remaining case is $p < 2$. Here we proceed in the same manner as for the case ($D > 2$, $p < p^*$), and we obtain (46) for $\beta = 0$. Theorem is proved.

### F. Proof of Theorem 3

Here we have $D \in [0, 2)$, $\beta > 0$ for $p > 1$; therefore $p^* = 2$, as in the previous case.

Let us start with the case $p > 2$. Now the competition between $I_1$ and $I_6 + I_7$ becomes crucial. We already know for $I_1$ from (39) that

$$n^{-p\,\alpha} I_1 = C_B n^{-\beta-1} \,.$$

To obtain the asymptotics for $n^{-p\,\alpha}(I_6 + I_7)$ we substitute $x^\beta$ in the left-hand side of (47)

$$\int\limits_{4n-Mn^{1/3}}^{4n+Mn^{1/3}} (w^{1/2}(x)\widehat{L}_n^{(\alpha)}(x))^{2p} x^\beta dx \simeq 2^{2\beta} n^{\frac{1-2p}{3}+\beta} C_A \,.$$

Now, instead of inequality (48) we have for $D > 4/3$ the solution $p = \tilde{p}$ of the equation (where $\beta$ is from (12))

$$-\beta - 1 = 1 - \frac{2p}{3} + \beta \Rightarrow \tilde{p} = \frac{-2+3D}{-4+3D} \,.$$

Thus, we have obtained (33) and (32).

Now let us consider that $p = 2$. In comparison with the previous cases, we have that the only contribution which plays a role is coming from the transition zone for the cosine-Airy regimes. Substituting $x^\beta$ in the left-hand sides of (50) and (51) we arrive at (31), $p = 2$.

Finally for $p \in (0, 2)$, we have

$$1 + \beta - p > -\beta - 1 \ ,$$

and

$$1 + \beta - p > \frac{1 - 2p}{3} + \beta \ .$$

Thus, only the oscillatory integral $I_3$ gives the contribution to the asymptotics of $N_{n,l}(D, p)$, and from (46) we complete proof of (31).

Theorem is proved.

## III. RÉNYI ENTROPY POWERS FOR RYDBERG $D$-DIMENSIONAL OSCILLATOR STATES

In this section the asymptotical results obtained in the previous section are applied to obtain the Rényi entropies (or better, the Rényi entropy powers, which have position physical units) of the Rydberg states of the multidimensional harmonic oscillator. The Rényi entropy powers, $\mathcal{N}_p[\rho]$, of the density $\rho$ is given by

$$\mathcal{N}_p[\rho] := e^{R_p[\rho]} = \left( \int \rho(x)^p \, dx \right)^{\frac{1}{1-p}}. \tag{52}$$

Taking into account Eqs. (2), (8), (9) and (11), we obtain the following expressions

$$\begin{aligned} R_p[\rho] &= \frac{1}{1-p} \ln \left[ 2^{p-1} \lambda^{\frac{D}{2}(p-1)} N_{n,l}(D,p) \right], \\ \mathcal{N}_p[\rho] &= \frac{1}{2} \lambda^{-\frac{D}{2}} \left[ N_{n,l}(D,p) \right]^{\frac{1}{1-p}} \end{aligned} \tag{53}$$

for the Rényi entropies and the Rényi entropy powers, respectively, of an arbitrary quantum state of the $D$-dimensional isotropic harmonic oscillator in terms of the $\mathcal{L}_p$-norms $N_{n,l}(D,p)$ of the orthonormal Laguerrre polynomials associated to the state wavefunction given by the three previous theorems. The involved parameters within the norms, $\alpha \equiv \alpha(l,D) = l + \frac{D}{2} - 1 \, (l = 0, 1, 2, \ldots)$ and $\beta \equiv \beta(p,D) = (p-1)(1-D/2)$, are taking from (12). Note that these information-theoretic quantities depend on the spatial dimension $D$ as well as on the order parameter $p$ for each pair $(n,l)$. In the numerical calculations performed heretoforth we will assume that $\lambda = 1$ without any loose of generality. Atomic units are used everywhere as already pointed out.

Let us now discuss these two Rényi-type quantities with $D \geq 2$ and $q \neq 1$ from Eqs. (53) in various ways. The Rényi entropies for the Rydberg states of the one-dimensional isotropic harmonic oscillator have been recently studied [68] in a monographic way, because the polynomials involved in this case are of Hermite type. The limiting case $p \to 1$ (Shannon entropy) will be analyzed separately elsewhere for any $D$-dimensional oscillator system.

First, in Figure 1 we study the variation of the Rényi entropy power, $\mathcal{N}_p[\rho]$, with respect to the order $p$ for the Rydberg oscillator state ($n = 50, l = 0$) with $D = 2(\blacksquare)$ and $D = 4(\odot)$. We observe that in both cases, the Rényi entropy power decreases monotonically as the order $p$ is increasing; in fact, this behavior holds for any dimensionality $D > 1$. Moreover it is very fast, indicating that the quantities with lowest orders (particularly the case $p = 2$, closely related with the disequilibrium) are most significant for the quantification of the spreading of the electron distribution of the system.

Second, we explore the dependence of the pth-order Rényi quantities of the Rydberg-state region in terms of the principal hyperquantum number $n$ when $(l,p,D)$ are fixed. To exemplify it, we will examine the case $p = 2$ for the Rydberg $(n, l = 0) \equiv (ns)$-states of the three-dimensional oscillator. From (8), (9), (11), (53) and Theorem 1, one has that for $p = 2$ and $D = 3$, the second-order Rényi entropy and the disequilibrium (the inverse of the Rényi entropy power) of the Rydberg state $(n,l)$ are given by

$$\begin{aligned} R_2[\rho] &= -\ln \left[ 2\lambda^{\frac{3}{2}} C_B \left( l + \frac{1}{2}, -\frac{1}{2}, 2 \right) n^{-\frac{1}{2}} \right] (1 + \bar{o}(1)), \\ \mathcal{D}[\rho] &= W_2[\rho] = \mathcal{N}_2[\rho]^{-1} \\ &= \left[ 2\lambda^{\frac{3}{2}} C_B \left( l + \frac{1}{2}, -\frac{1}{2}, 2 \right) n^{-\frac{1}{2}} \right] (1 + \bar{o}(1)) \end{aligned} \tag{54}$$

since the disequilibrium (or average density of the distribution $\rho$) is defined as $\mathcal{D}[\rho] := \int \rho(x)^2 \, dx$. Moreover, for the $(ns)$-states the $C_B$-constant given in (13) can be explicitly calculated, so that the second-order Rényi entropy and the disequilibrium of the Rydberg $(ns)$-states of the three-dimensional harmonic oscillator has the following behavior

$$\begin{aligned} R_2[\rho] &= \left[ -\ln \left( \frac{2\lambda^{\frac{3}{2}}}{\pi} \right) + \frac{1}{2} \ln n \right] (1 + \bar{o}(1)), \\ \mathcal{D}[\rho] &= \left[ \frac{2\lambda^{\frac{3}{2}}}{\pi} n^{-\frac{1}{2}} \right] (1 + \bar{o}(1)), \end{aligned} \tag{55}$$

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respectively. The case ($l = 0, p = 2, D = 2$) as well as the case ($l = 0, p = 2, D = 6$) are plotted in Figures 2-3, which gives the variation of the disequilibrium, $\mathcal{D}[\rho]$, with respect to $n$ for the Rydberg oscillator ($ns$)-states of the two- and six-dimensional harmonic oscillator, respectively. We observe that the behavior with respect to $n$ for the disequilibrium of these states has a decreasing (increasing) character in the two (six)-dimensional oscillator. On the other hand, one can realize from (53) and Theorem 1 (see the last lines of the comments to this theorem) that the disequilibrium for the case ($l = 0, p = 2, D = 4$) has the constant value 0.4053. So that, most interesting, we find the following phenomenon: the disequilibrium of the Rydberg ($ns$)-states of $D$-dimensional oscillator decreases (increases) as a function of the principal hyperquantum number $n$ when the dimensionlity $D$ is less (bigger) than 4, and it becomes constant when $D = 4$. In fact we should not be surprised that the disequilibrium as a function of $n$ changes when the spatial dimensionality is varying. This also happens for all physical properties of a quantum system at different spatial dimensionalities, since the physical solutions of their corresponding wave equations (e.g., Schrödinger) are so different (see e.g., [56]). The novelty is that the character of the disequilibrium behavior as a function of $n$ changes so much, pointing out the existence of a critical dimensionality at which it is constant.

In Figure 4, we illustrate the variation of the disequilibrium, $\mathcal{D}[\rho]$, as a function of $l$ for the Rydberg states ($n = 50, l$) of the four-dimensional harmonic oscillator. We observe that its behavior is monotonically decreasing when $l$ is increasing. In fact this property holds for $D \geq 2$. Then, it is interesting to point out that the electron distribution of the $D$-dimensional oscillator, within the region of the Rydberg $s$-states, becomes closer to equiprobability when $l$ is increasing, approaching what one would expect classically. Moreover, this trend is slightly moderated for Rydberg states other than $s$-states.

Third, finally, let us illustrate the behavior of the Rényi entropy power, $\mathcal{N}_p[\rho]$, of the Rydberg oscillator states as a function of the dimensionality $D$. We do that in Figure 5 for the disequilibrium $\mathcal{D}[\rho] = \mathcal{N}_2[\rho]^{-1}$ of the Rydberg state ($l = 0, p = 2, n = 50$) of the oscillator with various integer values of the dimensionality $D$. We observe that the disequilibrium has a *quasi-Gaussian* form when $D$ is increasing, so that finally it vanishes for a given, sufficiently large value of $D$. Most interesting is that the maximum of the Rényi entropy power is located at $D = 12$, which surprisingly corresponds to the universe dimensionality predicted by certain string theories [69]. Nevertheless, we should point out that for higher Rydberg states the maximum of the disequilibrium is located at larger dimensionalities. This indicates that the nearer the classical limit is, the larger is the dimensionality required for the disequilibrium (i.e., separation from equiprobability) to reach its maximum.

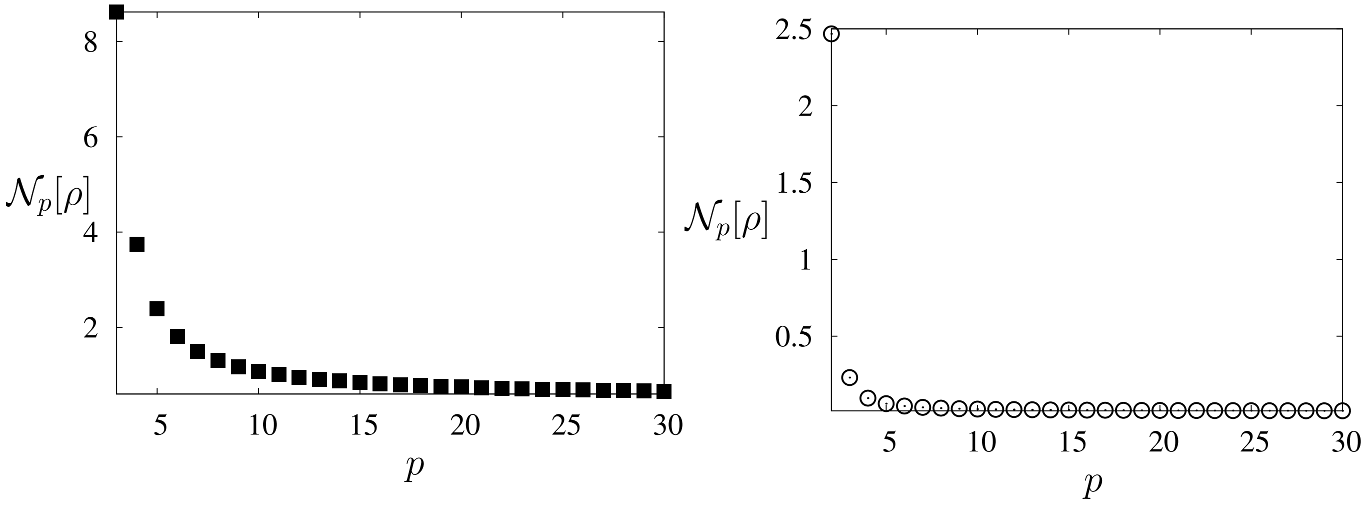

Fig. 1: Variation of the Rényi entropy power, $\mathcal{N}_p[\rho]$, with respect to $p$ for the Rydberg oscillator state ($n = 50$, $l = 0$) of the $D$-dimensional harmonic oscillator with $D = 2$(■) and $D = 4$(⊙).

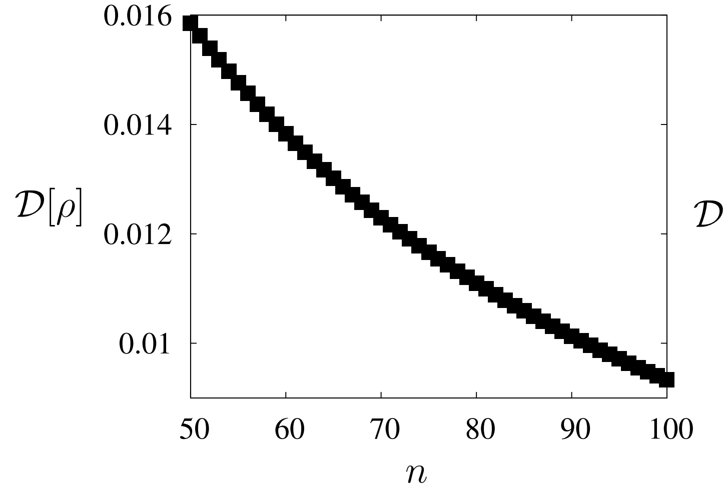

Fig. 2: Variation of the disequilibrium $\mathcal{D}[\rho]$ with respect to $n$ for the Rydberg oscillator $(ns)$-states of a two-dimensional harmonic oscillator. So, this is the case ($l = 0$, $p = 2$, $D = 2$).

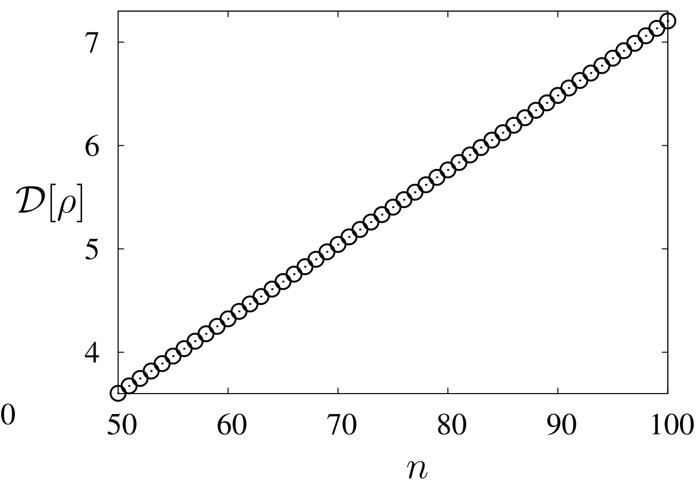

Fig. 3: Variation of disequilibrium $\mathcal{D}[\rho]$ with respect to $n$ for the Rydberg oscillator $(ns)$-states of a six-dimensional harmonic oscillator. So, this is the case ($p = 2$, $l = 0$, $D = 6$).

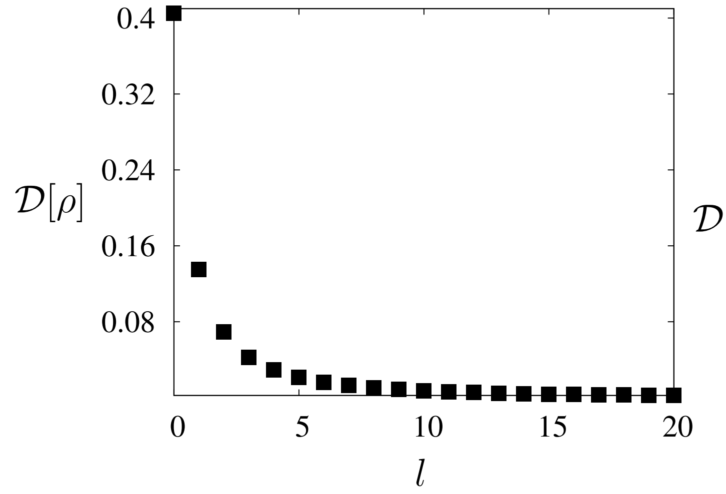

Fig. 4: Variation of the disequilibrium $\mathcal{D}[\rho]$ with respect to $l$ for the Rydberg oscillator state with $n = 50$ of the four-dimensional harmonic oscillator . So, this is the case ($p = 2$, $n = 50$, $D = 4$).

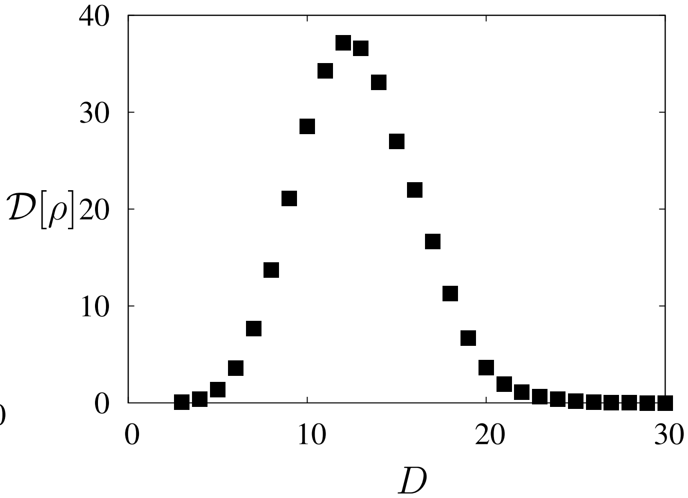

Fig. 5: Variation of the disequilibrium $\mathcal{D}[\rho]$ with respect to the dimensionality $D$ for the Rydberg oscillator state ($n = 50$, $l = 0$) of the $D$-dimensional harmonic oscillator . So, this is the case ($p = 2$, $n = 50$, $l = 0$).

## IV. CONCLUSIONS

The macroscopic properties of a quantum many-particle system essentially depend on the spreading of its quantum-mechanical Born one-particle distribution $\rho(\vec{r})$, as proved by the functional-density theory. This spreading can be completetely described by the knowledge of the moments $W_p[\rho]$ of $\rho(\vec{r})$ or by some closely related information-theoretic quantities, the Rényi entropies $R_p[\rho]$, which often describe some fundamental properties of the system and/or are experimentally observable. These quantities, however, cannot be analytically accessible, even not for the simplest harmonic systems unless we consider the ground state and the first few lowest-lying excited states. In 2012 the Shannon entropy, which corresponds to the limiting case $p \to 1$ of the Rényi entropy, was determined for the highest-lying (Rydberg) states of the one-dimensional harmonic oscillator [68] whose wavefunctions are controlled by

Hermite polynomials.

In this paper we extend this result in a two-fold way: we determine in an analytical way the Rényi entropies of all orders for the Rydberg states of a $D$-dimensional harmonic oscillator, whose wavefunctions are known to be controlled by Laguerre polynomials. To do that we first realize that the Rényi entropies can be explicitly expressed in terms of the $\mathcal{L}_p$-norms of the Laguerre polynomials, and then we develop a method to analytically calculate the leading term of the asymptotics of these norms when the polynomial degree is very high.

Later, a number of physical results are found. First, for a given Rydberg state the Rényi entropy has a very fast decreasing behavior as the parameter order is increasing, indicating that the Rényi entropies with lowest orders are most significant. Then, for illustration, we study in detail the second-order Rényi entropy (i.e., the disequilibrium) of the system, which quantifies the separation of the electron distribution from equiprobability. It is found that it has a bell-like quasi-Gaussian behavior in terms of $D$, its maximum being located at $D = 12$ which is the universe dimensionality predicted by certain string theories [69]. Let us here comment that geometrical quantities associated with $D$-dimensional hyperspheres (such as surface area) also exhibit this kind of behavior (with the corresponding bell-like function centered around a different $D$-value). This suggests that the behavior of the disequilibrium may have a geometrical origin in terms of basic properties of hyperspheres. Moreover, the disequilibrium of the Rydberg $(ns)$-states of $D$-dimensional oscillator decreases (increases) as a function of the principal hyperquantum number $n$ when the dimensionlity $D$ is less (bigger) than 4, and it becomes constant when $D = 4$. Needless to say that much more efforts have to be done before making exotic statements.

Finally, these results are potentially useful in the study of entropic uncertainty relations. Moreover, they might also be relevant in connection with quantitative entanglement indicators. Rényi entropies have been recently used for this purpose (see e.g., [70]). We believe that the analytical technology here developed could be useful in relation to entanglement-like studies in quantum information.

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## 3.9 Rényi, Shannon and Tsallis entropies of Rydberg hydrogenic systems

In this section we calculate in an explicit way the dominant term of the Rényi, Shannon and Tsallis entropies for all quantum-mechanically allowed Rydberg (i.e., highly excited) hydrogenic states in position space in terms of the nuclear charge $Z$ and the quantum numbers which characterize the corresponding state's wavefunctions. Moreover, note that:

- We have used a novel technique based on some ideas extracted from the modern approximation theory, which allows us to determine the asymptotics ($n \to \infty$) of the $\mathcal{L}_p$-norm, $N_{n,l}(p)$, of the Laguerre polynomials which control the associated wavefunctions,
- we have studied the behavior of the Rényi entropy for the Rydberg ($ns$)-states at various values of the involved parameters ($n, p, Z$), and
- we have found that this quantity (a) decreases as a function of $p$, indicating that the most relevant Rényi quantities of integer order are those associated with the Shannon entropy and the disequilibrium, (b) has an increasing character for all Rydberg values of $n$ as the parameter $p$ is increasing, which can be explained by the fact that the system tends to the classical regime as $n$ increases, and (c) decreases for all $p$'s as the nuclear charge is increasing when $n$ is fixed due to the fact that the probability distribution of the system tends to separate from equiprobability more and more as the electron number of the atom increases.

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# Rényi, Shannon and Tsallis entropies of Rydberg hydrogenic systems

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The Rényi entropies $R_p[\rho], 0 < p < \infty$ of the probability density $\rho_{n,l,m}(\vec{r})$ of a physical system completely characterize the chemical and physical properties of the quantum state described by the three integer quantum numbers $(n, l, m)$. The analytical determination of these quantities is practically impossible up until now, even for the very few systems where their Schrödinger equation is exactly solved. In this work, the Rényi entropies of Rydberg (highly-excited) hydrogenic states are explicitly calculated in terms of the quantum numbers and the parameter $p$. To do that we use a methodology which first connects these quantities to the $\mathcal{L}_p$-norms $N_{n,l}(p)$ of the Laguerre polynomials which characterize the state's wavefunction. Then, the Rényi, Shannon and Tsallis entropies of the Rydberg states are determined by calculating the asymptotics $(n \to \infty)$ of these Laguerre norms. Finally, these quantities are numerically examined in terms of the quantum numbers and the nuclear charge.

## I. INTRODUCTION

Recent years have witnessed a growing interest in the analytical information theory of finite quantum systems. A major goal of this theory is the explicit determination of the entropic measures (Fisher information and Shannon, Rényi and Tsallis entropies,...) in terms of the quantum numbers which characterize the state's wavefunction of the system. These quantities, which quantify the spatial delocalization of the single-particle density of the systems in various complementary ways, are most appropriate uncertainty measures because they do not make any reference to some specific point of the corresponding Hilbert space, in contrast to the variance and other dispersion measures. Moreover, they are closely related to numerous energetic and experimentally measurable quantities of the system [1–8] and they have been used as indicators of various atomic and molecular phenomena [10–15]. Since the Schrödinger equation can be exactly solved only for a few quatum-mechanical potentials which model most of the quantum chemical and physical phenomena, most of the efforts have been focused on the harmonic and hydrogenic systems up until now. Basically this is because the wavefunctions of their ground and excited states are controlled by the hypergeometric orthogonal polynomials (Hermite, Laguerre, Jacobi) whose analytical properties are under control.

Apart from the Fisher information whose explicit values have been found [16, 17], the entropic measures of the oscillator-like and hydrogenic systems have not yet been analytically determined for all quantum-mechanically-allowed states except for the ground and a few low-lying states [18–23] and for the high-lying states in the Shannon case (see Eq. (16) in [22]). In addition some rigorous bounds on these entropic measures, as well as some related uncertainty relations, have been found [24–27].

The Rényi entropies $R_p[\rho]$ and Tsallis entropies $T_p[\rho]$ of a probability density $\rho(\vec{r})$ are defined [40, 42] as

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

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

where $W_p[\rho]$ denotes the $p$-th entropic moment of $\rho(\vec{r})$ which is given by

$$W_p[\rho] = \int_{\mathbb{R}^3} [\rho(\vec{r})]^p \, d\vec{r}, \quad p \geq 0, \tag{3}$$

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These quantities completely characterize the density $\rho(\vec{r})$ [43, 44]. Note that these quantities include the Shannon entropy (since $S[\rho] := \int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r} = \lim_{p\to 1} R_p[\rho] = \lim_{p\to 1} T_p[\rho]$), and the disequilibrium, $\langle \rho \rangle = \exp(R_2[\rho])$, as two important particular cases. Moreover, they are mutually connected by the relation

$$T_p[\rho] \;=\; \frac{1}{1-p}[e^{(1-p)R_p[\rho]} - 1], \tag{4}$$

For a revision of the Rényi entropies properties see [25, 27, 36, 41, 43, 45] and the reviews [8, 9, 27]. 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 [8, 9, 38], ranging from the quantum-classical correspondence [24] and quantum entanglement [46] to pattern formation and Brown processes [47, 48], quantum phase transition [13], disordered systems [49] and multifractal thermodynamics [50]. Moreover, there exist various classical and quantum coding theorems [51, 52] which endow the Rényi and Tsallis entropies with an operational (so, experimentally verifiable) meaning.

In this work we analytically determine the Shannon, Rényi and Tsallis entropies of the highly-excited (Rydberg) hydrogenic states on the same footing, by use of a methodology based on the strong asymptotics of Laguerre polynomials. The Rydberg states [29, 30] play a relevant role from both fundamental and applicable points of view. Indeed they can be considered a fertile laboratory where to investigate the order-to-chaos transitions through the applications of electric fields and, because of their extraordinary properties, they are being presently used in many technological areas such as e.g. quantum information processing [31, 32]. The entropic moments and their associated Shannon, Rényi and Tsallis entropies quantify the internal disorder of the Rydberg atom as given by its quantum probability density in a complementary, but much more complete, way than the variance and other dispersion measures whose values have been already shown [21, 22].

The structure of this work is the following. First, in sec. II, we state the problem and the methodology to solve it. In section III we obtain the radial Rényi entropy $R_p[\rho_{n,l}]$ of the Rydberg hydrogenic states for all possible values of the involved parameters in an analytical way. Then in section IV, we obtain the final results of the Rényi, Tsallis and Shannon entropies for the Rydberg hydrogenic states and, in addition, we numerically compute the Rényi entropies for some specific Rydberg states and its variation with the nuclear charge of the atom. In section V, some conclusions are given.

## II. STATEMENT OF THE PROBLEM

Let us now determine the Rényi entropies of the Rydberg hydrogenic states characterized by the Coulombian potential $V_D(r) = -\frac{Z}{r}$. It is well-known that these states are given (see e.g., [22] and references therein) by the wavefunctions characterized by the energies $E_{n,l} = -\frac{Z^2}{2n^2}$ and the quantum probability densities

$$\rho_{n,l,m}(\vec{r}) = \frac{4Z^3}{n^4}\frac{\omega_{2l+1}(\tilde{r})}{\tilde{r}}[\widehat{L}_{n-l-1}^{(2l+1)}(\tilde{r})]^2\;|Y_{l,m}(\theta,\phi)|^2 \equiv \rho_{n,l}(\tilde{r})\,|Y_{l,m}(\theta,\phi)|^2, \tag{5}$$

where $\tilde{r} = \frac{2Z}{n}r$, $n = 1, 2, 3, \ldots$, $l = 0, 1, \ldots, n-1$, $m = -l, -l+1, \ldots, +l$, $\widehat{L}_n^{\alpha}(x)$ denotes the orthonormal Laguerre polynomials [53] with respect to the weight function $\omega_\alpha = x^\alpha e^{-x}$ on the interval $[0, \infty)$, and $Y_{l,m}(\theta, \phi)$ denotes the spherical harmonics [53] given by

$$Y_{l,m}(\theta,\phi) = \left(\frac{(l+\frac{1}{2})(l-|m|)![\Gamma(|m|+\frac{1}{2})]^2}{2^{1-2|m|}\pi^2(l+|m|)!}\right)^{\frac{1}{2}} e^{im\phi}(\sin\theta)^{|m|}C_{l-|m|}^{|m|+\frac{1}{2}}(\cos\theta). \tag{6}$$

Then, by keeping in mind Eqs. (2)-(3), the entropic moments of the hydrogenic state $(n, l, m)$ are

$$W_p[\rho_{n,l,m}] = \int_{\mathbb{R}^3}[\rho_{n,l,m}(\vec{r})]^p\,d\,\vec{r} = \int_0^\infty [\rho_{n,l}(r)]^p\,r^2\,dr \times \Omega_{l,m}(\theta,\phi), \tag{7}$$

where the angular part

$$\Omega_{l,m}(\theta,\phi) = \int_0^\pi\int_0^{2\pi}[Y_{l,m}(\theta,\phi)]^{2p}\sin\theta\,d\theta d\phi, \tag{8}$$

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and the Rényi entropies of the hydrogenic state $(n, l, m)$ can be expressed as

$$R_p[\rho_{n,l,m}] = R_p[\rho_{n,l}] + R_p[Y_{l,m}], \tag{9}$$

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

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \int_0^\infty [\rho_{n,l}(r)]^p \, r^2 dr, \tag{10}$$

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

$$R_p[Y_{l,m}] = \frac{1}{1-p} \ln \Omega_{l,m}(\theta, \phi), \tag{11}$$

which is the Rényi-entropic functional of the well-controlled spherical harmonics [53]. Since the radial part is the only component which depends on the principal quantum number $n$, the crucial problem for the calculation of the Rényi entropy $R_p[\rho_{n,l,m}]$ for the Rydberg states (i.e., states with a very large $n$) of hydrogenic systems is to determine the value of the radial Rényi entropy $R_p[\rho_{n,l}]$ in the limiting case $n \to \infty$. Taking into account (10), the explicit expression of $\rho_{n,l}(\tilde{r})$ given by (5), and that the $\mathcal{L}_p$-norm of the Laguerre polynomials $\widehat{L}_n^{(\alpha)}(x)$ is

$$N_n(\alpha, p, \beta) = \int_0^\infty \left( \left[ \widehat{L}_n^{(\alpha)}(x) \right]^2 w_\alpha(x) \right)^p x^\beta \, dx, \tag{12}$$

(with $\alpha > -1, p > 0$ and, to guarantee convergence at zero, $\beta + p\alpha > -1$), one has that the radial Rényi entropy can be expressed as

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \left[ \frac{n^{3-4p}}{2^{3-2p} Z^{3(1-p)}} N_{n,l}(\alpha, p, \beta) \right], \tag{13}$$

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

$$N_{n,l}(\alpha, p, \beta) = \int_0^\infty \left( \left[ \widehat{L}_{n-l-1}^{(\alpha)}(x) \right]^2 w_\alpha(x) \right)^p x^\beta \, dx, \tag{14}$$

with

$$\alpha = 2l + 1\,, \; l = 0, 1, 2, \ldots, n-1, \quad p > 0 \quad \text{and} \quad \beta = 2 - p\,. \tag{15}$$

Note that (15) guarantees the convergence of integral (14) since the condition $\beta + p\alpha = 2(1 + lp) > -1$ is always satisfied for the physically meaningful values of the parameters.

Thus, by keeping in mind Eqs. (9), (10), (11) and (13), the determination of the Rényi entropy $R_p[\rho_{n,l,m}]$ for the Rydberg states entails the calculation of the asymptotics $(n \to \infty)$ of the Laguerre norms $N_{n,l}(\alpha, p, \beta)$ given by Eqs. (14) and (15), which will be solved in the next section.

## III. RADIAL RÉNYI ENTROPY $R_p[\rho_{n,l}]$ OF RYDBERG STATES

Let us here determine the radial entropy of the Rydberg hydrogenic states, i.e. the asymptotics $(n \to \infty)$ of the radial Rényi entropy $R_p[\rho_{n,l}]$ which, according to Eq. (13), essentially reduces to the asymptotics $(n \to \infty)$ of the Laguerre norms $N_{n,l}(\alpha, p, \beta)$ given by (14) and (15).

To do that we use the method of Aptekarev et al which has been recently applied to oscillator-like systems [54]. This method allows us to find the asymptotics of the Laguerre functionals $N_n(\alpha, p, \beta)$ given by (12) with $\alpha > -1, p > 0$ and $\beta + p\alpha > -1$. It shows that the dominant contribution in the magnitude of the integral (12) comes from different regions of integration in (12); these regions depend on the different values of the involved parameters $(\alpha, p, \beta)$. This entails that we have to use various asymptotical representations for the Laguerre polynomials at different regions of the interval of orthogonality $(0, \infty)$.

Altogether there are five asymptotical regimes which can give (depending on $\alpha, \beta$ and $p$) the dominant contribution in the asymptotics of $N_n(\alpha, p, \beta)$. In three of them (which we call by Bessel, Airy and cosine regimes) the involved Laguerre norm $N_n(\alpha, p, \beta)$ grows according to a power law in $n$ with an exponent which depends on $\alpha, \beta$ and $p$. The Bessel regime corresponds to the neighborhood of zero (i.e., at the left extreme of the orthogonality interval), where the Laguerre polynomials can be asymptotically described by means of Bessel functions (taken for expanding scale of the variable). Then (to the right of zero) the oscillatory behavior of the polynomials (in the bulk region of zeros location) is asymptotically modelled by means of the trigonometric functions (cosine regime) and at the neighborhood of the extreme right zeros asymptotics is given by Airy functions (Airy regime). 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; that is, 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 $n$th-power laws in the Bessel, Airy and cosine regimes are controlled by the constants $C_B(\alpha, p, \beta)$, $C_A(p)$ and $C(\beta, p)$, respectively, whose values are given in Table I. Therein, we have used the notation

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

for the Bessel function, and

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

for the Airy function (see [55]). When the transition regimes dominate in integral (12), then the asymptotics of $N_n(\alpha, p, \beta)$ besides the degree on $n$ have the factor $\ln n$. It is also curious to mention that if these regimes dominate, then the gamma factors in the constant $C(\beta, p)$ for the oscillatory cosine regime explode. For the cosine-Bessel regime it happens for $\beta + 1 - p/2 = 0$, and for the cosine-Airy regime it happens for $1 - p/2 = 0$.

Tab. I: Asymptotic regimes†of the Laguerre norms $N_{n,l}(\alpha, p, \beta)$

| *Asymptotic regime* | *Constant* |
|---|---|
| Bessel regime | $C_B(\alpha, p, \beta) := 2 \int\limits_0^\infty t^{2\beta+1} \lvert J_\alpha \rvert^{2p}(2t)\, dt$ |
| Airy regime | $C_A(p) := \int_{-\infty}^{+\infty} \left[\frac{2\pi}{\sqrt[3]{2}} \mathrm{Ai}^2\left(-\frac{t\,\sqrt[3]{2}}{2}\right)\right]^p dt$ |
| Cosine regime | $C(p, \beta) := \frac{2^{\beta+1}}{\pi^{p+1/2}} \frac{\Gamma(\beta+1-p/2)\,\Gamma(1-p/2)\,\Gamma(p+1/2)}{\Gamma(\beta+2-p)\,\Gamma(1+p)}$ |

† There also exist two asymptotic transition regimes: cosine-Bessel and cosine-Airy; when they dominate, the asymptotics of $N_n(\alpha, p, \beta)$ has a factor $\ln n$ besides the $n$th-power law.

The application of this methodology [54] to the three-dimensional hydrogenic system has allowed us to find the asymptotics ($n \to \infty$) of the hydrogenic Laguerre norms $N_{n,l}(\alpha, p, \beta)$ given by (14) and (15), and thus the dominant term of $R_p[\rho_{n,l}]$ given by (13). We have obtained the following values for the radial Rényi entropy $R_p[\rho_{n,l}]$ of the Rydberg hydrogenic states for all possible values of $p$:

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \left[ \frac{n^{3-4p}}{2^{3-2p} Z^{3(1-p)}} \times \begin{cases} C(p,\beta)\,(2(n-l-1))^{3-2p}\,(1+\bar{\bar{o}}(1)) \Big], & p \in (0,2) \\ \frac{\ln(n-l-1)+\underline{\underline{O}}(1)}{\pi^2(n-l-1)} \Big], & p = 2 \\ C_B(\alpha,p,\beta)\,(n-l-1)^{-(3-p)}\,(1+\bar{\bar{o}}(1)) \Big], & p \in (2,\infty) \end{cases} \right. \tag{16}$$

Note that the Airy regime does not play a significant role at first order in our hydrogenic system. The reason is that for $p = 2$ the transition cosine-Bessel regime determines the asymptotics of $N_{n,l}(p = 2)$. Thus, we have (a) for $p \in (0, 2)$ the region of $\mathbb{R}_+$ where the Laguerre polynomials exhibit the cosine asymptotics contributes with the dominant part in the integral (12), and (b) for $p > 2$ the Bessel regime plays the main role.

Finally, from Eqs. (16) and taking into account the values $\alpha = 2l + 1$, $l = 0, 1, \ldots, n - 1$, and $\beta = 2 - p$ of the involved parameters, one has the following asymptotics for the radial Rényi entropies of the Rydberg states with the orbital quantum number $l << n$ (which are the most experimentally accesible ones [30]):

$$R_p[\rho_{n,l}] = \frac{1}{1-p} \ln \begin{cases} C(p)\,\frac{n^{6(1-p)}}{Z^{3(1-p)}}\,(1 + \bar{\bar{o}}(1)), & p \in (0,2) \\ \frac{n^{2-4p}}{2^{3-2p}Z^{3(1-p)}}\,\frac{\ln n + \underline{\underline{O}}(1)}{\pi^2}, & p = 2 \\ C_B(l,p)\,\frac{n^{-3p}}{2^{3-2p}Z^{3(1-p)}}\,(1 + \bar{\bar{o}}(1)), & p \in (2,\infty) \end{cases} \tag{17}$$

where $C(p) \equiv C(p, \beta = 2 - p)$ and $C_B(l, p) \equiv C_B(\alpha = 2l + 1, p, \beta = 2 - p)$.

## IV. RESULTS AND NUMERICAL DISCUSSION

In this section we obtain the Rényi, Shannon and Tsallis entropies of the Rydberg hydrogenic states in terms of the quantum numbers and the nuclear charge $Z$. Then, for illustration, we numerically discuss the Rényi entropy $R_p[\rho_{n,0,0}]$ of some Rydberg hydrogenic states $ns$ in terms of $n$, $p$ and $Z$.

First, by putting in Eq. (9) the values of the radial Rényi entropy $R_p[\rho_{n,l}]$ given by Eq. (16) and taking into account the angular Rényi entropy $R_p[Y_{l,m}]$ given by Eqs. (8) and (11), one obtains the total Rényi entropy $R_p[\rho_{n,l,m}]$ of the Rydberg states in a straightforward manner. Second, from the latter expression and Eq. (4) one can readily obtain the Tsallis entropy $T_p[\rho_{n,l,m}]$ of the Rydberg states.

Third, a most important case in the previous expressions is the limit $p \to 1$ since then the Rényi entropy $R_p[\rho]$ of a probability density $\rho$ is equal to the Shannon entropy $S[\rho]$, as already mentioned above. By keeping in mind Eq. (9), to investigate this limiting case for the Rényi entropy $R_p[\rho_{n,l,m}]$ of the Rydberg hydrogenic states we first take into account that

$$\begin{aligned} \lim_{p\to+1} R_p[\rho_{n,l}] &= \lim_{p\to+1} \frac{1}{1-p} \ln\left[\frac{n^{3-4p}}{2^{3-2p}Z^{3(1-p)}} C(p,\beta)\,(2n)^{1+\beta-p}\right] \\ &= 6\ln n - \ln 2 + \ln \pi - 3\ln Z, \end{aligned} \tag{18}$$

(where we used (16) and $l << n$ at the first equality), and

$$\lim_{p\to+1} R_p[Y_{l,m}] = \lim_{p\to+1} \frac{1}{1-p} \ln \Omega_{l,m}(\theta,\phi) = S[Y_{l,m}], \tag{19}$$

(remember (11) for the first equality) where $S[Y_{l,m}]$ is the Shannon-entropy functional of the spherical harmonics given [21, 56] by

$$S[Y_{l,m}] = \int_0^{\pi}\int_0^{2\pi} [Y_{l,m}(\theta,\phi)]^2 \,\ln\,[Y_{l,m}(\theta,\phi)]^2\,\sin\theta\,d\theta d\phi, \tag{20}$$

which is under control. Then the limit $p \to 1$ in Eq. (9) gives rise, keeping in mind Eq. (16), to the following value

$$S[\rho_{n,l,m}] = \lim_{p\to+1} R_p[\rho_{n,l,m}] = 6\ln n - \ln 2 + \ln\pi - 3\ln Z + S[Y_{l,m}] + o(1) \tag{21}$$

for the Shannon entropy of the Rydberg hydrogenic states. This expression has been previously obtained [22] by a different technique, what is a further checking of our results.

In particular, from the previous results we find that the following values

$$R_p[\rho_{n,0,0}] = R_p[\rho_{n,0}] + R_p[Y_{0,0}] = R_p[\rho_{n,0}] + \ln(4\pi) \tag{22}$$

for $p \neq 1$, and

$$S[\rho_{n,0,0}] = 6\ln n + \ln 2 + 2\ln\pi - 3\ln Z + o(1) \tag{23}$$

for the Rényi and Shannon entropy of the $(ns)$-Rydberg hydrogenic states, respectively. Here we have used that $S[Y_{0,0}] = \ln(4\pi)$ and the explicit values of $R_p[\rho_{n,0}]$ are given in Eq. (16).

Finally, for illustration we numerically study the variation 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 $Z$. Let us start with the variation of the $p$-th order Rényi entropy of these states in terms of the principal quantum number $n$ when $p$ is fixed. As an example, this quantity with $p = \frac{3}{4}(\triangle), 2(\bullet), \frac{7}{2}(\square)$ is plotted in Fig. 1. We observe that the behavior of the Rényi entropy of the Rydberg $(ns)$-states has an increasing character, which can be explained by the fact that the system tends to the classical regime as $n$ increases.

Then, we study in Figs. (2)-(3) the variation of the Rényi entropy, $R_p[\rho_{n,0,0}]$, with respect to the order $p$, with $p \in (0, 20)$, for the Rydberg hydrogenic state which corresponds to $n = 50$. Therein we observe that the Rényi entropy decreases as the order $p$ increases. This behavior (a) is not monotonic when $p \in (0, 2]$ because the decreasing at $p = 1$ and $p = 2$ is specially pronounced, and (b) is monotonic when $p > 2$. The monotonicity of the latter case is a consequence of the Bessel asymptotic regime. Moreover, by globally looking at the entropy values with integer $p$ we observe that the entropic quantities with the lowest orders (particularly when $p = 1$ and $p = 2$, closely related with the Shannon entropy and the desiquilibrium, respectively, as already mentioned) are most significant for the quantification of the spreading of the electron distribution of the system.

Finally, in Fig. 4, we study the behavior of the Rényi entropy, $R_p[\rho_{n,0,0}]$, as a function of the atomic number $Z$ of the Rydberg hydrogenic state with $n = 50$ for different values of the order parameter ($p = \frac{3}{2}(\triangle), 2(\bullet)$ and $4(\odot)$) when $Z$ is ranging from hydrogen ($Z = 1$) to lawrencium ($Z = 103$). We observe in all cases that the Rényi entropy decreases monotonically as $Z$ increases. In particular tha behavior of $R_2[\rho_{n,0,0}]$ (whose exponential gives the disequilibrium) points out the fact that the probability distribution of the system tends to separate from equiprobability more and more as the electron number of the atom increases; so, it nicely quantifies the complexity of the system as the atomic number grows.

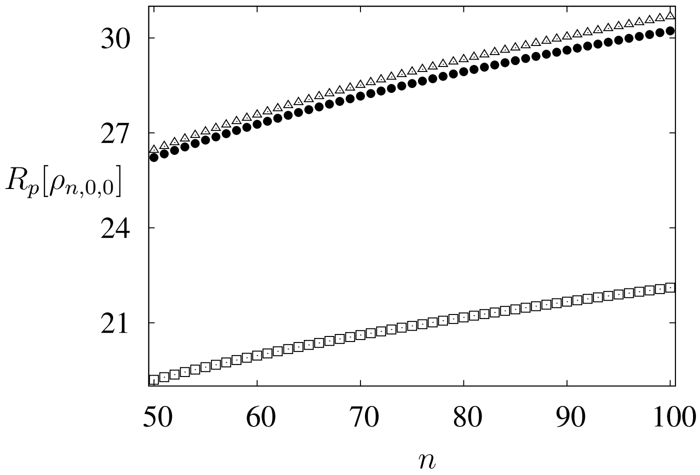

Fig. 1: Variation of the Rényi entropy, $R_p[\rho_{n,0,0}]$ for the Rydberg $(ns)$-states of the hydrogen atom ($Z = 1$) with respect to $n$, when $p = \frac{3}{4}(\triangle), 2(\bullet)$ and $\frac{7}{2}(\square)$.

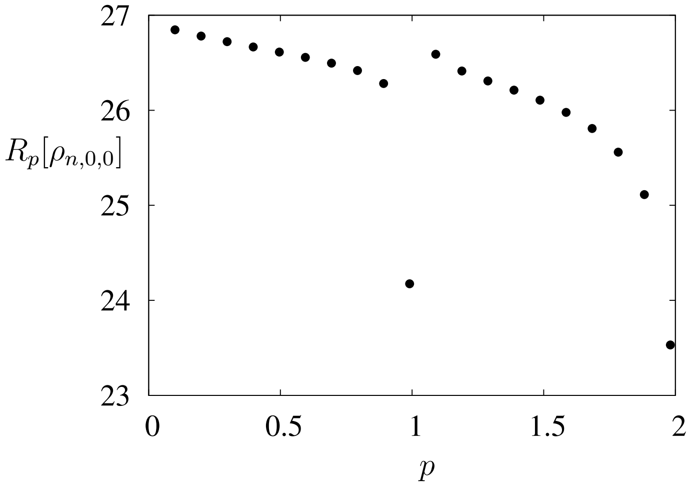

Fig. 2: Variation of the Rényi entropy, $R_p[\rho_{n,0,0}]$, with respect to $p$ for the Rydberg state with $n = 50$ of the hydrogen atom ($Z = 1$) when $p \in (0, 2)$.

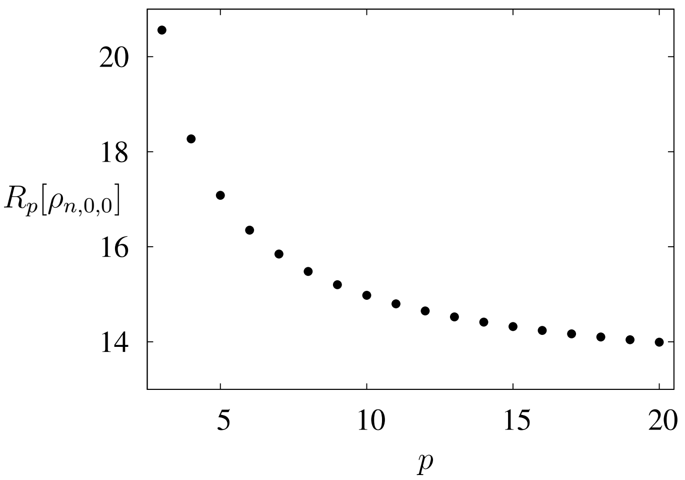

Fig. 3: Variation of the Rényi entropy, $R_p[\rho_{n,0,0}]$, with respect to $p$ for the Rydberg state with $n = 50$ of the hydrogen atom ($Z = 1$) when the integer $p \in (3, 20)$.

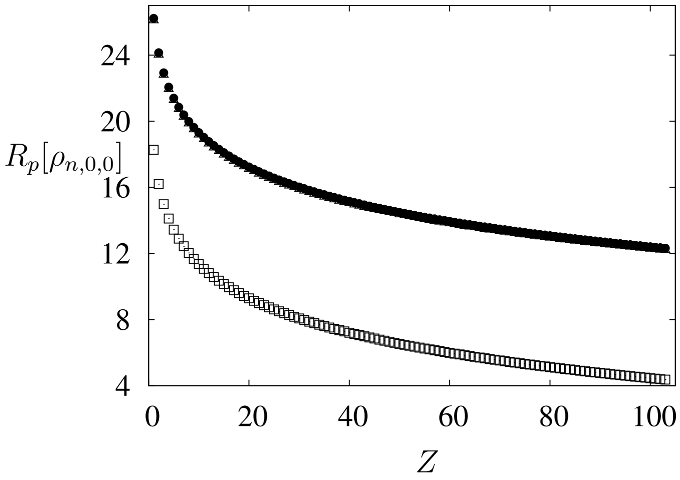

Fig. 4: Variation of the Rényi entropy, $R_p[\rho_{n,0,0}]$, with respect to the atomic number $Z$ for the Rydberg hydrogenic states with $n = 50$ when $p = \frac{3}{2}(\triangle), 2(\bullet)$ and $4(\odot)$.

## V. CONCLUSIONS

In this work we have explicitly calculated the dominant term of the Rényi, Shannon and Tsallis entropies for all quantum-mechanically allowed Rydberg (i.e., highly excited) hydrogenic states in terms of the nuclear charge $Z$ and the quantum numbers which characterize the corresponding state's wavefunctions. We have used a novel technique based on some ideas extracted from the modern approximation theory, which allows us to determine the asymptotics ($n \to \infty$) of the $\mathcal{L}_p$-norm, $N_{n,l}(p)$, of the Laguerre polynomials which control the associated wavefunctions. Finally, for illustration, we have studied the behavior of the Rényi entropy for the Rydberg ($ns$)-states at various values of the involved parameters $(n, p, Z)$. We have found that this quantity (a) decreases as a function of $p$, indicating that the most relevant Rényi quantities of integer order are those associated with the Shannon entropy and the disequilibrium, (b) has an increasing character for all Rydberg values of $n$ as the parameter $p$ is increasing, which can be explained by the fact that the system tends to the classical regime as $n$ increases, and (c) decreases for all $p$'s as the nuclear charge is increasing when $n$ is fixed.

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## 3.10 Quantum entanglement of Harmonium-type bosonic and fermionic systems

In this section we plan to show that some entanglement features of finite many-particle systems can be understood to a certain extent by purely kinematical considerations. We do it by explicitly analyzing the entanglement of the $N$-boson and $N$-fermion Harmonium systems. Our main objective is the analytical computation of the bosonic and fermionic ground-state entanglement of a single particle of the $N$-Harmonium system in terms of $N$ and the relative interaction strength.

Let us just mention some achievements:

- We complement and extend to harmonic systems with an arbitrary number of particles the study of entanglement recently done for various two-electron models [27, 78, 111, 117, 126, 161] as well as some helium-like systems [29, 48, 86, 99] and certain quantum complex networks [33], and
- we find that in the repulsive and attractive cases for relatively small values of the coupling constant, the entanglement of both bosonic and fermionic $N$-harmonium atoms grows when the number of particles increases, and that for the regime of strong coupling, the situation is exactly the opposite.

These results have been published in the article with coordinates: *C. L. Benavides-Riveros, I. V. Toranzo and J. S. Dehesa, Journal of Physics B: Atomic, Molecular and Optical Physics* ***47****, 195503 (****2014****)*, which is attached below.

# Entanglement in $N$-harmonium: bosons and fermions

***J. Phys. B: At. Mol. Opt. Phys. 47, 195503 (2014)***

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The ground-state entanglement of a single particle of the N-harmonium system (i.e., a completely-integrable model of $N$ particles where both the confinement and the two-particle interaction are harmonic) is shown to be analytically determined in terms of $N$ and the relative interaction strength. For bosons, we compute the von Neumann entropy of the one-body reduced density matrix by using the corresponding natural occupation numbers. There exists a critical number $N_c$ of particles so that below it, for positive values of the coupling constant, the entanglement grows when the number of particles is increasing; the opposite occurs for $N > N_c$. For fermions, we compute the one-body reduced density matrix for the closed-shell spinned case. In the strong coupling regime, the linear entropy of the system decreases when $N$ is growing. For fixed $N$, the entanglement is found (a) to decrease (increase) for negatively (positively) increasing values of the coupling constant, and (b) to grow when the energy is increasing. Moreover, the spatial and spin contributions to the total entanglement are found to be of comparable size.

## I. INTRODUCTION

The most precise determination of the properties of finite many-electron systems is usually done by means of a full-configuration-interaction (FCI) method, where the solution of the corresponding Schrödinger equation in a given one-electron basis is expressed in terms of a linear combination of all possible Slater determinants. Its application is naturally reduced to a bunch of small systems because of the enormous number of the involved determinants [1, 2].

Let us highlight that for all FCI approaches the correlation effects, which remain solely in the wave function, are not described by any correlation operator. Moreover, these effects are usually numerically computed as a difference of two variational energy bounds. Thus, up to now the electron correlation is widely and implicitly believed to be a purely methodical effect coming from the inadequate use of a trial wave function of multiconfiguration Hartree-Fock type; so, lacking of physical reality.

The application of quantum information ideas and techniques in electronic structure theory has recently allowed to conclude that the electron correlation is closely related to entanglement of electrons. Indeed, it has been proved that while the single Slater determinant in the monoconfigurational Hartree-Fock approximation is a disentangled state, the wavefunction of the multiconfiguration Hartree-Fock approximations (such as, e.g. FCI) accounts for entanglement effects. Therefore, entanglement plays an essential role not only in quantum communication between parties separated by macroscopic distances (see e.g., [3, 4]), but also it is essential to characterize quantum correlations at short distances. The latter problem, where one should necessarily consider the indistinguishable character of the involved particles, has received relatively less attention until a short time ago [5–10]. This is a serious lack because of its relevance for quantum information processing in various physical systems (see e.g., [5, 11]), to gain deeper insight into non-classical correlations of atomic and molecular systems as well as to fully understand the course of their dissociation processes and chemical reactions [10–12].

The main difficulty, however, stems from the fact that the Schrödinger equation of most quantum many-body systems cannot be solved analytically. Even numerically, the determination of the wavefunction is, in general, a serious problem. In the last three years an intense effort has been made to determine the entanglement of some real atomic and molecular species such as helium-like atoms [13–17], of a few processes of diatomic molecules [18] and elementary chemical reactions [19]. These works basically focus on the entanglement of bipartite systems, mainly because the characterization of this phenomenon for systems of many indistinguishable constituents is much less known, even at the level of the very notion of entanglement measure [20].

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Thus, the quantification of entanglement of bound states for model systems enabling analytic solutions of the associated Schrödinger equation is being a promising way to investigate correlation phenomena. Indeed, entanglement between the constituents of any bound system is most conveniently analyzed in such models, enabling to relate it to the bosonic or fermionic character. Up to now, however, only entanglement of some models of two bound electrons have been determined. We refer to the 2-harmonium (or Moshinsky) [21–25], Crandall and Hooke[13] atoms. In all these models the electron confinement is harmonic, and the electron-electron interaction is of harmonic (2-harmonium), $r_{12}^{-1}$ (Crandall), and Coulombic (Hooke) type. All of them show that when the spin degree of freedom and the indistinguishability of electrons are taken into account, new entanglement aspects[24] are encountered as compared to the model of distinguishable particles, although some further clarification is needed.

It is also worth noting that some entanglement features of the 2-harmonium atom are also qualitatively reproduced by the other two models, which give a good description for certain two-fermion systems (e.g., two electrons in a quantum dot is approximately described by the Hooke model). Namely, the growth of the entanglement when either the relative strength or the excitation energy is increasing. It is most interesting that recently the entanglement of some real helium-like atoms has been numerically shown to have an increasing dependence on the energy. This has been done both by the use of very accurate one-electron basis functions of Hylleraas-Kinoshita type [14, 17] and some Gaussian or Slater type orbital basis sets [6, 15]. As well it is observed from the models that the entanglement decrease of these systems in terms of the nuclear charge Z can also be understood as the result of the relative decrease of the electron-electron-interaction.

In this work we will study the entanglement of the one-body reduced density matrix of the N-harmonium model for bosons and fermions analytically. Von Neumann (for bosons) and linear (for fermions) entropies will be used. The one-body reduced matrix for the spinless fermionic case has been previously computed [26]. We obtain for the first time an explicit expression of the one-body reduced density matrix for the *closed-shell* spinned fermionic-case. This study will allow us to show that some entanglement features of finite many-particle systems can be understood by purely kinematical considerations to a certain extent. The N-particle harmonium is a completely-integrable system with an arbitrary number $N$ of particles where both the confinement and the two-particle interaction are harmonic. This model has been implicitly used to a certain extent to study cold atoms [27], to determine area laws of the ground-state entanglement of some one-dimensional chains [28] and to gain further insight into numerous phenomena of a variety of physical systems up to black holes (see e.g.,[21, 29–35]).

The paper is structured as follows. First, in Section II we briefly formulate the quantum-mechanical problem of the N-particle harmonium, showing its separability by using the appropriate set of normal coordinates [36], and fixing our notational settings. Then, in Section III we discuss the general mathematical structure of the one-body reduced density matrix in the bosonic case, obtaining its explicit expression. Moreover, we compute and discuss the analytical expression of the von Neumann entropy of the one-body reduced density matrix for the N-boson harmonium. Further, in Sections IV and V we obtain explicit expressions for the one-body reduced density matrix of the spinned N-fermion harmonium and analyze the linear entropy of the one-body reduced density matrix, with and without the spin degree of freedom. Finally, some concluding remarks and two appendices are given.

## II. THE N-HARMONIUM PROBLEM

The N-harmonium model is a system of $N$ interacting particles (fermions or bosons) which interact harmonically in a three-dimensional harmonic well. It is characterized by the Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} |\boldsymbol{p}_i|^2 + \frac{k}{2}\sum_{i=1}^{N} |\boldsymbol{r}_i|^2 + \frac{\delta}{2}\sum_{i<j}^{N} r_{ij}^2, \tag{1}$$

where $r_{ij} := |\boldsymbol{r}_i - \boldsymbol{r}_j|$, $k$ is the coupling constant of the harmonic well and $\delta$ the coupling of the harmonic interaction between the particles. The treatment of harmonically interacting bosons by means of this Hamiltonian represents the first exact solution of a N-particle system using only conditions on the reduced space of two-particle density matrices [37]. This system can be expressed in a separable form (i.e., as a system of uncoupled oscillators) using the set of normal coordinates $\{\boldsymbol{\xi}_1, ..., \boldsymbol{\xi}_N\}$ given by

$$\boldsymbol{\xi}_N := \frac{1}{\sqrt{N}}\sum_{i=1}^{N} \boldsymbol{r}_i \quad \text{and} \quad \boldsymbol{\xi}_m := \frac{1}{\sqrt{m(m+1)}}\sum_{i=1}^{m} (\boldsymbol{r}_i - \boldsymbol{r}_{m+1}), \tag{2}$$

with $m \in \{1, \ldots, N-1\}$. This is an orthogonal transformation of the position variables. A similar change of coordinates for momenta results in a canonical transformation, preserving the symplectic form. Let us call the new set of momenta $\{\boldsymbol{\Xi}_m\}$. A direct calculation shows that

$$\sum_{m=1}^{N-1} \boldsymbol{\xi}_m^2 = \frac{1}{N}\sum_{i<j}^{N} r_{ij}^2 = \sum_{m=1}^{N} \boldsymbol{r}_m^2 - \boldsymbol{\xi}_N^2, \tag{3}$$

so that the Hamiltonian (1) can be expressed in the following separable form

$$H = \mathcal{H}_N + \sum_{m=1}^{N-1} \mathcal{H}_m, \quad \text{where} \quad \mathcal{H}_N = \frac{1}{2}\boldsymbol{\Xi}_N^2 + \frac{1}{2}\omega^2 \boldsymbol{\xi}_N^2 \quad \text{and} \quad \mathcal{H}_m = \frac{1}{2}\boldsymbol{\Xi}_m^2 + \frac{1}{2}\mu^2 \boldsymbol{\xi}_m^2, \tag{4}$$

where $\omega^2 := k$, and $\mu^2 := k + N\delta$ depending on the number of particles. Then, the physical solutions of the associated Schrödinger equation (i.e., the wave functions $\Psi(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N)$), can be readily obtained. Here, let us first note that (a) there is a ground state whenever $\mu^2 > 0$, and (b) the particles are no longer bound if the relative interaction strength

$$\frac{\delta}{k} \leq -\frac{1}{N}. \tag{5}$$

On the other hand, let us comment here that the entanglement problem is formulated in terms of reduced density matrices. Either directly from the resulting one-particle reduced density matrix or, since the particles are assumed to interact pairwise, in terms of the two-particle density matrix

$$\rho(\boldsymbol{x}_1, \boldsymbol{x}_2; \boldsymbol{y}_1, \boldsymbol{y}_2) := \int d\boldsymbol{x}_3 \cdots d\boldsymbol{x}_N \; |\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \cdots, \boldsymbol{x}_N)\rangle\langle\Psi(\boldsymbol{y}_1, \boldsymbol{y}_2, , \boldsymbol{x}_3, \cdots, \boldsymbol{x}_N)|, \tag{6}$$

which carries all the necessary information required for calculating the quantum-mechanical properties of the whole system. The symbol $\boldsymbol{x}$ stands for spatial and spin coordinates, $\boldsymbol{x} := (\boldsymbol{r}, \varsigma)$. In particular, the ground state energy of the system can be computed by minimizing a simple linear functional of $\rho$. In passing, let us mention that the N-representability problem for this matrix has proved to be a major challenge for quantum chemistry [38]. The one-body density matrix, which is the basic variable in reduced density matrix functional theory [39], is then given as

$$\rho_1(\boldsymbol{x}; \boldsymbol{y}) := \int \rho(\boldsymbol{x}, \boldsymbol{x}_2; \boldsymbol{y}, \boldsymbol{x}_2) d\boldsymbol{x}_2. \tag{7}$$

By means of the spectral theorem, $\rho_1(\boldsymbol{x}; \boldsymbol{y})$ can be decomposed in terms of its natural spin orbitals $\{\phi_i(\boldsymbol{x})\}$ and its eigenvalues $\{n_i\}$, the *natural occupation numbers*: $\rho_1(\boldsymbol{x}; \boldsymbol{y}) = \sum_i n_i \phi_i(\boldsymbol{x})\phi_i(\boldsymbol{y})$, where $\sum_i n_i = 1$, with (for fermions) $0 \leq n_i \leq 1/N$.

For the case of an assembly of bosons we will compute the von Neumann entropy of the one-body reduced density matrix finding explicitly the occupation numbers of the system, as described in the next section. Recently, there has been a renewed interest in formulating the reduced density matrix theory using Wigner quasidistributions [25, 40, 41]. Our treatment for bosons will be done by using the Wigner function in phase space, what is a natural procedure for these systems. Let us advance that there exists a critical value for the number of particles. Below this critical value (around 3.5), we will show that for positive values of the coupling constant $\delta$ the first occupation number decreases (and consequently the von Neumann entropy grows) as the number of particles is increasing. Above this value, the first occupation number increases as the number of particles is increasing. Moreover, the first occupation number tends to 1 (and the entropy tends to 0) in the limit when the number of particles tends to infinity.

Later on, for fermions we use the one-body reduced density matrix to compute an explicit expression for its purity and its linear entropy as well. Let us advance that we will show that in the region of negative coupling $\delta$, the entropy grows when the number of particles is increasing. A similar situation is observed in the attractive case for small values of the coupling constant. For large values of $\delta/k$ the situation is the opposite: when particles are added to the system the entropy decreases. In both bosonic and fermionic cases, we will show that it is possible to calculate these two measures of entanglement as a function of the coupling constant $\delta/k$ and the number of particles.

## III. THE N-BOSON HARMONIUM: VON NEUMANN ENTROPY

In this section we determine the von Neumann entropy of the N-boson harmonium ground state in terms of $N$ and the relative interaction strength $\delta/k$. Taking into account the Gaussian character of the ground-state oscillator wave function, the ground state distribution on phase space is characterized by the Wigner N-body density function

$$\begin{aligned} W_{\text{gs}}^b(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N; \boldsymbol{p}_1, \ldots, \boldsymbol{p}_N) &= \frac{1}{\pi^{3N}}\, e^{-2\mathcal{H}_N/\omega} e^{-2\sum_{m=1}^{N-1}\mathcal{H}_m/\mu} \\ &= \frac{1}{\pi^{3N}} \exp\left[ -(\omega - \mu)\, \boldsymbol{\xi}_N^2 - \mu \sum_{i=1}^{N} \boldsymbol{r}_i^2 + \frac{\omega - \mu}{\omega\mu}\, \boldsymbol{\Xi}_N^2 - \frac{1}{\mu}\sum_{i=1}^{N} \boldsymbol{p}_i^2 \right]. \end{aligned} \tag{8}$$

The energy of the ground state is the total sum of the contributions of each individual oscillator, i.e. $E^b_{\rm gs} = \frac{3}{2}\big[\omega + (N-1)\mu\big]$. On the other hand the one-body density factorizes as a product of two separable quantities, to wit:

$$\begin{aligned} d^b_1(\boldsymbol{r};\boldsymbol{p}) :=& \int W^b_{\rm gs}(\boldsymbol{r},\boldsymbol{r}_2,\dots,\boldsymbol{r}_N;\boldsymbol{p},\boldsymbol{p}_2,\dots,\boldsymbol{p}_N)\, \prod_{m=2}^{N} d\boldsymbol{r}_m d\boldsymbol{p}_m \\ &= e^{-\mu \boldsymbol{r}^2 - \frac{1}{\mu}\boldsymbol{p}^2}\, \Delta^{\boldsymbol{r}}(\boldsymbol{r},\mu,\omega,N)\, \Delta^{\boldsymbol{p}}(\boldsymbol{p},\mu,\omega,N). \end{aligned} \tag{9}$$

It can be shown that the $\Delta$-function fulfills the following recursion relation:

$$\begin{aligned} \Delta^{\boldsymbol{r}}(\boldsymbol{r},\mu,\omega,N) :=& \frac{1}{\pi^{3N/2}} \int \exp\bigg[-\frac{\omega-\mu}{N}\Big(\boldsymbol{r}+\sum_{m=2}^{N}\boldsymbol{r}_m\Big)^2 - \mu\sum_{m=2}^{N}\boldsymbol{r}^2_m\bigg] \prod_{m=2}^{N} d\boldsymbol{r}_m \\ =& \frac{1}{\mu_1^{3/2}}\frac{1}{\pi^{3(N-1)/2}} \int \exp\bigg[-\frac{\omega-\mu}{N}\frac{\mu}{\mu_1}\Big(\boldsymbol{r}+\sum_{m=2}^{N-1}\boldsymbol{r}_m\Big)^2 - \mu\sum_{m=2}^{N-1}\boldsymbol{r}^2_m\bigg] \prod_{m=2}^{N-1} d\boldsymbol{r}_m \\ =& \frac{1}{\mu_1^{3/2}}\frac{1}{\pi^{3(N-1)/2}} \int \exp\bigg[-\frac{\omega-\mu_1}{N-1}\frac{\mu}{\mu_1}\Big(\boldsymbol{r}+\sum_{m=2}^{N-1}\boldsymbol{r}_m\Big)^2 - \mu\sum_{m=2}^{N-1}\boldsymbol{r}^2_m\bigg] \prod_{m=2}^{N-1} d\boldsymbol{r}_m \\ =& \,(\text{const.})\, \Delta^{\boldsymbol{r}}\bigg(\sqrt{\frac{\mu}{\mu_1}}\boldsymbol{r},\mu_1,\omega,N-1\bigg), \end{aligned} \tag{10}$$

where $\mu_m := \frac{m}{N}\,\omega + \frac{N-m}{N}\mu$. The constant (const.) will be determined by normalization so that it will depend on the number of particles as well as on the frequencies. Therefore,

$$\begin{aligned} \Delta^{\boldsymbol{r}}(\boldsymbol{r},\mu,\omega,N) &= (\text{const.})\, \Delta^{\boldsymbol{r}}\bigg(\sqrt{\frac{\mu}{\mu_1}}\boldsymbol{r},\mu_1,\omega,N-1\bigg) = (\text{const.})\, \Delta^{\boldsymbol{r}}\bigg(\sqrt{\frac{\mu}{\mu_2}}\boldsymbol{r},\mu_2,\omega,N-2\bigg) \\ &= \ldots = (\text{const.})\, \exp\bigg(-\frac{\omega-\mu}{N}\frac{\mu}{\mu_{N-1}}\boldsymbol{r}^2\bigg), \end{aligned} \tag{11}$$

and in addition that

$$\Delta^{\boldsymbol{p}}(\boldsymbol{p},\mu,\omega,N) \equiv \Delta^{\boldsymbol{r}}(\boldsymbol{p},\mu^{-1},\omega^{-1},N), \tag{12}$$

so that the expression (9) can be transformed as:

$$d^b_1(\boldsymbol{r};\boldsymbol{p}) = \frac{N^3}{\pi^3}\bigg(\frac{\omega\mu}{\mathcal{A}_N}\bigg)^{3/2} \exp\bigg(-\frac{N\omega\mu}{(N-1)\,\omega+\mu}\,\boldsymbol{r}^2 - \frac{N}{\omega+(N-1)\,\mu}\,\boldsymbol{p}^2\bigg), \tag{13}$$

where $\mathcal{A}_N = [(N-1)\,\omega+\mu][\omega+(N-1)\,\mu]$.

Let us now diagonalize this expression by decomposing it into its set of natural orbitals as well as into its occupation numbers. The task is made easier by noting that the one-body quasidensity is a linear combination of Laguerre polynomials (the phase-space counterpart of the Hermite polynomials). To see that, let us define

$$\gamma_N := (\omega\mu)^{1/4}\bigg[\frac{\omega+(N-1)\,\mu}{(N-1)\,\omega+\mu}\bigg]^{1/4}, \qquad \lambda_N := \frac{N\sqrt{\omega\mu}}{\sqrt{\mathcal{A}_N}}, \tag{14}$$

as well as the symplectic transformation

$$S_N := \begin{pmatrix} \gamma_N & 0 \\ 0 & \gamma_N^{-1} \end{pmatrix} \quad \text{and} \quad U := S_N \boldsymbol{u} \quad \text{where} \quad \boldsymbol{u}^T = (\boldsymbol{r},\boldsymbol{p}). \tag{15}$$

Then the one-body quasidensity function can be rewritten in the Gaussian way as follows,

$$d^b_1(U) = \frac{\lambda^3_N}{\pi^3}e^{-\lambda_N U^2}, \tag{16}$$

showing that it is actually a *Gibbs state.* Note that $\lambda_N \leq 1$ for all $N$, since $\omega+\mu \geq 2\sqrt{\omega\mu}$ and $\mathcal{A}_N \geq N^2\omega\mu$ and that $\lambda_N \to 1$ when $N \to \infty$.

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It is known that associated to any symplectic transformation (say, $S_N$), there is a unitary operator acting on the Hilbert space [42]. Let us use this transformation to find the set of occupation numbers in the basis of Wigner eigenfunctions of the harmonic oscillator. Since the one-body quasidensity function factorizes completely, from now on we work in one dimension. From the series formula

$$(1-t)\sum_{r=0}^{\infty} L_r(x)\, e^{-x/2}\, t^r = e^{-\frac{1+t}{1-t}\frac{x}{2}}, \tag{17}$$

where $L_r(x)$ is the Laguerre polynomial, it follows that

$$d_1^b(U) = \sum_{r=0}^{\infty} \frac{(-1)^r}{\pi} L_r(2U^2)\, e^{-U^2}\, n_r, \tag{18}$$

where the occupation numbers are equal to

$$n_r = \frac{2\lambda_N}{1+\lambda_N}\left(\frac{1-\lambda_N}{1+\lambda_N}\right)^r =: (1-t_N)\, t_N^r, \tag{19}$$

fulfilling $\sum_r n_r = 1$ as one should expect.

For the sake of completeness we plot the numerical behavior of the one-body quasidensity function of the N-boson harmonium in Figure 1 for different values of the number of bosons. We observe that, as the number of bosons grows, the profiles of the position and momentum densities become narrower and wider, respectively. This clearly indicates that the more precisely the particles are localized in position space, the larger the localization in momentum space, as one should expect according to the position-momentum uncertainty principle. There is no relevant difference for negative values of the coupling constant $\delta$ except that in this case it can be plotted only when $\delta/k \geq -1/N$.

Finally we can compute the von Neumann entropy of the N-boson harmonium explicitly in terms of $N$ and the relative interaction strength $\delta/k$, obtaining the value

$$\begin{aligned} S(N) &:= -\sum_{r=0} n_r \log n_r = -\log(1-t_N) - \frac{t_N \log(1-t_N)}{1-t_N} \\ &= -\frac{\sqrt{\mathcal{A}_N} + N\sqrt{\omega\mu}}{2N\sqrt{\omega\mu}} \log\left[\frac{2N\sqrt{\omega\mu}}{\sqrt{\mathcal{A}_N} + N\sqrt{\omega\mu}}\right], \end{aligned} \tag{20}$$

which complements and extends a similar formula encountered by other means in a black-hole context[31].

This entanglement measure is numerically examined in Figure 2 in terms of the number $N$ of bosons and $\delta/k$. As it is stated in (5) the minimum value of this relative strength is $-1/N$. There is a critical point around $N_c \sim 3.5$, where the entanglement acquires its maximum value. This is more clearly seen in Figure 3, where the explicit dependence of the von Neuman entropy on $N$ is shown. To investigate it in a closer way, we study the dependence of the occupation numbers on the number of bosons and the relative interaction strength. In particular, we plot the first occupation number separately in terms of $N$ and the relative strength. This is done in Figure 4. Therein, we note that below a critical value of number of particles (around $N_c \sim 3.5$), for *positive* values of the coupling constant $\delta/k$, the first occupation number decreases as the number of particles increases. Beyond this value the situation is reversed: the value of the first occupation number increases as the number of particles increases. This implies that $n_0 \sim 1$ in the limit when the number of particles tends to infinite, which is a necessary condition for the existence of a Bose-Einstein condensation [43].

In summary, the critical point around $N \sim 3.5$ where the von Neumann entropy is maximum is closely connected with the minimum of the first occupation number occurring at such position. It is found that above this critical value the spatial entanglement decreases when we add up more and more particles to the system, so that the degrowth rate increases when the coupling constant is increasing. Moreover, it can be shown that the entropy vanishes when $N$ goes to infinite.

## IV. THE SPINLESS N-FERMION HARMONIUM: LINEAR ENTROPY

In this section we study the spatial entanglement of the N-fermion harmonium (i.e., entanglement without taking into account the spin degree of freedom of the constituents) using the linear entropy of the one-particle density matrix as measure of entanglement of one particle. This measure is a first order approximation of the von Neumann entropy of the reduced one-body density of the system. In fact, it is a lower bound of this entropy. We will consider the

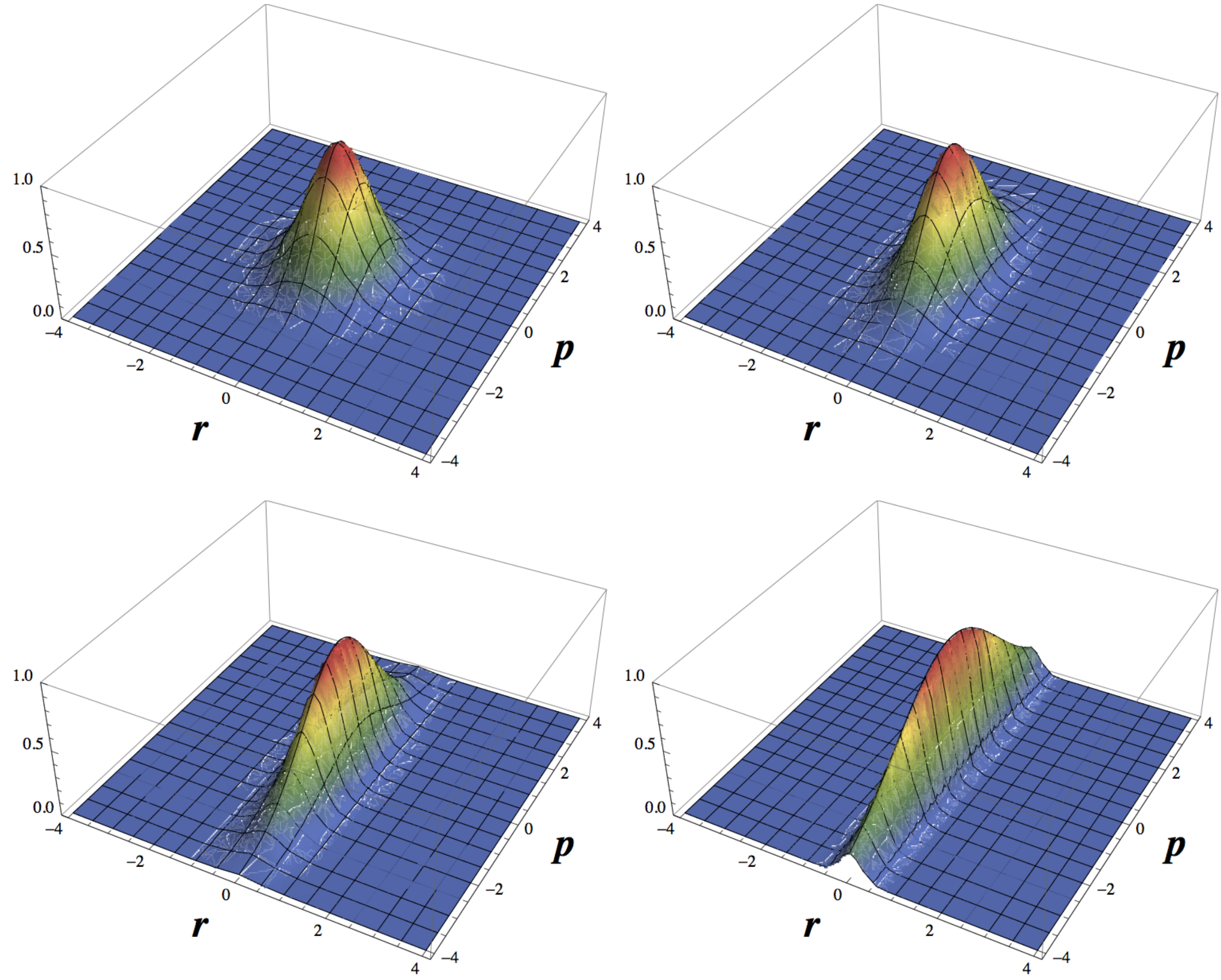

FIG. 1: The one-body quasidensity function (13) is plotted for different values of the number of bosons. Since the one-body quasidensity function factorizes completely, we plot it in one spatial dimension (two dimensions in phase space). The strength $\delta/k$ is taken to be equal to 1. Note that as the number of bosons grows, the profiles of the position and momentum densities become narrower and wider, respectively.

case in which the spinless fermions are confined in a one-dimensional well, mainly because the antisymmetric fermion case requires more elaborate computations. Here we have to consider the antisymmetry under exchange of position coordinates $\{r_1, \ldots, r_N\}$.

Taking into account the Hamiltonian (1) for the N-fermion harmonium, one has that the ground-state energy of the system is

$$E^f_{\rm gs} = \tfrac{1}{2}\omega + \sum_{j=1}^{N-1} \mu\big(m + \tfrac{1}{2}\big) = \tfrac{1}{2}\omega + \tfrac{1}{2}\mu(N^2 - 1) \tag{21}$$

and the corresponding eigenfunction can be expressed as

$$\Psi^f(\xi_1, \ldots, \xi_N) = \frac{1}{\sqrt{N!}} \sum_{J \in S_N} (-)^J J \left[ \phi^{\omega}_{n_N}(\xi_N) \prod_{m=1}^{N-1} \phi^{\mu}_{n_m}(\xi_m) \right], \tag{22}$$

where $n_m \in \{0, \cdots, N-1\}$, so that $n_i \neq n_j$ whenever $i \neq j$. The symbol $J$ denotes an element of the permutation group $S_N$ of $N$ elements (acting on the $r$-coordinates), and $\phi^{\nu}_n$ is the single-particle wave function given by an

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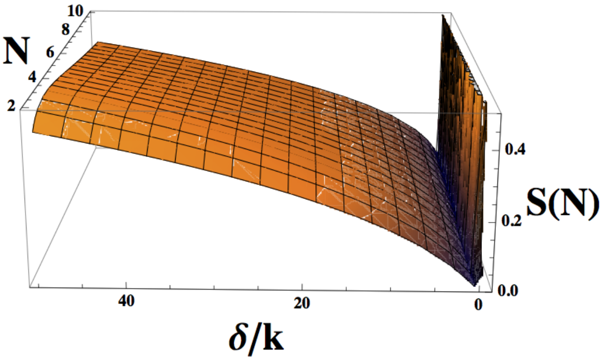

FIG. 2: Von Neumann entropy of the one-body reduced density matrix for the N-boson harmonium is plotted as a function of the number of bosons $N$ and the relative interaction strength $\delta/k$. It is apparent that there is a critical point around $N_c \sim 3.5$, where the entanglement acquires its maximum value.

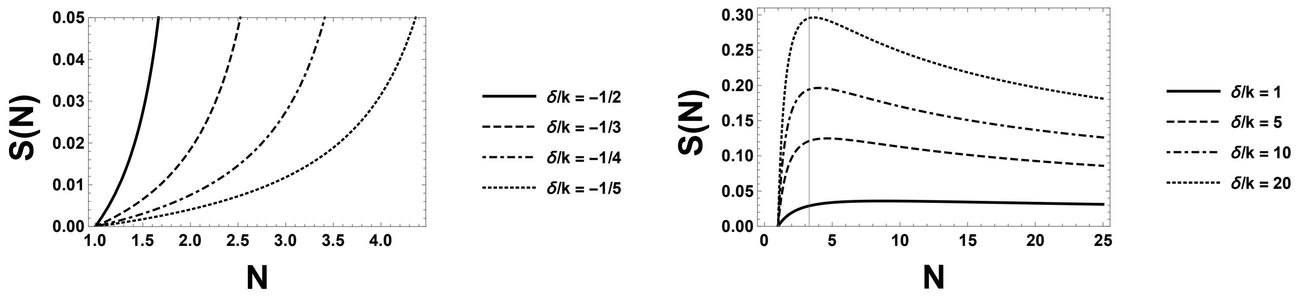

FIG. 3: Von Neumann entropy of the one-body reduced density matrix for the N-boson harmonium, whose explicit formula is given in Eq. (20), is plotted as a function of the number of particles for eight different values of the relative interaction strength $\delta/k$. Note that for each value of the relative strength there is a peak around the critical value $N_c$.

Hermite function of degree $n$ with frequency $\nu$. The collective mode $\xi_N$ is symmetric under any exchange of the position coordinates. Therefore, one has $n_N = 0$; otherwise one would have $n_m = 0$ for some $m \neq N$, and the wave function would not be totally antisymmetric. This eigenfunction can be rewritten as

$$\Psi^f_{\mathrm{gs}}(\xi_1, ..., \xi_N) = (\mathrm{const.}) \sum_{J \in S_N} (-)^J J \left[ \prod_{m=1}^{N-1} H_{n_m}(\sqrt{\mu}\, \xi_m) \right] e^{-\frac{\omega}{2}\xi_N^2 - \frac{\mu}{2}\sum_{m=1}^{N-1}\xi_m^2}, \tag{23}$$

where $H_n$ is the Hermite polynomial of degree $n$ and now $n_m \in \{1, \cdots, N-1\}$. The exponential power of (23) is the bosonic wave function, counterpart of the Wigner function in (8).

As an illustrative case let us consider the 3-harmonium system. To produce an antisymmetric wave function there is only one possibility for the degree of the polynomials, namely $n_1 = 1$ and $n_2 = 2$. Then the ground-state eigenfunction is

$$\Psi^f_{\mathrm{gs}}(\xi_1, \xi_2, \xi_3) = (\mathrm{const.}) \sum_{J \in S_3} (-)^J J \big[ \psi(\xi) \big]\, e^{-\frac{\omega}{2}\xi_3^2 - \frac{\mu}{2}(\xi_1^2 + \xi_2^2)}, \tag{24}$$

where $\psi(\xi) := H_1(\sqrt{\mu}\, \xi_1) H_2(\sqrt{\mu}\, \xi_2)$ and $\xi := (\xi_1, \xi_2)$. Note that the six elements of the permutation group $S_3$ are

$$p_1 = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}, \;\; p_2 = \begin{pmatrix} 2 & 1 & 3 \end{pmatrix}, \;\; p_3 = \begin{pmatrix} 2 & 3 & 1 \end{pmatrix},$$
$$p_4 = \begin{pmatrix} 1 & 3 & 2 \end{pmatrix}, \;\; p_5 = \begin{pmatrix} 3 & 1 & 2 \end{pmatrix}, \;\; p_6 = \begin{pmatrix} 3 & 2 & 1 \end{pmatrix}.$$

The coordinate $\xi$ transforms under the representation of the permutation group in the following form:

$$R(p_1)\xi = \xi, \;\; R(p_2)\xi = M_1\xi, \;\; R(p_3)\xi = M_1M_2\xi,$$
$$R(p_4)\xi = M_2\xi, \;\; R(p_5)\xi = M_1M_3\xi, \;\; R(p_6)\xi = M_3\xi,$$

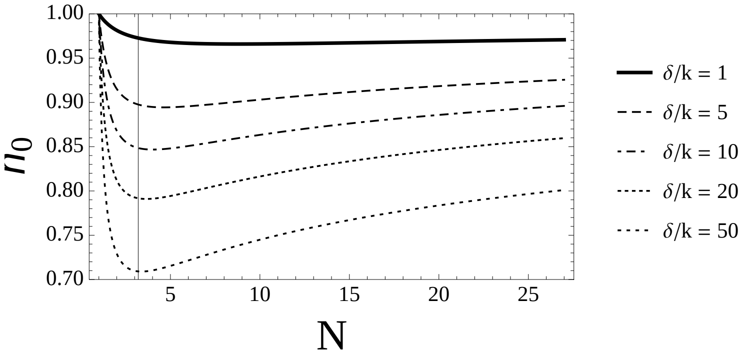

FIG. 4: Plot of the first occupation number $n_0 = 1 - t_N$ as a function of the number of particles for different *positive* values of $\delta/k$. As it is displayed, $n_0$ takes its minimum value around a critical value in the number of particles ($\sim 3.5$).

where

$$M_1 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad M_2 = \begin{pmatrix} \cos\pi/3 & \sin\pi/3 \\ \sin\pi/3 & -\cos\pi/3 \end{pmatrix} \quad M_3 = \begin{pmatrix} \cos\pi/3 & -\sin\pi/3 \\ -\sin\pi/3 & -\cos\pi/3 \end{pmatrix}.$$

Note that $\det M_i = -1$ and $M^t M = 1$. Any matrix

$$M_\phi = \begin{pmatrix} \cos\phi & \sin\phi \\ \sin\phi & -\cos\phi \end{pmatrix}$$

is a reflection in the axis $\theta = \phi/2$. In our case, this means $\theta = \pi/2, \pi/6, -\pi/6$; i.e., three reflection axes at 60-degree angles to each other. The rotations $R(p_3)$ and $R(p_5)$ are products of two reflections each. Thus, the eigenfunction transforms as follows:

$$\begin{aligned} \Psi^f_{\text{gs}}(\xi_1, \xi_2, \xi_3) &= (\text{const.})\, e^{-\frac{\omega}{2}\xi_3^2 - \frac{\mu}{2}(\xi_1^2+\xi_2^2)} \sum_{i=1}^{6} (-)^{i+1} \psi(R(p_i)\xi) \\ &= (\text{const.})\, e^{-\frac{\omega-\mu}{2}\xi_3^2 - \frac{\mu}{2}(r_1^2+r_2^2+r_3^2)} \sum_{i=1}^{6} (-)^{i+1} \psi(R(p_i)\xi) \\ &= (\text{const.})\, e^{-\frac{\omega-\mu}{2}\xi_3^2 - \frac{\mu}{2}(r_1^2+r_2^2+r_3^2)} (r_1 - r_2)(r_1 - r_3)(r_2 - r_3). \end{aligned} \tag{25}$$

Notice that the last equality has been possible because

$$\frac{1}{12\sqrt{2}} \frac{1}{\mu^{3/2}} \sum_{i=1}^{6} (-)^{i+1} \psi(\sqrt{\mu}\, R(p_i)\xi) = -\frac{1}{\sqrt{2}}(\xi_1^3 - 3\xi_1\xi_2^2) = (r_1 - r_2)(r_1 - r_3)(r_2 - r_3) \tag{26}$$

is a Vandermonde determinant. This 3-fermion result can be extended to the N-fermion system. In fact, general results of the theory of antisymmetric functions ensure that the wave function of a system of spinless fermions is equal to the wave function of the corresponding bosonic system multiplied by the $N$-variable Vandermonde determinant (see Section 3.1 of [44]). So, the ground-state wave function of the spinless N-fermion harmonium described by the Hamiltonian (1) has the form:

$$\Psi^f(r_1, \cdots, r_N) = (\text{const.}) \prod_{i<j} (r_i - r_j) \, \exp\left[ -\frac{\omega - \mu}{2}\, \xi_N^2 - \frac{\mu}{2} \sum_{i=1}^{N} r_i^2 \right], \tag{27}$$

where the product-like symbol on the right hand of this expression denotes the Vandermonde determinant:

$$\mathcal{V}_{(r_1, \cdots, r_N)} := \begin{vmatrix} 1 & \cdots & 1 \\ r_1 & \cdots & r_N \\ \vdots & \ddots & \vdots \\ r_1^{N-1} & \cdots & r_N^{N-1} \end{vmatrix} = \prod_{1 \le i < j \le N} (r_i - r_j). \tag{28}$$

Concrete calculations [30, 34] have borne out this fact several times. On the other hand, it has been pointed out by several authors that this function is actually a generalization of Laughlin's wave function for the fractional quantum Hall effect[45]. This is not surprising since in the Hall effect the magnetic field can be understood as a harmonic potential acting on the electrons. Let us also point out that the Wigner function corresponding to the Gaussian one on the right-hand side of (27) is nothing but the Wigner N-body quasidensity given by (8).

Let us now calculate the one-body density of the one-dimensional spinless N-fermion harmonium, which is defined by

$$\rho_1(r;r') = \int dr_2 \cdots dr_N \; \Psi^f(r, r_2, \cdots, r_N)\Psi^f(r', r_2, \cdots, r_N). \tag{29}$$

For this purpose it is convenient to rewrite the eigenfunction (27) as:

$$\Psi^f(r_1, \cdots, r_N) = (\text{const.})\, \mathcal{V}_{(r_1,\cdots,r_N)}\, e^{-a(r_1^2+\cdots+r_N^2)+b_N(r_1+\cdots+r_N)^2}, \tag{30}$$

with $a = \frac{\mu}{2}$ and $b_N = \frac{\mu-\omega}{2N}$. Moreover, we will use the Hubbard-Stratonovich transformation

$$e^{\alpha\zeta^2} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} dz\, e^{-\alpha z^2 + 2\alpha z\zeta}, \quad \text{with} \quad \alpha \in \mathbb{C} \quad \text{and} \quad \mathrm{Re}(\alpha) > 0, \tag{31}$$

where $\zeta = r_2 + \cdots + r_N$ and $\alpha = 2b_N$. Then the one-body density reads:

$$\begin{aligned} \rho_1(r;r') = k_N\, e^{-(a-b_N)(r^2+r'^2)} \int dz\, e^{-2b_N z^2} e^{(N-1)\frac{b_N^2}{2a}(r+r'+2z)^2} \\ \times \int dz_2 \cdots dz_N \mathcal{V}_{(z_r, z_2, \cdots, z_N)}\, \mathcal{V}_{(z'_r, z_2, \cdots, z_N)} \prod_{j=2}^{N} e^{-z_j^2}, \end{aligned} \tag{32}$$

where $k_N$ denotes the normalization constant (to be calculated later), and $z_j := \sqrt{2a}\big[r_j - \frac{b_N}{2a}(r + r' + 2z)\big]$ is a convenient change of coordinates. A key observation [26] is that the last expression on the right-hand side is the multiplication of two Slater determinants and therefore, the computation of the reduced density matrix can be done using well-known methods in quantum chemistry. Indeed, with the notation

$$\begin{aligned} \beta_N := \sqrt{\frac{\mu - \omega}{(N-1)\omega + \mu}}, \qquad q_{(r,r')} := \sqrt{\mu}\big[r - \tfrac{1}{2}\beta_N^2(r + r')\big] \\ \text{and} \quad c_N := \frac{(\mu-\omega)^2}{(N-1)\omega + \mu}\frac{N-1}{2N}, \end{aligned} \tag{33}$$

one can express the one-body density as

$$\rho_1(r;r') = k_N\, e^{-a_N(r^2+r'^2)+2c_N r r'} \int du\, e^{-u^2} \sum_{j=0}^{N-1} \frac{1}{2^j j!} H_j[q_{(r,r')} - \beta_N u] H_j[q_{(r',r)} - \beta_N u], \tag{34}$$

with $a_N := a - b_N - c_N$. This expression can be calculated analytically with the help of the following general formula derived in Appendix A:

$$\begin{aligned} &\int_{-\infty}^{\infty} e^{-u^2} H_k(q_{(r,r')} - \beta_N u) H_k(q_{(r',r)} - \beta_N u)\, du \\ &= \sum_{\substack{n_1,n_2=0 \\ n_1+n_2\,\text{even}}}^{k} (2\beta_N)^{n_1+n_2} \binom{k}{n_1}\binom{k}{n_2} H_{k-n_1}(-q_{(r,r')}) H_{k-n_2}(-q_{(r',r)})\, \Gamma\left(\frac{n_1+n_2+1}{2}\right). \end{aligned} \tag{35}$$

Then the integral at the right-hand side of (34) can be expressed as the following power sum:

$$\int du\, e^{-u^2} \sum_{j=0}^{N-1} \frac{1}{2^j j!} H_j[q_{(r,r')} - \beta_N u] H_j[q_{(r',r)} - \beta_N u] = \sqrt{\pi} \sum_{t=0}^{N-1} \sum_{s=0}^{2t} c_{t,s}^N\, r^{2t-s} r'^s, \tag{36}$$

where the expansion coefficients $c^N_{r,s}$ depend on the frequencies $\omega$, $\mu$ and the number of particles. When $r+s$ is an odd number or bigger than $2(N-1)$, $c^N_{r,s}=0$. By symmetry it is clear that $c^N_{t,s}=c^N_{s,t}$. In the one fermion case there is only one coefficient $c^1_{0,0}=1$. For $N$ fermions, the rank of the quadratic form of the $c_{r,s}$ is $2N-1$. In particular, when $N=2$, we have the expansion coefficients

$$c^2_{0,0}=\frac{2\mu}{\omega+\mu},\quad c^2_{1,1}=\frac{\mu(\mu^2+2\mu\omega+5\omega^2)}{(\omega+\mu)^2}\quad\text{and}\quad c^2_{2,0}=c^2_{0,2}=\frac{\mu(\omega-\mu)(3\omega+\mu)}{2(\omega+\mu)^2}. \tag{37}$$

For completeness, let us mention that the reader will have no difficulty in verifying that $\rho_1(r,r)$ —the diagonal of (29)— coincides (except for the difference in the normalization conventions) with the one obtained in [25, Sect. V] by the Wigner function method. Moreover, for $N=3$ the non-vanishing expansion coefficients are:

$$\begin{aligned}
c^3_{0,0}&=\frac{3}{2}\left[1+\frac{(\omega-\mu)^2}{(2\omega+\mu)^2}\right],\quad c^3_{1,1}=\frac{\mu(-15\omega^3+51\mu\omega^2+15\mu^2\omega+3\mu^3)}{(2\omega+\mu)^3},\\
c^3_{2,2}&=\frac{\mu^2(363\omega^4+168\mu\omega^3+90\mu^2\omega^2+24\mu^3\omega+3\mu^4)}{4(2\omega+\mu)^4},\\
c^3_{2,0}=c^3_{0,2}&=-\frac{\mu(39\omega^3-3\mu\omega^2+15\mu^2\omega+3\mu^3)}{2(2\omega+\mu)^3},\quad c^3_{4,0}=c^3_{0,4}=\frac{\mu^2(5\omega+\mu)^2(\omega-\mu)^2}{8(2\omega+\mu)^4}\\
\text{and}\quad c^3_{3,1}=c^3_{1,3}&=\frac{\mu^2(\omega-\mu)(65\omega^3+33\mu\omega^2+9\mu^2\omega+\mu^3)}{2(2\omega+\mu)^4}.
\end{aligned} \tag{38}$$

Except for the difference in the normalization and notation conventions, these coefficients coincide with the ones found in [26].

Keeping all this in mind and determining the normalization constant $k_N$ by imposing that $\int\rho_1(r;r)\,dr=1$, one finally has the expression

$$\rho_1(r;r')=\frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{N}}\sqrt{\frac{\omega\mu}{(N-1)\omega+\mu}}\,e^{-a_N(r^2+r'^2)+2c_N rr'}\sum_{t=0}^{N-1}\sum_{s=0}^{2r}c^N_{t,s}\,r^{2t-s}r'^s \tag{39}$$

for the one-body density of the one-dimensional spinless N-fermion harmonium.

Let us now quantify the entanglement of the system by means of the linear entropy associated to the one-body density [46]:

$$S_L=1-N\,\mathrm{Tr}[\rho_1^2], \tag{40}$$

where $\Pi_N=N\,\mathrm{Tr}[\rho_1^2]$ is the *purity* of the system. This entanglement measure, which is a non-negative quantity that vanishes if and only if the state has Slater rank 1 and it is therefore separable, has been recently used in various two-fermion systems [13, 24] as well as for various helium-like systems [14, 16, 17] in both ground and excited states. Let us also point out that the linear entropy is a linearization of the von Neumann entropy, and gives a lower bound for this logarithmic entropy. Moreover, in our systems it turns out that

$$\mathrm{Tr}[\rho_1^2]=\int\rho_1(r;r')\rho_1(r';r)\,dr'\,dr=k_N^2\sum_{t,e=0}^{N-1}\sum_{s=0}^{2t}\sum_{f=0}^{2e}c^N_{t,s}c^N_{e,f}\,\mathcal{I}_{(2t-s+f,2e-f+s)}, \tag{41}$$

where, as shown in Appendix B,

$$\begin{aligned}
\mathcal{I}_{(n,m)}&=\mathcal{I}_{(m,n)}\\
&=\int_{-\infty}^{\infty}r^n r'^m e^{-2a_N(r^2+r'^2)+4C_N rr'}\,dx\,dy\\
&=2\sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}(-1)^j\lambda_1^{-(n+m-i-j+1)/2}\lambda_2^{-(i+j+1)/2}\\
&\quad\times\Gamma\Big(\frac{n+m-i-j+1}{2}\Big)\Gamma\Big(\frac{n+m+1}{2}\Big)\frac{1}{4}[1+(-1)^{n+m-i-j}][1+(-1)^{i+j}],
\end{aligned} \tag{42}$$

with $\lambda_1=4(a_N-c_N)$ and $\lambda_2=4(a_N+c_N)$.

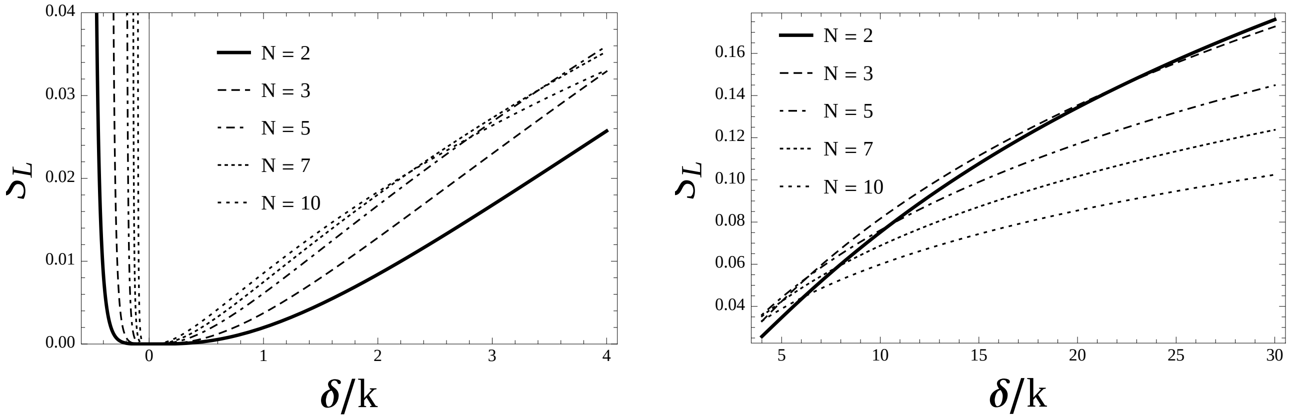

FIG. 5: Linear entropy of the one-particle density matrix of the N-fermion harmonium as a function of the coupling constant for five different values of $N$. Note the change of behavior when the strength grows.

Using expressions (40), (41) and (42), we have investigated the dependence of the linear entropy of the system on the relative interaction strength $\delta/k$, as well as on the energy. The results are given in Figure 5. A first basic observation is that for fixed $N$ the entanglement decreases (increases) when the relative interaction strength is increasing in the negative (positive) region. Moreover, for negative values of the coupling constant, the spatial entanglement of the N-fermion harmonium grows when $N$ is increasing. For small positive values of the coupling constant (i.e., when the fermions attract each other); herein we find that for very small values of $\delta/k$ the entanglement grows again with increasing $N$. In general, we observe that for positive values of the strength we have various regimes of dependence on $N$. In the strong-coupling regime, the linear entropy grows as the number of particles is increasing since the purity decreases with increasing number of particles. For instance, for $\delta/k = 10$ the purity is 0.92 for $N = 2$ and 0.94 for $N = 10$, whereas for $\delta/k = 1$ is 0.998 and 0.992 respectively.

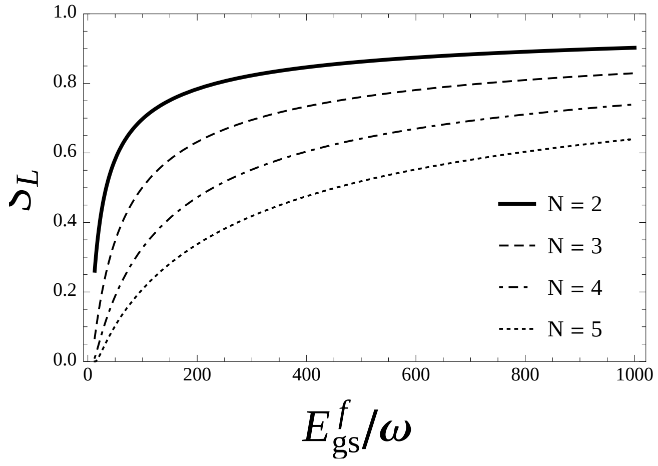

FIG. 6: Linear entropy $S_L$ of the N-fermion harmonium versus the ground-state energy $E^f_{\rm gs}/\omega$ for different values of $N$. The relation between the relative strength $\delta/k$ and the energy is stated in (43). The entanglement grows when the energy increases.

Figure 6 displays the dependence of the linear entropy of the system on the ground state energy $E^f_{\rm gs}/\omega$ for various values of the number of fermions $N$. We should keep in mind that the relation between the relative interaction strength and the energy is given by

$$\delta/k = \left[\frac{2E^f_{\rm gs}/\omega - 1}{N^2 - 1}\right]^2 - 1. \tag{43}$$

We find that the entanglement grows when the energy increases. For $N = 2$ this behavior has been recently observed not only in the Moshinsky or 2-fermion harmonium atom but also in other 2-fermion systems [13–17]. The novelty is that this behavior appears to be true also for heavier N-fermion harmonium atoms.

It is worth noting that our results can be considered as a generalization of previous results for the entanglement entropy of the fractional quantum Hall effect based in an exact matrix-product representation of the Laughlin wave function [47–49]. This well-known wave function, formulated by R. Laughlin to explain the fractional quantum Hall effect, consists of a lone Slater determinant and reads as in (27) except that there is no coupling between the electrons, that is, $\omega = \mu$ or $\delta = 0$, and the domain is the complex space.

## V. TOTAL ENTANGLEMENT OF THE SPINNED N-FERMION HARMONIUM

So far, we have considered only spinless particles. This means that in the two previous sections we have determined the spatial entanglement of the N-boson and N-fermion harmonia. Nevertheless, our conclusions for the bosonic system also apply to the total entanglement from a qualitative point of view, because the spin part of the ground-state eigenfunction fully factorizes. For fermionic systems this is no longer true, at least when they are isolated. In fact, for the ground state of two fermions is the product of a two-boson state and an antisymmetric spin state. For a system of fermions with spin in presence of a strong magnetic field, the spin part of the eigenfunction factorizes and so the spatial part must be antisymmetric [26]. In general, however, for the isolated fermionic system the spatial and spin parts of the ground-state wave function are not separable, and antisymmetry must take into consideration both spin and position coordinates.

Let us now calculate the total entanglement of the N-fermion harmonium (i.e., the entanglement of both spatial and spin degrees of freedom) using the linear entropy as measure of entanglement. For simplicity, we consider one-dimensional models with an even number (say $2N$) of spinned electrons from now on. The total spin of the system is zero, and all the spatial orbitals are doubly occupied (restricted configuration). This will eventually allow for an easy generalization to closed-shell three-dimensional systems. We define the set of spin natural orbitals in the following way:

$$\varphi_j(x) = \begin{cases} \phi_{\frac{j-1}{2}}(r)\uparrow, & \text{if } j \text{ is odd,} \\ \phi_{\frac{j}{2}}(r)\downarrow, & \text{if } j \text{ is even.} \end{cases}$$

The symbols $\uparrow$ and $\downarrow$ mean spin up and spin down, respectively, and we denote $x := (r, \varsigma)$, $\varsigma$ being the spin coordinate.

Let us begin with the consideration of the simpler non-interacting case; that is, when $\delta = 0$, and hence $\mu = \omega$. The corresponding ground-state eigenfunction is then given by the expression

$$\begin{aligned} \Psi^f(x_1, \ldots, x_N) &= \frac{1}{\sqrt{2N!}} \sum_{J \in S_{2N}} (-)^J \left[ \prod_{i=1}^{2N} \varphi_{i-1}(x_{J(i)}) \right] \\ &= \frac{1}{\sqrt{2N!}} \sum_{J \in S_{2N}} (-)^J \, J \left[ \prod_{i=1}^{N} \uparrow_{2i-1} \downarrow_{2i} \phi^{\omega}_{i-1}(r_{2i-1})\, \phi^{\omega}_{i-1}(r_{2i}) \right]. \end{aligned} \tag{44}$$

In the non-interacting case, the basis of the one-particle Hilbert space is the set of Hermite functions whose degree is less than $N$. Moreover, let us define

$$\begin{aligned} H &= \{ j \in S_{2N} : j \text{ fixes } 1, \ldots, N \} \simeq S_N \\ K &= \{ j \in S_{2N} : j \text{ fixes } N+1, \ldots, 2N \} \simeq S_N \end{aligned}$$

and $\tilde{S}_N = H \times K$ the direct product of these two subgroups. The set $S'_{2N} = S_{2N}/\tilde{S}_N$ is the set of right cosets in $S_{2N}$, giving the following equivalence relation: $J \sim J'$ if and only if there exists $(j, j') \in \tilde{S}_N$ such that $J' = (j, j')J$.

Therefore we can reorganize the expression (44) in the following form:

$$\begin{aligned} \Psi^f(x_1, \ldots, x_N) &= \frac{1}{\sqrt{2N!}} \sum (-)^J \prod_{i=1}^{N} \uparrow_{J(i)} \prod_{i=N+1}^{2N} \downarrow_{J(i)} \\ &\quad \times \begin{vmatrix} \phi^{\omega}_0(r_{J(1)}) & \cdots & \phi^{\omega}_0(r_{J(N)}) \\ \vdots & \ddots & \vdots \\ \phi^{\omega}_N(r_{J(1)}) & \cdots & \phi^{\omega}_N(r_{J(N)}) \end{vmatrix} \begin{vmatrix} \phi^{\omega}_0(r_{J(N+1)}) & \cdots & \phi^{\omega}_0(r_{J(2N)}) \\ \vdots & \ddots & \vdots \\ \phi^{\omega}_N(r_{J(N+1)}) & \cdots & \phi^{\omega}_N(r_{J(2N)}), \end{vmatrix}, \end{aligned} \tag{45}$$

where the sum runs over a representative of each coset. The choice of the representative $J \in [J] \in S'_{2N}$ is immaterial. The number of summands is

$$\left|S_{2N}/\tilde{S}_N\right| = \frac{|S_{2N}|}{|\tilde{S}_N|} = \frac{(2N)!}{(N!)^2} = \binom{2N}{N}.$$

For instance, for the four-harmonium ($N = 4$), the eigenfunction can be written in the alternative form:

$$\begin{aligned}\Psi^f(x_1, x_2, x_3, x_4) = \frac{\omega^2}{\pi}\frac{1}{\sqrt{3!}}e^{-\frac{\omega}{2}(r_1^2+r_2^2+r_3^2+r_4^2)}&[(\uparrow_1\uparrow_2\downarrow_3\downarrow_4 + \downarrow_1\downarrow_2\uparrow_3\uparrow_4)\mathcal{V}_{(1,2)}\mathcal{V}_{(3,4)} \\ &- (\uparrow_1\uparrow_3\downarrow_2\downarrow_4 + \downarrow_1\downarrow_3\uparrow_2\uparrow_4)\mathcal{V}_{(1,3)}\mathcal{V}_{(2,4)} + (\uparrow_1\uparrow_4\downarrow_2\downarrow_3 + \downarrow_1\downarrow_4\uparrow_2\uparrow_3)\mathcal{V}_{(1,4)}\mathcal{V}_{(2,3)}].\end{aligned}$$

The one-body reduced density matrix corresponding to the wave function (45) is diagonal in spin space and is given by the expression

$$\rho_1(x, x') = \begin{pmatrix} \rho_1^{\uparrow\uparrow}(r, r') & 0 \\ 0 & \rho_1^{\downarrow\downarrow}(r, r') \end{pmatrix}. \tag{46}$$

Moreover, it is clear that

$$\begin{aligned}\rho_1^{\uparrow\uparrow}(r, r') = \rho_1^{\downarrow\downarrow}(r, r') &= \int dx_2 \cdots dx_{2N}\, \Psi^f(r, \varsigma_1, x_2, \ldots, x_N)\Psi^f(r', \varsigma_1, x_2, \ldots, x_N)|_{\varsigma_1=\uparrow} \\ &= \frac{1}{2N}\frac{1}{(N-1)!}\int dr_2 \cdots dr_N \begin{vmatrix} \varphi_0(r) & \cdots & \varphi_0(r_N) \\ \vdots & \ddots & \vdots \\ \varphi_N(r) & \cdots & \varphi_N(r_N) \end{vmatrix} \begin{vmatrix} \varphi_0(r') & \cdots & \varphi_0(r_N) \\ \vdots & \ddots & \vdots \\ \varphi_N(r') & \cdots & \varphi_N(r_N) \end{vmatrix} \\ &= \frac{1}{2N}\sum_{i=0}^{N-1} \varphi_i(r)\varphi_i(r').\end{aligned} \tag{47}$$

The occupation numbers appear twice, what is a well-known result for atomic and molecular scientists.

Let us now consider the general interacting case, for which $\delta \neq 0$, and hence $\mu \neq \omega$. The ground-state eigenfunction for the Hamiltonian (1) is similar to (22), except that each spatial orbital is doubly occupied. For the same reasons as in the spinless case, the collective mode $\xi_{2N}$ occupies the Hermite function of degree zero. The other coordinates $\{\xi_m\}_{m=1}^{2N-1}$ occupy the other spatial orbitals in such a way that the total wave function is totally antisymmetric under interchange the coordinates $\{x_m\}_{m=1}^{2N}$. The ground-state eigenfunction schematically reads

$$\Psi^f(x_1, ..., x_{2N}) = \frac{1}{\sqrt{2N!}}\sum_{J\in S_{2N}} (-)^J \left[\prod_{i=1}^{N} \uparrow_{J(i)} \prod_{i=N+1}^{2N} \downarrow_{J(i)}\right] J\left[\phi_0^\omega(\xi_{2N})\phi_0^\mu(\cdot)\prod_{m=1}^{N} \phi_m^\mu(\cdot)\phi_m^\mu(\cdot)\right]. \tag{48}$$

For instance, in the particular case $N = 4$ the eigenfunction has the form

$$\begin{aligned}\Psi^f(x_1, x_2, x_3, x_4) &= \frac{1}{\sqrt{4!}}\sum_{J\in S_4} (-)^J \uparrow_{J(1)}\uparrow_{J(2)}\downarrow_{J(3)}\downarrow_{J(4)} J\left[\phi_0^\omega(\xi_4)\phi_1^\mu(\xi_1)\phi_0^\mu(\xi_3)\phi_1^\mu(\xi_2)\right] \\ &= (\text{const.})\sum_{J\in S_4} (-)^J \uparrow_{J(1)}\uparrow_{J(2)}\downarrow_{J(3)}\downarrow_{J(4)} J\left[\xi_1\xi_2\right] e^{-\frac{\omega}{2}\xi_4 - \frac{\mu}{2}(\xi_1^2+\xi_2^2+\xi_3^2)} \\ &= (\text{const.})\sum_{S'_4} (-)^J \uparrow_{J(1)}\uparrow_{J(2)}\downarrow_{J(3)}\downarrow_{J(4)} \mathcal{V}_{(J(1),J(2))}\mathcal{V}_{(J(3),J(4))} e^{-\frac{\omega}{2}\xi_4 - \frac{\mu}{2}(\xi_1^2+\xi_2^2+\xi_3^2)}.\end{aligned}$$

Using again that an antisymmetric polynomial is equal to a symmetric polynomial multiplied by a Vandermonde determinant [44], we can write the ground-state eigenfunction of the general interacting spinned N-fermion system as:

$$\begin{aligned}\Psi^f(x_1, \ldots, x_{2N}) = &(\text{const.})\, e^{-\frac{\omega-\mu}{2}\xi_{2N}^2 - \frac{\mu}{2}\sum_{i=1}^{2N} r_i^2} \\ &\times \sum_{S'_{2N}} (-)^J \left[\prod_{i=1}^{N} \uparrow_{J(i)} \prod_{i=N+1}^{2N} \downarrow_{J(i)}\right] \mathcal{V}_{(J(1),\ldots,J(N))}\mathcal{V}_{(J(N+1),\ldots,J(2N))}.\end{aligned} \tag{49}$$

and the corresponding energy is $E^f_{\rm gs} = \frac{1}{2}(\omega+\mu)+\mu(N^2-1)$. Let us define $\eta = r+r_2+\cdots+r_N$ and $\eta' = r'+r_2+\cdots+r_N$. To compute the one-density we use twice the Hubbard-Stratonovich identity. First to compute $N$ integrals with $\zeta' = r_{N+1}+\cdots+r_{2N}$, and second to compute $N-1$ integrals with $\zeta = r_2+\cdots+r_N$. Each diagonal element of the one-body density matrix reads:

$$\begin{aligned}
&\rho_1^{\uparrow\uparrow}(r,r') = \rho_1^{\downarrow\downarrow}(r,r') \\
&= (\text{const.})\, e^{-a(r^2+r'^2)} \int dr_2\cdots dr_N\, e^{-2a(r_2^2+\cdots+r_N^2)+b_{2N}(\eta^2+\eta'^2)} \int dz\, e^{-2b_{2N}z^2} e^{N\frac{b_{2N}^2}{2a}(\eta+\eta'+2z)^2} \\
&\qquad \times \mathcal{V}_{(r,,2,\ldots,N)}\, \mathcal{V}_{(r',2,\ldots,N)} \int dz_{N+1}\cdots dz_{2N}\, \mathcal{V}^2_{(z_{N+1},\ldots,z_{2N})} \prod_{j=N+1}^{2N} e^{-z_j^2},
\end{aligned} \tag{50}$$

where $z_j := \sqrt{2a}\big[r_j - \frac{b_{2N}}{2a}(\eta+\eta'+2z)\big]$. Once again, the expression on the right is the total integral of the product of two Slater determinants, that is,

$$\int dz_{N+1}\cdots dz_{2N}\mathcal{V}^2_{(z_{N+1},\ldots,z_{2N})} \prod_{j=N+1}^{2N} e^{-z_j^2}$$

is a real constant. Therefore

$$\begin{aligned}
&\rho_1^{\uparrow\uparrow}(r,r') = \rho_1^{\downarrow\downarrow}(r,r') \\
&= (\text{const.})\, e^{-a(r^2+r'^2)} \int dr_2\cdots dr_N\, e^{-2a(r_2^2+\cdots+r_N^2)+b_{2N}(\eta^2+\eta'^2)+d_N(\eta+\eta')^2}\, \mathcal{V}_{r,,2,\ldots,N}\, \mathcal{V}_{r',2,\ldots,N} \\
&= (\text{const.})\, e^{-a(r^2+r'^2)+b_{2N}(r^2+r'^2)+d_N(r+r')^2} \int dz\, e^{-2g_N z^2}\, e^{(N-1)\frac{g_N^2}{2a}(r+r'+2z)^2} \\
&\qquad \times \int dz_2\cdots dz_N\, \mathcal{V}_{z_r,,z_2,\ldots,z_N}\, \mathcal{V}_{z'_r,z_2,\ldots,z_N} \prod_{j=2}^{N} e^{-z_j'^2},
\end{aligned} \tag{51}$$

where $z'_j := \sqrt{2a}\big[r_j - \frac{g_N}{2a}(r+r'+2z)\big]$, $d_N = \frac{1}{8N}\frac{(\mu-\omega)^2}{\mu+\omega}$ and $g_N = \frac{\mu-\omega}{2N}\frac{\mu}{\mu+\omega}$. As in the spinless case, let us define

$$\tilde{q}_{(r,r')} = \sqrt{\mu}\big[r - \tfrac{1}{2}\beta_{2N}^2(r+r')\big] \quad \text{and} \quad \tilde{c}_{2N} = \frac{(\mu-\omega)^2}{(2N-1)\omega+\mu}\frac{2N-1}{8N} \tag{52}$$

with $\beta_N$ as defined in (33). Then

$$\begin{aligned}
\rho_1^{\uparrow\uparrow}(r,r') = \rho_1^{\downarrow\downarrow}(r,r') &= \frac{1}{2\pi}\frac{1}{\sqrt{N}}\sqrt{\frac{2\omega\mu}{(2N-1)\omega+\mu}} \\
&\times e^{-a'_N(r^2+r'^2)+2\tilde{c}_{2N}rr'} \int du\, e^{-u^2} \sum_{j=0}^{N-1} \frac{1}{2^j j!} H_j[\tilde{q}_{(r,r')} - \beta_{2N}u] H_j[\tilde{q}_{(r',r)} - \beta_{2N}u],
\end{aligned} \tag{53}$$

with $a'_N := a - b_{2N} - \tilde{c}_{2N}$.

The expression (53) is similar to (34), except that we have an even number of fermions: $N \to 2N$ and $c_N \to \tilde{c}_{2N}$. It is now clear that the conclusions for the spinless fermionic case also hold for the full spin case from a qualitative point of view. Figure 7 plots the linear entropy for the spinless and the spinned cases as functions of the relative strength.

For completeness, we have numerically investigated the dependence of the linear entropy on the number of particles for some specific values of the relative coupling in both spinless and spinned cases (i.e., for spatial and total entanglements). Figure 8 exhibits the results for $\delta/k \in \{-1/15, 2, 4, 22\}$. In the spinned case the behavior is similar to the spinless system, so that the total entanglement behaves similarly as the spatial entanglement. In fact, for small values of the coupling the entropy grows when increasing the number of particles, while in the strong-coupling regime the situation is the opposite. The inclusion of the spin tends to enhance the entropy of the system, being most important this phenomenon for small values of the coupling constant. Note that in turn the contributions of the spin and the spatial one are of comparable size.

Finally, let us investigate the relative behavior of entanglement and energy. This is done in Figure 9, where the linear entropy as a function of the ground-state energy is shown for some values of the number of particles. Let us

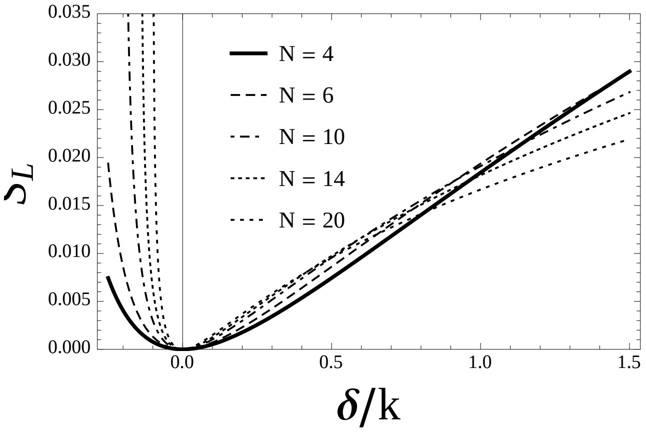

FIG. 7: Linear entropy of the spinned N-fermion harmonium as a function of the relative coupling constant for various values of $N$. Qualitatively, it is similar to the spinless case in Fig. 5.

recall here that the relation between the relative coupling and the energy is given by

$$\delta/k = \left[\frac{2E^f_{\mathrm{gs}}/\omega - 1}{2N^2 - 1}\right]^2 - 1. \tag{54}$$

As in the spinless case, the entropy grows when increasing the ground-state energy. For very large values of the dimensionless energy $E^f_{\mathrm{gs}}/\omega$ (i.e., very large values of the relative strength $\delta/k$) the gap between the spinless and spinned cases decreases.

## VI. CONCLUDING REMARKS

In this work we have shown that some entanglement features of finite many-particle systems can be understood to a certain extent by purely kinematical considerations. This is done by explicitly analyzing the entanglement of the N-boson and N-fermion harmonium systems. This has been possible because for these harmonic systems we have been able to calculate analytically not only the one-body reduced matrix for bosons and fermions, but also the von Neumann entropy in the bosonic case as well as the linear entropy in the fermionic case. In doing so, we complement and extend to harmonic systems with an arbitrary number of particles the study of entanglement recently done for various two-electron models [13, 21–25] as well as some helium-like systems [6, 14, 15, 17] and certain quantum complex networks [50].

We have determined the entanglement of these harmonic systems for both spatial and spin degrees of freedom analytically in terms of the number of particles and the relative interaction strength (or coupling constant). We have used the von Neumann entropy and the linear entropy as entanglement quantifiers in the bosonic and fermionic systems, respectively. We have found that for positive couplings the entanglement of the 3-boson harmonium atom is bigger than the one of the 2-boson system, but in general the entanglement of the N-boson harmonium decreases when $N$ is increasing. Moreover, the entanglement of a given N-boson system grows when the positive coupling constant is increasing; that is, when the positive value if the strength of interparticle interaction relative to the confinement well is increasing. On the other hand, globally speaking the spatial entanglement of the N-fermion harmonium grows when $N$ is increasing for both negative and sufficiently small positive values of the coupling constant. Moreover, the entanglement behavior is opposite in the positive strong-coupling regime. On the other hand, entanglement of a given N-fermion system grows when the coupling constant is increasing. The contribution of the spin degree of freedom to the entanglement of the N-fermion system is shown to be of positive comparable size to the contribution of the spatial degrees of freedom.

Summarizing, we have shown that in the repulsive case and in the attractive case for relatively small values of the coupling constant, the entanglement of both bosonic and fermionic N-harmonium atoms grows when the number of particles is increasing, basically because purity decreases. However, in the regime of strong coupling the situation is exactly the opposite: purity increases (and hence entanglement decreases) by adding particles to the system.

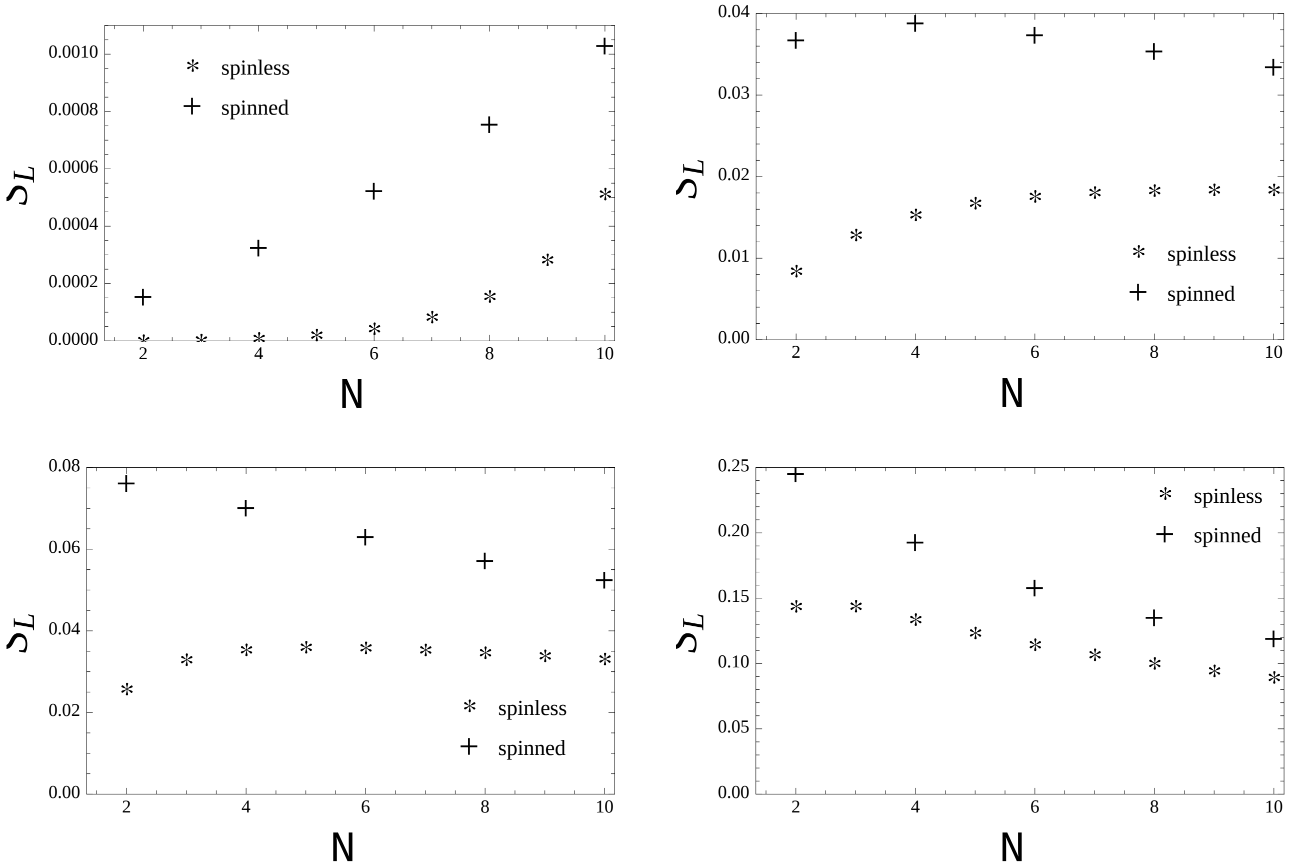

FIG. 8: Linear entropy of the one-body reduced density matrix for the spinless and spinned N-fermion harmonium as a function of the number of particles for different values of $\delta/k$. From left to right and from top to bottom $\delta/k = -1/15, 2, 4, 22$.

### Acknowledgments

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## Appendix A: Calculation of the integral $\int_{-\infty}^{\infty} e^{-u^2} H_k(a-cu) H_k(b-cu)\, du$

In this section we calculate the integral

$$\int_{-\infty}^{\infty} e^{-u^2} H_k(a-cu) H_k(b-cu)\, du, \tag{A1}$$

where $a$, $b$ and $c$ are real numbers and $H_k(x)$ is the Hermite polynomial of degree $k$. We use the following property of the Hermite polynomials

$$H_n(-z) = (-1)^n H_n(z),$$

as well as the power series of these polynomials around $z = z_0$

$$H_n(z) = \sum_{k=0}^{n} 2^k \binom{n}{k} H_{n-k}(z_0)(z-z_0)^k.$$

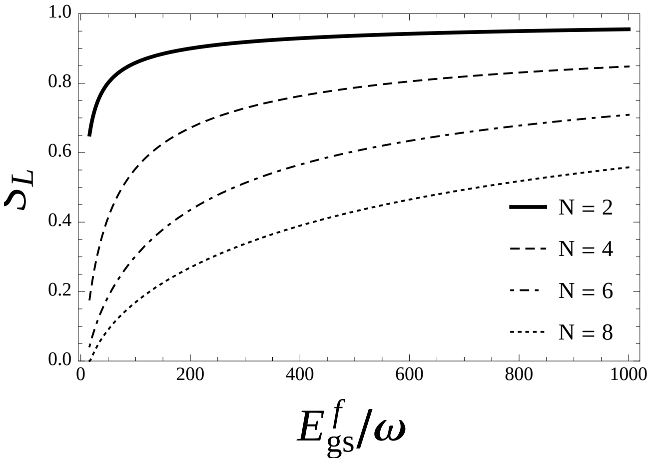

FIG. 9: Linear entropy $S_L$ of the N-fermion spinned harmonium versus the ground-state energy $E^f_{\rm gs}/\omega$ for different values of $N$. The relation between the relative strength $\delta/k$ and the energy is stated in (54).

This expression allows us to rewrite each Hermite polynomial in the following form:

$$H_k(a-cu) \underset{z_0=-a}{=} (-1)^k \sum_{n_1=0}^{k} (2c)^{n_1} \binom{k}{n_1} H_{k-n_1}(-a) u^{n_1}. \tag{A2}$$

Inserting (A2) into (A1) we obtain

$$\begin{aligned}
&\int_{-\infty}^{\infty} e^{-u^2} H_k(a-cu) H_k(b-cu)\, du \\
&= \int_{-\infty}^{\infty} e^{-u^2} (-1)^k \sum_{n_1=0}^{k} (2c)^{n_1} \binom{k}{n_1} H_{k-n_1}(-a) u^{n_1}\, (-1)^k \sum_{n_2=0}^{k} (2c)^{n_2} \binom{k}{n_2} H_{k-n_2}(-b) u^{n_2} \\
&= \sum_{\substack{n_1,n_2=0 \\ n_1+n_2 \text{ even}}}^{k} (2c)^{n_1+n_2} \binom{k}{n_1} \binom{k}{n_2} H_{k-n_1}(-a) H_{k-n_2}(-b)\, \Gamma\left(\frac{n_1+n_2+1}{2}\right).
\end{aligned} \tag{A3}$$

## Appendix B: The Gaussian integral $\mathcal{I}_{(n,m)}$

In the following, we calculate the integral

$$\mathcal{I}_{(n,m)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^n y^m e^{-a(x^2+y^2)+2cxy}\, dx\, dy. \tag{B1}$$

Here we perform the change of coordinates

$$x = u + v \quad \text{and} \quad y = u - v \tag{B2}$$

and the integral now reads:

$$\mathcal{I}_{(n,m)} = 2 \sum_{i=0}^{n} \sum_{j=0}^{m} \binom{n}{i} \binom{m}{j} (-1)^j \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u^{n+m-i-j} v^{i+j}\, e^{-\lambda_1 u^2 - \lambda_2 v^2}\, du\, dv, \tag{B3}$$

with $\lambda_1 = 2(a-c)$ and $\lambda_2 = 2(a+c)$. From the form of the (double) integral, on using polar coordinates in the $(u,v)$-plane, $u = R\cos\phi$ and $v = R\sin\phi$, since the exponential is an even function of $\phi$, the double integral vanishes if $i+j$ is odd. Switching $u$ and $v$ in the polar coordinates we likewise see that it vanishes if $(m+n)-(i+j)$ is odd.

The integral thus becomes

$$\begin{aligned}\mathcal{I}_{(n,m)}&\\ &= 2\sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}(-1)^j\lambda_1^{-(n+m-i-j+1)/2}\lambda_2^{-(i+j+1)/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}u^{n+m-i-j}v^{i+j}\,e^{-u^2-v^2}\,du\,dv\\ &= 2\sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}(-1)^j\lambda_1^{-(n+m-i-j+1)/2}\lambda_2^{-(i+j+1)/2}\\ &\quad\times\Gamma\Big(\frac{n+m-i-j+1}{2}\Big)\Gamma\Big(\frac{n+m+1}{2}\Big)\frac{1}{4}[1+(-1)^{n+m-i-j}][1+(-1)^{i+j}].\end{aligned}\tag{B4}$$

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## 3.11 Quantum entanglement of Spherium-like two-electron systems

In this section we explore the entanglement-like features of the $(d-1)$-Spherium system. This quantum system consists of two electrons interacting via a Coulomb potential and confined to the surface of a $d$-dimensional ball (that is, a $(d-1)$-hypersphere) of radius $R$. This system is quasi-exactly solvable, because its Schrödinger eigenvalue equation can be solved in a closed analytical fashion for particular values of the radius $R$ and particular eigenstates.

Here the targets are:

- The analytical calculations of the amount of entanglement exhibited by $s$-states of the Spherium model, and
- characterize the entanglement in terms of the quantized radius $R$, the energy $E$ of the system and the spatial dimensionality $d$.

Some achievements are:

- The explicit computation of various entanglement measures of the ground state of Spherium in terms of the radius $R$ and of the space dimension $d$, and
- these ground-state entanglement measures increase with the radius $R$ (fulfilling a general property exhibited by other two-electron systems), decrease with the spatial dimensionality $d$, and tend to increase with the energy $E$ of the system.

These results have been published in the article with coordinates: *I. V. Toranzo, A. R. Plastino and J. S. Dehesa, Journal of Physics A: Mathematical and Theoretical **48**, 475302 (**2015**)*, which is attached below.

# Quantum Entanglement in $(d-1)$-Spherium

***J. Phys. A: Math. Theor. 48, 475302 (2015)***

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There are very few systems of interacting particles (with continuous variables) for which the entanglement of the concomitant eigenfunctions can be computed in an exact, analytical way. Here we present analytical calculations of the amount of entanglement exhibited by $s$-states of *spherium*. This is a system of two particles (electrons) interacting via a Coulomb potential and confined to a $(d-1)$-sphere (that is, to the surface of a $d$-dimensional ball). We investigate the dependence of entanglement on the radius $R$ of the system, on the spatial dimensionality $d$, and on energy. We find that entanglement increases monotonically with $R$, decreases with $d$, and also tends to increase with the energy of the eigenstates. These trends are discussed and compared with those observed in other two-electron atomic-like models where entanglement has been investigated.

## I. INTRODUCTION

It has been recently shown by Loos and Gill [1, 2] that "spherium", a system consisting of two electrons trapped on the surface of a sphere and interacting through a Coulomb potential, belongs to the family of quasi-exactly solvable quantum mechanical models. These are models whose Schrödinger eigenvalue equation admits an explicit analytical solution for a finite portion of the energy spectrum. This kind of models are of considerable interest both for illuminating the properties of more complex or realistic systems and for testing and developing approximate treatments, such as those related to density functional theory. Indeed, spherium has found interesting applications in the study of correlated quantum systems (see [1] and references therein). Spherium is related to another widely studied semi-solvable two-body model, the Hooke atom, which consists of a pair of electrons repelling Coulombically and confined by a harmonic external potential (this system has direct experimental relevance as a model of a two-electron quantum dot with parabolic confinement). Here we are going to consider a $(d-1)$-dimensional version of spherium, where the two electrons are trapped on a $(d-1)$-sphere of radius $R$. By a $(d-1)$-sphere we mean the surface of a $d$-dimensional ball.

Exactly solvable and semi-solvable systems provide a valuable arena for the exploration of the entanglement properties of quantum systems of interacting particles. In particular, they provide useful insights for illuminating the entanglement-related features of natural and artificial atomic systems. Unfortunately, there are few such systems

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where entanglement measures can be evaluated analytically. In point of fact, to the best of our knowledge, the only system of two interacting particles with continuous variables where entanglement has been calculated in an exact analytical way is the Moshinsky model [3, 4]. Even for the Hooke atom, entanglement calculations are based upon the numerical evaluation of rather complex multi-dimensional integrals [5].

In the present contribution we show that spherium is a highly exceptional model, where the amount of entanglement exhibited by some of its eigenstates can be determined in an exact and fully analytical way. As far as we know, spherium is the only two-body system with Coulomb interaction where this goal has been achieved.

Entanglement is nowadays regarded as one of the most fundamental phenomena in Quantum Physics [6–8]. Entangled states of multipartite quantum systems are endowed with non-classical correlations that give rise to a variegated family of physical phenomena of both fundamental and technological significance. Quantum entanglement can be viewed in two complementary ways. On the one hand, entanglement constitutes a valuable resource. The controlled manipulation of entangled states is central to several quantum information technologies. On the other hand, entanglement can be regarded as a fundamental ingredient for the physical characterization of natural quantum systems such as, for instance, atoms and molecules. These two points of view are closely related to each other, although the latter is somehow less developed than the former. Concerning the second of the approaches mentioned above, several researchers have investigated in recent years the phenomenon of entanglement in two-electron atomic models and related systems [3–5, 8–30]. Most works dealing with entanglement in two-electron systems have been restricted to the associated ground state wavefunctions. However, the entanglement properties of excited states of two-electron atomic models have also been investigated [3, 5]. The most detailed results concerning the entanglement of excited states have been obtained from analytical investigations of exactly soluble models, in particular the Moshinsky one [3].

The main entanglement-related features exhibited by these models share some common trends. First, one observes that entanglement increases with the strength of the interaction between the particles. Alternatively, for a constant interaction strength, entanglement decreases with the strength of the confining potential (this behaviour has also been verified in numerical studies of entanglement in Helium-like atoms with increasing nuclear charge). These effects are clearly two sides of the same coin, and can usually be described jointly in terms of the dependence of entanglement on an appropriate dimensionless parameter corresponding to the relative strengths of the interaction and the confining potentials. In the case of atomic-like models with an external harmonic confining potential, such as the Moshinsky and the Hooke ones, it is also observed that entanglement tends to increase with energy. This last property hold for the majority of states. However there are a few entanglement "level-crossings" where a state has more entanglement than another state of higher energy [3]. Aside from these rare exceptions, the general monotonically increasing behaviour of entanglement with energy has been observed in harmonically confined models endowed with different types of particle interaction (i.e., harmonic interaction in the Moshinsky system, Coulomb interaction in the Hooke atom; and a $r^{-2}$-interaction potential in the Crandall model). Another trend exhibited by two-electron models with harmonic confinement (which also holds for different interaction laws between the constituent particles) is that the amount of entanglement associated with excited states does not always vanish in the limit of a vanishing interaction [22].

The goal of the present paper is to calculate analytically the amount of entanglement of the ground state of $(d-1)$-spherium. The paper is organized as follows. In Section II, we briefly review the concept of entanglement in systems consisting of identical fermions. In Section III, we show the technical details of the calculations performed in this work. In Section IV, we describe our main results. Finally, some conclusions are drawn in Section V.

## II. ENTANGLEMENT IN SYSTEMS OF IDENTICAL FERMIONS

There is a natural and physically meaningful measure of entanglement for pure states of systems consisting of two identical fermions. It is based on the Schmidt decomposition for fermions [31, 32], which reads

$$|\Psi\rangle = \sum_i \sqrt{\frac{\lambda_i}{2}} \left( |2i\rangle |2i+1\rangle - |2i+1\rangle |2i\rangle \right), \tag{1}$$

where $\{|i\rangle, i = 0, 1, \ldots\}$ is an appropriate orthonormal basis of the single-particle Hilbert space, and $0 \leq \lambda_i \leq 1$ with $\sum_i \lambda_i = 1$. The entanglement of the pure state $|\Psi\rangle$ can then be expressed in terms of the above fermionic Schmidt coefficients, as

$$\xi[|\Psi\rangle] = 1 - \sum_i \lambda_i^2 = 1 - 2\,\mathrm{Tr}(\rho_1^2), \tag{2}$$

where $\rho_1 = Tr_2|\Psi\rangle\langle\Psi|$ is the single-particle reduced density matrix obtained from the global, two-particle density matrix $\rho = |\Psi\rangle\langle\Psi|$. The Schmidt coefficients $\lambda_i$ are the eigenvalues (each one two-fold degenerate) of $\rho_1$. The entanglement measure (2) is (up to appropriate additive and multiplicative constants) basically given by the linear entropy $S_L(\rho_1) = 1 - Tr(\rho_1^2)$ of the single-particle density matrix $\rho_1$. Alternatively, one could consider an entanglement measure based upon the von Neumann entropy of the density matrix $\rho_1$, given by $S_{\mathrm{vN}}(\rho_1) = -Tr\rho_1 \ln \rho_1$. This last measure is extremely difficult to evaluate analytically for systems with continuous variables. Even in the case of the Moshinsky model, which is the atomic model where entanglement has been studied more systematically [3, 4], the entanglement measure based on the von Neumann entropy has been determined in an exact analytical way only for the ground state [9, 14]. It is highly unlikely that in systems with Coulomb interactions the entanglement measure based on the von Neumannn entropy can be calculated analytically. In these cases the (exact) analytical approach seems basically intractable. Entanglement measures based on the linear entropy have many computational advantages, both from the analytical and the numerical points of view. In particular, and in contrast with measures based on the von Neumann entropy, measures based on the linear entropy can be evaluated directly from $\rho_1$, without the need of first determining $\rho_1$'s eigenvalues. They constitute a practical tool for assessing the amount of entanglement that has been applied to the study of a variety of systems (see [3–5, 31] and references therein).

An important property of the entanglement measure (2) is that correlations between the two particles that are solely due to the antisymmetry of the fermionic state do not contribute to the state's entanglement. In fact, the amount of entanglement exhibited by a two-fermion state is given, basically, by the quantum correlations that the state has beyond the minimum correlations required by the antisymmetric constraint on the fermionic wavefunction [31–38]. Consequently, the entanglement of a pure state of two identical fermions that can be written as a single Slater determinant is zero.

We apply now the above measure to a pure state of a two-electron system. In order to analyze the entanglement of the eigenstates of spherium we have to consider states described by wavefunctions of the form,

$$\psi(\mathbf{r}_1, \mathbf{r}_2)\chi(\sigma_1, \sigma_2), \tag{3}$$

with the total wavefunction factorized as the product of a coordinate wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2)$ and a spin wavefunction $\chi(\sigma_1, \sigma_2)$. Here $\mathbf{r}_1$ and $\mathbf{r}_2$ stand for the vector positions of the two electrons. The density matrix corresponding to a wavefunction of the form (3) is given by

$$\rho = \rho^{(coord.)} \otimes \rho^{(spin)} \tag{4}$$

where the matrix elements of $\rho^{(coord.)}$ are

$$\langle \mathbf{r}_1', \mathbf{r}_2' | \rho^{(coord.)} | \mathbf{r}_1, \mathbf{r}_2 \rangle = \psi(\mathbf{r}_1', \mathbf{r}_2')\psi^*(\mathbf{r}_1, \mathbf{r}_2). \tag{5}$$

Even if we are going to investigate the entanglement features only of pure states of spherium, it is conceptually convenient to consider the corresponding density matrix (proyector) (4) in order to obtain from it the single-particle reduced density matrix, in terms of which the entanglement measure to be used can be clearly formulated. For a state with a wavefunction of the form (3) (and a density matrix of the form (4)) the entanglement measure (2) reads,

$$\begin{aligned} \xi[|\Psi\rangle] &= 1 - 2\mathrm{Tr}\left[\rho_1^2\right] \\ &= 1 - 2\,\mathrm{Tr}\left[\left(\rho_1^{(coord.)}\right)^2\right] \mathrm{Tr}\left[\left(\rho_1^{(spin)}\right)^2\right], \end{aligned} \tag{6}$$

where $\rho_1 = \rho_1^{(coord.)} \otimes \rho_1^{(spin)}$ is the single-particle reduced density matrix, and $\rho_1^{(coord.)}$ and $\rho_1^{(spin)}$ are, respectively, the marginal density matrices obtained after tracing the matrices $\rho^{(coord.)}$ and $\rho^{(spin)}$ over the degrees of freedom of one of the two particles. It is clear that the entanglement between the two electrons described by (3) involves both the translational and the spin degrees of freedom of electrons.

To calculate the entanglement measure (6), it is necessary to consider separately the cases of a spin wavefunction corresponding to parallel spins or antiparallel spins. When spins are parallel (that is, when the coordinate wavefunction is antisymmetric and the spin wavefunction is either $\chi_{++}$ or $\chi_{--}$), one has $Tr[(\rho^{(spin)})^2] = 1$, and the entanglement measure (6) of a two-electron state of the form (3) is

$$\xi[|\Psi\rangle] = 1 - 2\int |\langle \mathbf{r}_1'|\rho_1^{(coord.)}|\mathbf{r}_1\rangle|^2 \, d\mathbf{r}_1' d\mathbf{r}_1 \tag{7}$$

On the other hand, when the spins are anti-parallel (when the coordinate wavefunction is symmetric and the spin wavefunction is $\frac{1}{\sqrt{2}}(\chi_{+-} - \chi_{-+})$, or alternatively, when the coordinate wavefunction is antisymmetric and the spin wavefunction is $\frac{1}{\sqrt{2}}(\chi_{+-} + \chi_{-+})$), one has $Tr[(\rho^{(spin)})^2] = \frac{1}{2}$, and the entanglement is

$$\xi[|\Psi\rangle] = 1 - \int |\langle \mathbf{r}_1'|\rho_1^{(coord.)}|\mathbf{r}_1\rangle|^2 \, d\mathbf{r}_1' d\mathbf{r}_1 \tag{8}$$

In equations (7) and (8) we have

$$\langle \mathbf{r}_1'|\rho_1^{(coord.)}|\mathbf{r}_1\rangle = \int \psi(\mathbf{r}_1', \mathbf{r}_2)\psi^*(\mathbf{r}_1, \mathbf{r}_2)\, d\mathbf{r}_2 \tag{9}$$

for the matrix elements of the *coordinate* marginal matrix density.

In the above discussion we have considered two-electron states that are separable with respect to the spin and spatial degrees of freedom. Moreover, among these states we only considered states where the spin parts of the wavefunction correspond to the standard singlet and triplet states. When studying two-electron systems with a Hamiltonian not depending on spin, and energy levels with no degeneracy arising from the spatial part of the Hamiltonian, it is standard and natural to focus on eigenstates of the above described forms. However, even in these cases the spin-independence of the Hamiltonian leads to degeneracy of the energy spectra, and to the existence of eigenstates with the spin part of the wavefunction different from the ones just mentioned. For instance, one can have as spin wavefunction a linear combination of the triplet states. The corresponding (global) eigenstate would have an amount of entanglement different from the ones given by equations (7-8). But the difference would be due solely to the spin part, and would not correspond to any specific feature of the particular two-electron system under consideration. If the Hamiltonian includes spin-orbit interaction terms, coupling the spin and the spatial degrees of freedom, the situation becomes much more complex. The eigenstates would not, in general, have the spin and the spatial parts disentangled. In such cases both types of degrees of freedom need to be considered jointly in order to evaluate the entanglement between the two electrons constituting the system. These situations are outside the scope of the present work. The spherium Hamiltonian does not depend on spin, and we shall consider only *s*-states, where the spatial part of the wavefunction is symmetric, and the spin part is given by the singlet state.

## III. $(d-1)$-SPHERIUM: DESCRIPTION

As already mentioned, spherium consists of two identical particles ("electrons") interacting via a Coulomb potential and confined to the surface of a $(d-1)$-sphere of radius $R$. The corresponding Hamiltonian, expressed in atomic units, reads,

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} + \frac{1}{r_{12}}, \tag{10}$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the interelectronic distance (a brief review of some basic aspects of the spherium Hamiltonian is given in Appendix A). ${}^1S$ states (*s*-states) have a wavefunction $\Psi(r_{12})$ that depends only on the inter-electronic distance. The corresponding Schrödinger equation can be cast in the form,

$$\left[\frac{u^2}{4R^2} - 1\right]\frac{d^2\Psi}{du^2} + \left[\frac{u(2d-3)}{4R^2} - \frac{d}{u}\right]\frac{d\Psi}{du} + \frac{\Psi}{u} = E\Psi, \tag{11}$$

where $u = r_{12}$. As was recently proved by Loos and Gill in [1], equation (11) admits closed analytical solutions for particular, discrete values of the radius $R = R_{n,m}$. These exact eigenfunctions of the spherium system have a polynomial form,

$$\Psi_{n,m}(r_{12}) = \sum_{k=0}^{n} s_{k,m} r_{12}^k, \tag{12}$$

where the coefficients $s_{k,m} \equiv s_{k,m}(d)$ are determined by the recurrence relation

$$s_{k+2,m} = \frac{s_{k+1,m} + \left[k(k+2(d-1)-2)\frac{1}{4R_{n,m}^2} - E_{n,m}\right] s_{k,m}}{(k+2)(k+(d-1))}, \tag{13}$$

with the starting values $s_{0,m} = 1$ and $s_{1,m} = \frac{1}{(d-1)-1} \equiv \gamma$. The integer parameter $n$ has values $n = 1, 2, \ldots$ and $m$ is the number of roots that the polynomial (12) has in the range $[0, 2R]$. That is, the wavefunction (12) corresponds to the $m$-th excited $s$-state.

For a given $n$, the energies are obtained by finding the roots of the equation $s_{n+1,m} = 0$, which is a polynomial in $E$, of degree $(n+1)/2$. The corresponding radius $R_{n,m}$ is found through the relation

$$R_{n,m}^2 E_{n,m} = \frac{n}{2}\left(\frac{n}{2} + (d-1) - 1\right). \tag{14}$$

We see that the special $R$-values for which the $s$-states of spherium can be obtained in a closely analytical way arise from an expansion of the wavefunction in powers of $r_{12}$ that, for the mentioned $R$-values, becomes a finite polynomial (for a full discussion see [1, 2] and references therein). Of course, the spherium system is well defined for any value of $R$, and the corresponding Schrödinger equation can be solved numerically, leading to results that interpolate between those corresponding to the special $R$-values yielding analytical solutions.

The (unnormalized) wavefunction, radius and energy for the ground state ($m = 0$) and $n = 1$ are given by

$$\Psi_{1,0}(r_{12}) = s_0 + s_1\, r_{12}, \quad R_{1,0}^2 = \frac{\delta}{4\gamma}, \quad E_{1,0} = \gamma\,, \tag{15}$$

where from now on we have denoted $s_{k,0} \equiv s_k$. The parameters $\delta$ and $\gamma$ are tabulated in Table I.

| State | $(n,m)$ | Configuration | $\chi(\mathbf{\Omega_1}, \mathbf{\Omega_2})$ | $\delta$ | $\gamma$ |
|---|---|---|---|---|---|
| $^1S$ | (1,0) | $s^2$ | 1 | $2(d-1)-1$ | $\frac{1}{(d-1)-1}$ |

TABLE I: Ground state for $n = 1$ of $(d-1)$-spherium.

The (unnormalized) ground state wavefunctions for $n = 2, 3$ are the following,

$$\begin{aligned} \Psi_{2,0}(r_{12}) &= s_0 + s_1\, r_{12} + s_2\, r_{12}^2 & (16) \\ \Psi_{3,0}(r_{12}) &= s_0 + s_1\, r_{12} + s_2\, r_{12}^2 + s_3\, r_{12}^3, & (17) \end{aligned}$$

where the coefficients $s_k \equiv s_{k,0}(d)$, obtained through the recurrence relation (13), are analytically given in Appendix A for $k = 1, 2, 3$ and numerically shown in Table II for $d = 3 - 6$.

| $d$ | $s_0$ | $s_1$ | $s_2$ | $s_3$ |
|---|---|---|---|---|
| 3 | 1 | 1 | 0.178571 | 0.012946 |
| 4 | 1 | 0.5 | 0.053030 | 0.002703 |
| 5 | 1 | 0.333333 | 0.025 | 0.000968 |
| 6 | 1 | 0.25 | 0.014474 | 0.000449 |

TABLE II: Numerical values of the expansion coefficients $s_k \equiv s_{k,0}$ for $d = 3, 4, 5, 6$ and $n = 1, 2, 3$.

In order to compute the entanglement of the spherium's eigenstates (with $m = 0$) we are going to work with appropriately normalized eigenfunctions,

$$\psi_{n,0} = \frac{\Psi_{n,0}}{R^{d-1} N_n^{1/2}}, \tag{18}$$

where $N_n = \int |\Psi_{n,0}|^2 \, d\Omega_1 d\Omega_2$. The wavefunctions $\psi_{n,0}$ are now normalized to one over the surface of a hyper-sphere of radius $R$: $\int |\psi_{n,0}|^2 \, R^{2(d-1)} d\Omega_1 d\Omega_2 = 1$. The analytical values of the constant $N_n$ are determined in the next section.

## IV. ENTANGLEMENT IN $(d-1)$-SPHERIUM

Let us now evaluate in an analytical way the entanglement for the wavefunctions $\psi_{n,0}(r_{12})$ of the $(d-1)$-spherium as described in the two previous sections. For this purpose we need to calculate first the constant $N_n = \int |\Psi_{n,0}|^2 \, d\Omega_1 d\Omega_2$, and then the trace $Tr\left[\left(\rho_1^{(coord.)}\right)^2\right]$ which is given by the following multidimensional definite integral

$$\begin{aligned} Tr\left[\left(\rho_1^{(coord.)}\right)^2\right] \; = \; \int_{\mathbb{R}^{4(d-1)}} & \psi_{n,0}(\mathbf{r}_1', \mathbf{r}_2)\psi_{n,0}^*(\mathbf{r}_1, \mathbf{r}_2) \times \\ & \psi_{n,0}^*(\mathbf{r}_1', \mathbf{r}_2')\psi_{n,0}(\mathbf{r}_1, \mathbf{r}_2') \times \\ & R^{4(d-1)} d\Omega_1 d\Omega_2 d\Omega_1' d\Omega_2', \end{aligned} \tag{19}$$

where $R^{d-1} d\Omega_k$, $k = 1, 2$ are area elements on the surface of a $(d-1)$-hypersphere, and $d\Omega_k$ are elements of hyper-spherical angle, given by

$$d\Omega_k = \left( \prod_{j=1}^{d-2} \sin^{d-j-1} \theta_j^{(k)} \right) d\phi^{(k)}. \tag{20}$$

in terms of the hyperspherical angular coordinates of the two particles $\{\theta_1^{(k)}, ..., \theta_{d-2}^{(k)}, \phi^{(k)}\}$, with $0 \leq \theta_j^{(k)} \leq \pi$ for $j = 1, \ldots, d-2$, and $0 \leq \phi^{(k)} \leq 2\pi$. Atomic units will be used throughout the rest of the paper.

Here a comment concerning coordinates is in order. In Section II, when discussing general aspects of entanglement, the integrals involved in the calculation of entanglement were expressed in cartesian coordinates. However, in the particular case of spherium, it is clear that the most natural coordinates to employ are the hyper-spherical ones. Hence, as already indicated by the elements $d\Omega_i$ appearing in (19), in the present work we are going to formulate all the relevant integrals first in terms of hyper-spherical coordinates on the $(d-1)$-sphere where the two electrons are confined. For technical reasons we are also going to define a new set of angular variables in order to actually compute the aforementioned integrals.

To solve some of the integrals appearing in the study of entanglement in spherium we shall apply the methodology recently developed by Ruiz [39] to deal with atomic-related integrals. Let us first calculate the normalization constant $N_1$ of the ground state wavefunction $\Psi_{1,0}(r_{12})$ given by eq. (15); that is,

$$N_1 = \int |\Psi_{1,0}|^2 \, d\Omega_1 d\Omega_2 = J_0 + 2\gamma J_1 + \gamma^2 J_2, \tag{21}$$

where the symbols $J_k, k = 0, 1, 2$, denote the integral functions

$$J_k \equiv \int r_{12}^k \, d\Omega_1 d\Omega_2, \quad k = 0, 1, 2 \tag{22}$$

To evaluate these integrals we begin by doing a change of variables. Consider the triangle formed by the vectors $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_{12}$, where the last one stands for the relative vector position of particle 2 with respect to particle 1 (see Fig. 1). Following an idea originally advanced by Calais and Löwdin [40], we rotate the coordinate frame used to define the angular spherical coordinates of the vector $\mathbf{r}_2$. The $z$ axis of the new frame is the line joining the origin (which is the same as in the original frame) with particle 1, with the positive direction towards particle 1. The angular coordinates of $\mathbf{r}_2$ in the new frame are now denoted $\{\theta_1^{(12)}, ..., \theta_{d-2}^{(12)}, \phi^{(12)}\}$ (see Figure 1 for a three dimensional illustration of this change of reference frame). The integration variables concerning particle 2 are then transformed as: $\theta_i^{(2)} \to \theta_i^{(12)}$, and $\phi^{(2)} \to \phi^{(12)}$. The volume element associated to electron 2 can then be re-cast as,

$$\begin{aligned} d\Omega_2 &= \left( \prod_{j=1}^{d-2} \sin^{d-j-1} \theta_j^{(2)} \right) d\phi^{(2)} \\ &= \left( \prod_{j=1}^{d-2} \sin^{d-j-1} \theta_j^{(12)} \right) d\phi^{(12)} \\ &= d\Omega_{12}. \end{aligned} \tag{23}$$

Moreover, we use the Cohl representation [41] for $r_{12}^p$ in terms of the orthogonal Gegenbauer polynomials $C_n^{\alpha}(x)$:

$$\begin{aligned} r_{12}^p = & \sum_{n=0}^{\infty} \frac{(d+2n-2)\, 2^{d+p-3}\, \Gamma\left(\frac{d-2}{2}\right) \left(-\frac{1}{2}\right)_n R^p}{\sqrt{\pi}\, \Gamma\left(d+n+\frac{p}{2}-1\right)} \\ & \times \Gamma\left(\frac{1}{2}(d+p-1)\right) C_n^{d/2-1}(\cos\theta_{12}) \\ = & \sum_{n=0}^{\infty} -\frac{\pi^{\frac{d}{2}-1} 2^{d+p-2} \Gamma\left(n-\frac{1}{2}\right) R^p \Gamma\left(\frac{1}{2}(d+p-1)\right)}{\Gamma\left(d+n+\frac{p}{2}-1\right)} \\ & \times \sum_{\{\mu\}} \mathcal{Y}_{n,\{\mu\}}^*(\Omega_2) \mathcal{Y}_{n,\{\mu\}}(\Omega_1), \; p = 1, 2, \ldots, \end{aligned} \tag{24}$$

where $\Omega_k = (\theta_1^{(k)}, \theta_2^{(k)}, \ldots, \theta_{d-2}^{(k)}, \theta_{d-1}^{(k)} \equiv \phi^{(k)})$, and $\mathcal{Y}_{n,\{\mu\}}$ denote the known hyperspherical harmonics, which have the following expression [42–44]

$$\begin{aligned} \mathcal{Y}_{l,\{\mu\}}(\Omega_{d-1}) &= A_{l,\{\mu\}} e^{im\phi} \prod_{j=1}^{d-2} C_{\mu_j - \mu_{j+1}}^{\alpha_j + \mu_{j+1}}(\cos\theta_j) \\ & \qquad \times (\sin\theta_j)^{\mu_{j+1}} \\ &= \frac{1}{\sqrt{2\pi}} e^{im\phi} \prod_{j=1}^{d-2} \tilde{C}_{\mu_j - \mu_{j+1}}^{\alpha_j + \mu_{j+1}}(\cos\theta_j) \\ & \qquad \times (\sin\theta_j)^{\mu_{j+1}}, \end{aligned} \tag{25}$$

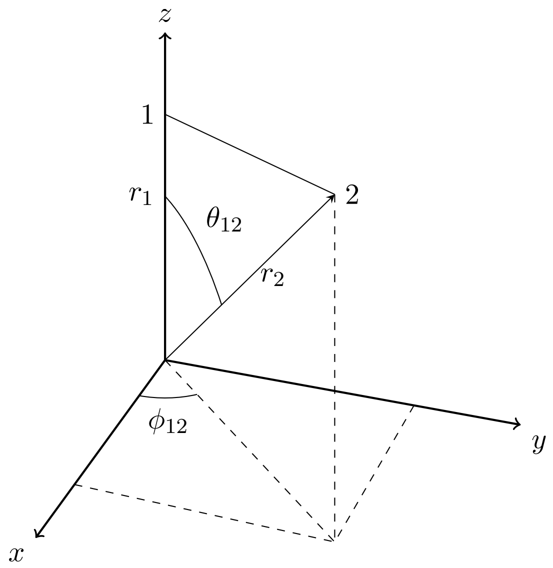

FIG. 1: Definition of the electron's coordinates used for the evaluation of entanglement-related integrals

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

$$\begin{aligned} |A_{l,\{\mu\}}|^2 &= \frac{1}{2\pi}\prod_{j=1}^{d-2}\frac{(\alpha_j+\mu_j)(\mu_j-\mu_{j+1})![\Gamma(\alpha_j+\mu_{j+1})]^2}{\pi\, 2^{1-2\alpha_j-2\mu_{j+1}}\Gamma(2\alpha_j+\mu_j+\mu_{j+1})} \\ &\equiv \frac{1}{2\pi}\prod_{j=1}^{d-2} A^{(j)}_{\mu_j,\mu_{j+1}} \, . \end{aligned} \tag{26}$$

The symbols $C_m^{\alpha}(x)$ and $\tilde{C}_m^{\alpha}(x)$ denote the orthogonal and orthonormal Gegenbauer polynomials [45] of degree $m$ and parameter $\alpha$ with respect to the weight function $\omega^*_\alpha = (1-x^2)^{\alpha-\frac{1}{2}}$ on the interval $[-1,+1]$, respectively, so that

$$\tilde{C}_m^{\alpha}(x) = \left(\frac{m!(m+\alpha)\Gamma^2(\alpha)}{\pi\, 2^{1-2\alpha}\Gamma(2\alpha+m)}\right)^{\frac{1}{2}} C_m^{\alpha}(x). \tag{27}$$

Then, by using the expressions (22) and (24) as explained in detail in Appendix B, we obtain that the integrals $J_k, k = 0-2$, are given by

$$J_0 = \left(\frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})}\right)^2, \tag{28}$$

$$J_1 = \frac{2^{d+1}\pi^{d-\frac{1}{2}}}{\Gamma\left(d-\frac{1}{2}\right)}R \tag{29}$$

and

$$J_2 = \frac{8\pi^d}{\Gamma\left(\frac{d}{2}\right)^2}R^2 \tag{30}$$

respectively. Finally, these values together with eq. (21) allows us to write the normalization constant as

$$N_1 = 4\pi^d\left(\frac{1+2\gamma^2R^2}{\Gamma\left(\frac{d}{2}\right)^2} + \frac{2^d\gamma}{\sqrt{\pi}\,\Gamma\left(d-\frac{1}{2}\right)}R\right) \tag{31}$$

Replacing the analytical expressions for the spherium state $\psi_{1,0}(r_{12})$, into the general expression for $Tr[(\rho_1^{(coord.)})^2]$ one gets,

$$\begin{aligned} & Tr[(\rho_1^{(coord.)})^2] \\ = & R^{2d-2}\int |\rho_1^{(coord.)}(\mathbf{r}_1', \mathbf{r}_1)|^2 \, d\Omega_1' d\Omega_1 \\ = & R^{4d-4}\int \psi_{1,0}(\mathbf{r}_1', \mathbf{r}_2)\psi_{1,0}^*(\mathbf{r}_1, \mathbf{r}_2)\psi_{1,0}^*(\mathbf{r}_1', \mathbf{r}_2') \times \\ & \psi_{1,0}(\mathbf{r}_1, \mathbf{r}_2') \, d\Omega_1 d\Omega_2 \, d\Omega_1' d\Omega_2' \\ = & N_1^{-2}\int_{\mathbb{S}^{d-1}} (1+\gamma\, r_{12})(1+\gamma\, r_{12'}) \times \\ & (1+\gamma\, r_{1'2})(1+\gamma\, r_{1'2'}) \, d\Omega_1 d\Omega_2 \, d\Omega_1' d\Omega_2' \\ = & N_1^{-2}\int \Bigg[ 1+\gamma(r_{12}+r_{12'}+r_{1'2}+r_{1'2'}) \\ + & \gamma^2(r_{12}r_{12'}+r_{12}r_{1'2}+r_{12'}r_{1'2}+r_{12}r_{1'2'} \\ + & r_{12'}r_{1'2'}+r_{1'2}r_{1'2'}) \\ + & \gamma^3(r_{12}r_{12'}r_{1'2}+r_{12}r_{12'}r_{1'2'}+r_{12}r_{1'2}r_{1'2'} \\ + & r_{12'}r_{1'2}r_{1'2'})+\gamma^4\, r_{12}r_{12'}r_{1'2}r_{1'2'} \Bigg] \\ \times & \; d\Omega_1 d\Omega_2 d\Omega_1' d\Omega_2' \end{aligned} \tag{32}$$

For convenience and taking into account the symmetries of the integrand of (32), we rewrite this expression as

$$Tr[(\rho_1^{(coord.)})^2] = N_1^{-2}(I_0 + 4\gamma\, I_1 + 6\gamma^2\, I_2 + 4\gamma^3 I_3 + \gamma^4\, I_4), \tag{33}$$

where the symbols $I_i, i = 1-4$, denote the following integral functions:

$$I_0 \equiv \int d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'}, \tag{34}$$

$$I_1 \equiv \int r_{12}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'}, \tag{35}$$

$$I_2 \equiv \int r_{12}\, r_{12'}\; d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'}, \tag{36}$$

$$I_3 \equiv \int r_{12}\, r_{12'}\, r_{1'2}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'}, \tag{37}$$

$$I_4 \equiv \int r_{12}\, r_{12'}\, r_{1'2}\, r_{1'2'}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'}. \tag{38}$$

These integrals have been analytically evaluated by means of the methodology described in Appendix B, obtaining the following values:

$$
\begin{aligned}
I_0 &= \left(\frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})}\right)^4 && (39)\\
I_1 &= \frac{2^{d+3}\pi^{2d-\frac{1}{2}}}{\Gamma\left(d-\frac{1}{2}\right)\Gamma\left(\frac{d}{2}\right)^2}R && (40)\\
I_2 &= \frac{4^{d+1}\pi^{2d-1}}{\Gamma\left(d-\frac{1}{2}\right)^2}R^2 && (41)\\
I_3 &= \frac{2^{3d+1}\pi^{2d-\frac{3}{2}}\Gamma\left(\frac{d}{2}\right)^2}{\Gamma\left(d-\frac{1}{2}\right)^3}R^3 && (42)\\
I_4 &= 2^{4d-3}\pi^{2d-2}\left[\frac{\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(d+\frac{1}{2}\right)}\right]^4 R^4 \times
\end{aligned}
$$

$$
\left[{}_5F_4\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},d-1;d+\frac{1}{2},d+\frac{1}{2},d+\frac{1}{2},d+\frac{1}{2};1\right)\right.
+8\left(d-\frac{1}{2}\right)^4 \times
\left.{}_5F_4\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},d-2;d-\frac{1}{2},d-\frac{1}{2},d-\frac{1}{2},d-\frac{1}{2};1\right)\right] \quad (43)
$$

Then, taking into account (8) and (33) we obtain that the entanglement measure for the spherium state $\psi_{1,0}(r_{12})$ is given by

$$
\begin{aligned}
\xi[|\psi_{1,0}\rangle] &= 1 - Tr[(\rho_1^{(coord.)})^2]\\
&= 1 - N_1^{-2}(I_0 + 4\gamma\, I_1 + 6\gamma^2\, I_2 + 4\gamma^3 I_3\\
&\quad + \gamma^4\, I_4) \qquad (44)
\end{aligned}
$$

The calculations required for evaluating the normalization constants $N_n$ and the integrals $I_i, i = 1-4$ involved in the determination of the amount of entanglement of the spherium $s$-eigenstates $\psi_{n,0}(r_{12})$ with $n \geq 2$ are similar to those for the state $\psi_{1,0}(r_{12})$, following the lines indicated in Appendix B. In particular, the above explained analytical techniques can be readily applied to the $n = 2$ and $n = 3$ $s$-states, with the wavefunctions given by Eqs. (16)-(17) and Table II.

The results obtained for the amount of entanglement exhibited by the $(d-1)$-spherium (singlet) ground state are summarized in Table III and in Figures 3- 6. In Table III we provide the amounts of entanglement and the energies corresponding to the ground state of $(d-1)$-spherium for various dimensionalities. The analytical procedure for calculating the entanglement of $s$-states of spherium has been checked by the numerical computation of entanglement for some of these states.

It can be seen in Table III that, for a given dimensionality $d$, the amount of entanglement associated with the ground state of spherium increases with the radius $R$. This trend is akin with what has been recently observed in other two-electron models [5]; see also the recent review [8]. In fact, we know from previous experience with two-electron systems that, for a constant strength of the interaction between the particles, entanglement tends to increase when the confinement becomes weaker. This behaviour has been observed in several systems, such as the Moshinsky model, the Hooke atom, the Crandall model, and the Helium iso-electronic series [5]. The connection between entanglement and confinement has also been detected in two-electron systems in a uniform magnetic field [4]. In these systems confinement decreases, and entanglement increases, when the intensity of the applied magnetic field becomes weaker. In spherium confinement decreases, and entanglement increases, for increasing values of the radius $R$. In Figure 2 we plotted, for $d = 3$ (that is, when the two electrons are confined to an ordinary two-dimensional sphere), the wavefunction $\psi_{10}(\theta_1, \phi_1, \theta_2, \phi_2)$ as a function of the angular coordinates $(\theta_1, \phi_1)$ of one of the particles, keeping constant the values of the coordinates $(\theta_2, \phi_2)$ of the other particle (here we use the standard notation for

| State | $d$ | $R_{n,0}$ | $E_{n,0}$ | $\xi[\lvert\Psi_{n,0}\rangle]$ |
|---|---|---|---|---|
| $n=1$ | 3 | 0.866025 | 1 | 0.0677386 |
|  | 4 | 1.58114 | 0.5 | 0.0436006 |
|  | 5 | 2.29129 | 0.333333 | 0.0323117 |
|  | 6 | 3. | 0.25 | 0.0256836 |
| $n=2$ | 3 | 2.64575 | 0.285714 | 0.235892 |
|  | 4 | 4.06202 | 0.181818 | 0.160622 |
|  | 5 | 5.47723 | 0.133333 | 0.121691 |
|  | 6 | 6.89202 | 0.105263 | 0.0979235 |
| $n=3$ | 3 | 5.43118 | 0.127128 | 0.391247 |
|  | 4 | 7.51536 | 0.0929523 | 0.293556 |
|  | 5 | 9.61594 | 0.0729996 | 0.232591 |
|  | 6 | 11.7241 | 0.0600194 | 0.191796 |

TABLE III: Radius, energy and entanglement values of the of the $(d-1)$-dimensional spherium with singlet ground-state wavefunctions $\Psi_{n,0}(r_{12})$, $n=1,2,3$, for various dimensionalities $d=3,4,5,6$.

the polar and azimuthal coordinates on a two dimensional sphere). Since the wavefunction is in this case real, we depict in Fig. 2 the wave function $\psi_{10}$ itself, not its squared modulus. In Fig. 2 we have $\theta_2=0$; $\phi_2=0$ (upper left) and $\theta_2=\frac{\pi}{2}$;$\phi_2=0$ (upper right); $\theta_2=\frac{\pi}{2}$; $\phi_2=\frac{\pi}{2}$ (lower left) and $\theta_2=\frac{\pi}{4}$;$\phi_2=\frac{\pi}{2}$ (lower right). Figure 2 provides an illustration of the entangled character of the associated two-electron state. If it were a non-entangled state, it would be of the form $\Phi(\theta_1,\phi_1)\Phi(\theta_2,\phi_2)\frac{1}{\sqrt{2}}(\chi_{+-}-\chi_{-+})$. We would have a factorizable spatial wavefunction (remember that the spatial parts of the wavefunctions corresponding to the states that we are considering are symmetric) and a singlet spin wavefunction. With a factorized spatial wavefunction the four graphics depicted in Figure 2 would be identical. All of them would correspond to $\Phi(\theta_1,\phi_1)$. The differences between the four graphics in Figure 2 constitute a concrete pictorial illustration of the entanglement of the concomitant two-electron state.

The connection between entanglement and the radius $R$ of the spherium system can be appreciated in Fig. 3. In this Figure we plotted the amount of entanglement versus the radius of the confining sphere for several singlet states wavefunctions $\psi_{n,0}(r_{12})$ of the 2-dimensional ($d=3$) spherium, with the integer parameter $n$ (characterizing the radius' values $R_{n,m}$ leading to exact analytical solutions) adopting values $n=1,\ldots,6$. We observe that entanglement grows with the radius. The dependence of entanglement on the spherium radius is, however, nonlinear. For small values of $R$ (corresponding to small values of the parameter $n$) the rate of growth of entanglement with $R$ is greater than for larger values of $R$. The monotonically increasing behaviour of entanglement with $R$ illustrated in Fig. 3 corresponds to the particular case $d=3$. However, the same trend is observed for other values of the spatial dimensionality $d$, as can be seen in Table III for dimensions up to $d=6$.

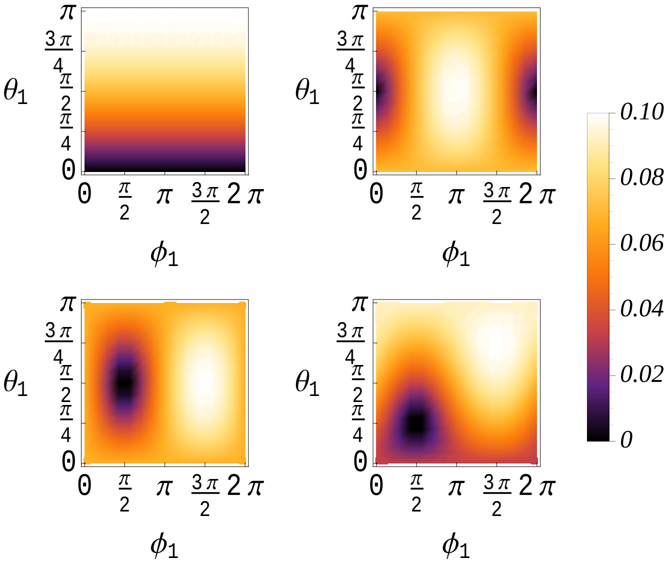

FIG. 2: Wave function $\psi(\theta_1, \phi_1, \theta_2, \phi_2)$ as a function of the angular coordinates $\theta_1, \phi_1$ of one the electrons for constant values $\theta_2$ and $\phi_2$ of the coordinates of the other electron. On the upper left plot we have $\theta_2 = 0$ and $\phi_2 = 0$ and on the upper right one $\theta_2 = \frac{\pi}{2}$ and $\phi_2 = 0$. The lower left plot corresponds to $\theta_2 = \frac{\pi}{2}$ and $\phi_2 = \frac{\pi}{2}$ and the lower right one to $\theta_2 = \frac{\pi}{4}$ and $\phi_2 = \frac{\pi}{2}$. The different aspect of the four figures illustrates the fact that the wavefunction $\psi$ is entangled.

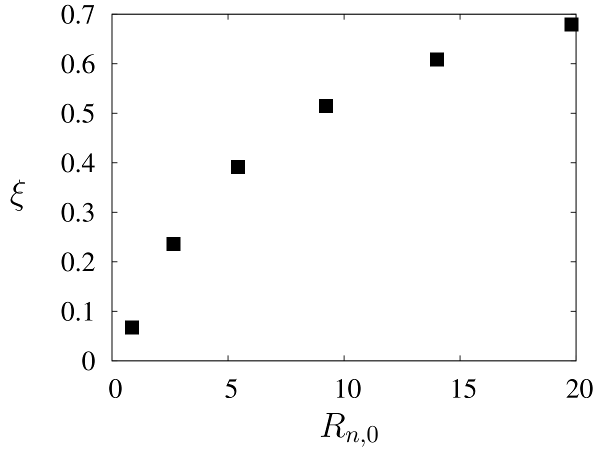

FIG. 3: Entanglement against the radius $R$ for the singlet state wavefunctions $\psi_{n,0}(r_{12})$, $n = 1, \ldots, 6$, of $(d-1)$-dimensional spherium with $d = 3$.

The observed decreasing rate of growth of entanglement with the spherium's radius $R$ does not rule out the possibility that the (increasing) entanglement measure $\xi$ tends to its maximum possible value ($\xi = 1$) in the limit $R \to \infty$. Unfortunately, the case by case (exact) evaluation of the entanglement of each exactly solvable eigenstate of spherium does not allow us to analytically determine the aforementioned limit value. However, the behaviour of other two-electron systems suggests that entanglement in spherium does indeed approach its maximum value as $R \to \infty$. In the $d = 3$ case the $R \to \infty$ limit of spherium can be related to a limit case of the two dimensional Hooke atom. In the $R \to \infty$ limit, as the radius of curvature of the confining sphere tends to zero, the Schrödinger equation describing spherium approaches that of two electrons moving in a two dimensional Euclidean plane. This suggests that the limit value of entanglement in $d = 3$ spherium should coincide with the limit value of entanglement in the two dimensional Hooke system when the confining potential becomes negligible compared with the electron-electron interaction potential. Results reported by Kościk and Hassanabadi in [18] provide numerical evidence that the entanglement of the two dimensional Hooke system tends to its maximum value in this limit.

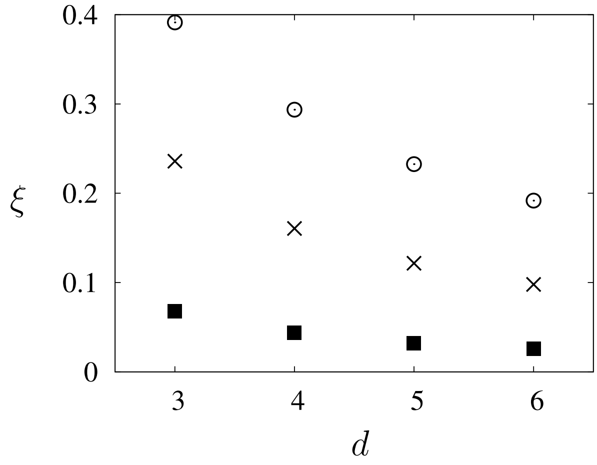

FIG. 4: Entanglement against dimensionality for the singlet state wavefunctions $\psi_{n,0}(r_{12})$ with $n = 1$ (■), $n = 2\,(\times)$, $n = 3\,(\odot)$, of $(d-1)$-dimensional spherium with $d = 3, \ldots, 6$.

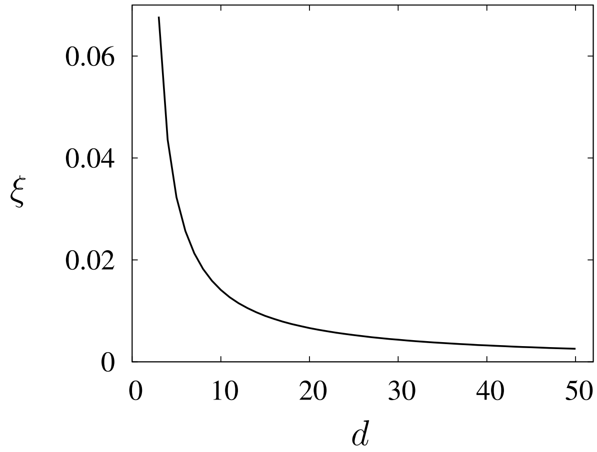

FIG. 5: Entanglement against dimensionality for the singlet state wavefunction $\psi_{1,0}(r_{12})$.

In Fig. 4 the ground state's entanglement is plotted against the spatial dimensionality $d$. We have computed the entanglement measure based on the linear entropy of the single particle reduced density matrix for spatial dimensionalities in the range $3 \leq d \leq 6$, and for $n = 1, 2, 3$. We see that the range of possible values of entanglement, as well as the largest adopted value (for the above range of $n$-values) decreases with $d$.

It can be appreciated from Fig. 4 that, for given constant values of the integer parameter $n$ determining the special radius $R_{n,m}$ for which spherium admits closed analytical solutions, the amount of entanglement exhibited by the ground state of spherium decreases monotonically with the spatial dimensionality. We conjecture that entanglement behaves in this way for all values of the parameter $n$. In the particular case of $n = 1$, since we have an analytical expression for $R_{10}$, we can obtain a closed analytical expression for the entanglement of the states $\psi_{10}$ for all values of the spatial dimension $d$. The corresponding behaviour of entanglement as a function of $d$ is shown in Fig. 5, where it can be seen that entanglement decreases with $d$. This trend might be related to a well-known, but counterintuitive, feature of multi-dimensional spheres: the surface area of a $(d-1)$-hypersphere of radius 1 (that is, the total hyper-solid angle $\int_{\text{sphere}} d\Omega$) tends to zero as $d \to \infty$ (for an interesting discussion on the physical implications of the geometry of hyperspheres see, for instance, [46] and references therein). The above can be construed as implying that, as far as the hyperspherical angular degrees of freedom are concerned, the particles constituting the spherium system can be regarded as becoming more confined as $d$ increases. These geometrical considerations suggest a tentative explanation of the behaviour of entanglement with spatial dimensionality $d$ in spherium: entanglement decreases with $d$, because an increasing spatial dimensionality tends to make the system more confined. Then, according to this explanation, the entanglement-dimensionality relation in spherium would be another instance of the entanglement-confinement relation observed in several two-electron systems [5]. These considerations have some plausibility in connection with the behaviour of entanglement with dimensionality for large values of $d$. However, a simple, direct connection between entanglement and the area of the unit hyper-sphere seems unlikely, since for $n = 1$ entanglement decreases monotonically with the spatial dimension for all $d$-values, while the surface area of a unit hyper-sphere does not behave monotonically with $d$: for moderately small values of $d$ it first increases with $d$, reaching a maximum for $d \approx 7$, and then decreases monotonically for all $d$. The decreasing behaviour of entanglement with spatial dimension in spherium might be related to the properties of other quantum mechanical models where the limit of high dimensionality leads to classical behaviour [47].

The effect of space dimensionality on entanglement has also been studied in the Hooke atom by Kośćik and Hassanabadi [18]. These authors studied the behaviour of entanglement in the Hooke system for one, two, and three spatial dimensions. The dependence of entanglement on spatial dimension is not as clear in the Hooke atom as it is in spherium. Indeed, the dependence of entanglement with dimension in the Hooke system depends on the strength of the electron-electron interaction (as compared with the strength of the confining potential). This more complicated behaviour is probably due to the fact that in the Hooke atom the entanglement features of the system's eigenstates depend on both the radial and angular behaviours of the concomitant wavefunctions. In spherium, in contrast, the effective configuration space solely involves the angular variables.

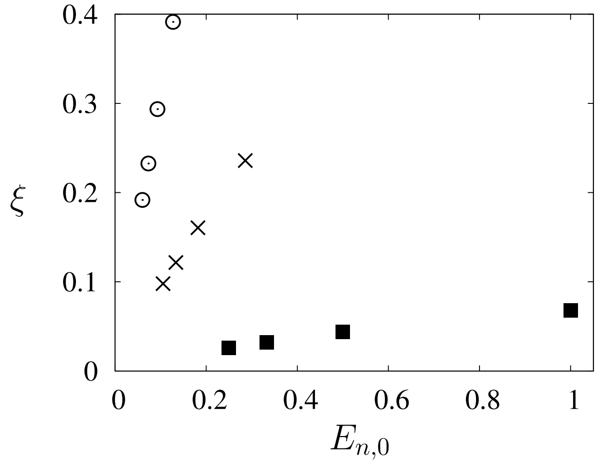

FIG. 6: Entanglement against energy for the singlet state wavefunctions $\psi_{n,0}(r_{12})$ with $n = 1$ (■), $n = 2$ ($\times$), $n = 3$ ($\odot$) of the $(d-1)$-dimensional spherium with $d = 3 - 6$.

In Fig. 6 we depict the amount of entanglement against the energy of the singlet state for $d = 3, 4, 5$ and 6. We observe that entanglement of $(d-1)$-dimensional spherium tends to increase with energy. A similar behaviour has been observed in other models, such as the Crandall and the Hooke ones [5], as well as for the singlet states of the Helium atom employing high-quality, state-of- the-art wavefunctions [12] (although for more general states of Helium the energy-entanglement connection seems to be much more complicated [28, 29]).

Finally, let us comment on the excited states of the spherium. There are no excited states for the singlet wavefunction with $n = 1$ and $n = 2$. This is due to the fact that the equation allowing for the calculation of the energy for each $n$ has only one root which correspond to $m = 0$. For $n \geq 3$ the excited states begin to appear because the equation mentioned above has a degree equal or greater than 2. So e.g., for $n = 3$ there are two possible values for $m = 0, 1$, and therefore one exact analytical excited state can be obtained (corresponding to $m = 1$).

## V. CONCLUSIONS

We have explored the entanglement related features of $(d-1)$-spherium. This quantum system consists of two electrons interacting via a Coulomb potential and confined to the surface of a $d$-dimensional ball (that is, a $(d-1)$-hypersphere) of radius $R$. This system is quasi-exactly solvable: its Schrödinger eigenvalue equation can be solved in a closed analytical fashion for particular values of the radius $R$ and particular eigenstates. In the present contribution we computed in an exact analytical way the amount of entanglement (as measured by the linear entropy of the single-particle reduced density matrix) of the ground state of spherium, for several values of the radius $R$

(corresponding to different values of the parameter $n$) and of the space dimension $d$. To the best of our knowledge this is the first two-electron system with Coulomb interaction for which exact entanglement calculations have been done. We investigated the dependence of entanglement on the radius $R$ of the spherium system and on the spatial dimensionality $d$. The relation between entanglement and energy was also considered.

We have found that the amount of entanglement of the ground state of spherium increases with the radius $R$ of the hypersphere where the particles are confined. This behaviour is consistent with a general property exhibited by other two-electron systems: entanglement tends to increase when, for a given value of the interaction strength, the confinement due to the external common fields acting on both particles decreases. For instance, in the helium isoelectronic series the entanglement of the ground state increases when one considers decreasing values of the nuclear charge $Z$ [5, 12]. Likewise, in the three-dimensional Moshinsky model with a uniform magnetic field the entanglement of the ground state increases for decreasing values of the applied magnetic field [4].

The results reported in the present work indicate that in spherium the amount of entanglement exhibited by the ground state decreases with the spatial dimensionality $d$, a behaviour that can also be related to the entanglement-confinement connection. In addition, we have observed that entanglement of spherium tends to increase with energy. This relation between entanglement and energy is similar to what is observed in other two-electron models, such as the Moshinsky system, the Hooke atom, and the Crandall model [5].

We hope that the techniques developed in the present work may stimulate new analytical approaches to the study of entanglement in systems with Coulomb interactions. Any further developments in this direction will be very welcome.

### Acknowledgments

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### Appendix A: $(d-1)$-Spherium Hamiltonian

Here we are going to briefly review some basic aspects of the Hamiltonian describing the two-electron system spherium. For more details on spherium and the solutions of the concomitant Schrödinger equation see [1, 2] and references therein. Spherium consists of two electrons confined to a $(d-1)$-sphere (that is, the surface of a $d$-dimensional ball) and interacting via a Coulomb potential. The corresponding Schrödinger eigenvalue equation reads,

$$-\left(\frac{\hbar^2}{2m}\right)\frac{1}{R^2}\left[\Delta^{(1)}_{S^{d-1}}+\Delta^{(2)}_{S^{d-1}}\right]\Psi+\frac{e^2}{r_{12}}\Psi=E\Psi, \tag{A1}$$

where $R$ is the radius of the $(d-1)$-sphere, $r_{12}$ is the distance between the two electrons (evaluated in the $d$-dimensional euclidean space in which the $(d-1)$-sphere is embedded), $\Psi$ is the two-electron eigenfunction, $E$ is the corresponding eigenenergy, and $\Delta^{(1,2)}_{S^{d-1}}$ are the angular Laplacian operators acting on the angular coordinates of each electron. Note that the wavefunction $\Psi$ is a function of the hyper-spherical angular coordinates of both electrons, $\{\theta^{(k)}_1,...,\theta^{(k)}_{d-2},\phi^{(k)}\}$, with $0\leq\theta^{(k)}_j\leq\pi$ for $j=1,\ldots,d-2$, and $0\leq\phi^{(k)}\leq 2\pi$. The upper index $k=1,2$ refers to the two electrons. The spherical Lapacian operator (Laplace-Beltrami operator on the $(d-1)$-sphere) acts on a function $f$ defined on the $(d-1)$-sphere according to the following recurrence relation,

$$\begin{aligned}\Delta_{S^{d-1}}f(\theta_1,\zeta) &= (\sin\theta_1)^{2-d}\frac{\partial}{\partial\theta_1}\left[(\sin\theta_1)^{d-2}\frac{\partial f}{\partial\theta_1}\right]\\ &+ (\sin\theta_1)^{-2}\Delta_\zeta f,\end{aligned} \tag{A2}$$

where $\zeta=\{\theta_2,...,\theta_{d-2},\phi\}$ denotes the set of all the angular coordinates on the $(d-1)$-sphere except $\theta_1$, and $\Delta_\zeta$ is the spherical Laplacian corresponding to a $(d-2)$-sphere with hyper-spherical coordinates $\zeta=\{\theta_2,...,\theta_{d-2},\phi\}$. That is, the operator $\Delta_\zeta$ only involves derivatives with respect to the coordinates appearing in the set $\zeta$. For instance, for $d=3$ the spherical Laplacian adopts the well known form,

$$\Delta_{S^2} f(\theta,\phi) = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2}. \tag{A3}$$

It is convenient to recast the Schrödinger equation (A1) in a dimensionless form, using atomic units. In order to do that we divide equation (A1) by the constant $me^4/\hbar^2$ (which has dimensions of energy) obtaining,

$$-\frac{1}{2\tilde{R}^2}\left[\Delta^{(1)}_{S^{d-1}} + \Delta^{(2)}_{S^{d-1}}\right]\Psi + \frac{1}{\tilde{r}_{12}}\Psi = \tilde{E}\Psi, \tag{A4}$$

where,

$$\begin{aligned} \tilde{R} &= \frac{me^2}{\hbar^2}R & \text{(A5)}\\ \tilde{r}_{12} &= \frac{me^2}{\hbar^2}r_{12} & \text{(A6)}\\ \tilde{E} &= \frac{\hbar^2}{me^4}E. & \text{(A7)} \end{aligned}$$

Note that in its dimensionless form (A4) the Schrödinger equation for spherium only has one parameter, the dimensionless radius $\tilde{R}$ given by (A5). This parameter is a dimensionless quantity involving the parameter $e^2$, measuring the strength of the interaction between the electrons, and the radius $R$ of the confining sphere. When studying entanglement in spherium we investigate, among other things, its dependence on the dimensionless parameter $\tilde{R}$, which can be regarded as proportional to the quotient between the quantities $e^2$ (interaction strength) and $1/R$ (amount of confinement). In the rest of the present article, since we are going to deal exclusively with the dimensionless form (A4) of the spherium's Schrödinger equation, we are going to drop the upper "tilde" from $R$, $r_{12}$ and $E$ (as in equation (10)).

In the case of $s$-states, the solutions of spherium's Schrödinger equation are functions of the inter-particle distance $r_{12}$. That is, one has $\Psi = \Psi(r_{12})$, with

$$r_{12} = R\sqrt{2(1-\cos\alpha)}, \tag{A8}$$

where $\cos\alpha$ can be expressed in terms of the hyper-spherical coordinates of the two electrons,

$$\begin{aligned} \cos\alpha &= \cos\theta_1^{(1)}\cos\theta_1^{(2)}\\ &+ \sin\theta_1^{(1)}\sin\theta_1^{(2)}\cos\theta_2^{(1)}\cos\theta_2^{(2)}\\ &+ \sin\theta_1^{(1)}\sin\theta_1^{(2)}\sin\theta_2^{(1)}\sin\theta_2^{(2)}\\ \cdots\\ &+ \sin\theta_1^{(1)}\sin\theta_1^{(2)}\cdots\sin\theta_{d-2}^{(1)}\sin\theta_{d-2}^{(2)}\cos\phi^{(1)}\cos\phi^{(2)}.\\ &+ \sin\theta_1^{(1)}\sin\theta_1^{(2)}\cdots\sin\theta_{d-2}^{(1)}\sin\theta_{d-2}^{(2)}\sin\phi^{(1)}\sin\phi^{(2)}. \end{aligned} \tag{A9}$$

For $s$-states the Schrödinger equation (A1) can be re-expressed in terms of the derivatives of the wavefunction with respect to the variable $u = r_{12}$ [1, 2],

$$\left[\frac{u^2}{4R^2} - 1\right]\frac{d^2\Psi}{du^2} + \left[\frac{u(2d-3)}{4R^2} - \frac{d}{u}\right]\frac{d\Psi}{du} + \frac{\Psi}{u} = E\Psi. \tag{A10}$$

### Appendix B: Expansion coefficients of spherium $s$-eigenstates $\Psi_{n,0}(r_{12})$ with $n = 1, 2, 3$

The analytical expression for the expansion coefficients $s_k \equiv s_{k,0}(d)$ of the spherium $s$-eigenstates $\Psi_{n,0}(r_{12})$ with $n = 1, 2, 3$, have the following form:

$$\begin{aligned}
s_0 &= 1 \\
s_1 &= \frac{1}{d-2} \equiv \gamma \\
s_2 &= \frac{1-2d}{-8d^3+34d^2-46d+20} \\
s_3 &= \frac{1}{48600}\Bigg( -\frac{5520}{(d-2)^2} - \frac{5400}{d-1} + \frac{1600}{1-2d} + \frac{2393}{d-2} \\
&\quad -\frac{4050}{d^2} + \frac{24975}{d} - \frac{42336}{2d+1} \\
&\quad + \frac{900(d(14d-23)+6)\sqrt{\frac{d(d(64(d-2)d+169)-78)+9}{d^2(d(3-2d)+2)^2}}}{(d-2)(d-1)d(2d-1)}\Bigg).
\end{aligned} \tag{B1}$$

They have been obtained from the recurrence relation (13).

### Appendix C: Evaluation of the multidimensional integrals involved in the entanglement of spherium

Here we first give some further details of the calculation of the relevant integrals involved in the determination of the normalization constant $N_1$ of the ground state wavefunction $\Psi_{1,0}(r_{12})$ given by Eq. (15). Later on, we provide with further information of the derivation of the integral functions involved in the determination of the entanglement measure of such a state. Finally, we give indications for the similar calculation of the normalization constant $N_n$ and the entanglement measure of the general wavefunctions $\Psi_{n,0}(r_{12})$, $n \geq 2$, of the $d$-dimensional spherium.

*Derivation of the normalization constant $N_1$ given by Eq. (31).* This issue reduces to prove that the two-center integrals $J_i, i = 0 - 2$, defined by expressions (22) have the values given by Eqs. (28), (29) and (30), respectively. The value (28) of the integral $J_0$ is straightforward since it is the product of the volumes of the hyperspheres for each electron. To obtain the values (29) and (30) of $J_1$ and $J_2$, respectively, we use the Cohl expansion (24) for $r_{12}^p$ in terms of the Gegenbauer polynomials, $C_m^\alpha(x)$, and then we apply the orthogonality property of these polynomials which reads [45] as

$$\int_{-1}^{1} (1-t^2)^{\alpha-\frac{1}{2}} C_n^\alpha(x) C_m^\alpha(x)\, dx = \frac{\pi\, 2^{1-2\lambda}\Gamma(n+2\lambda)}{n!(n+\lambda)[\Gamma(\lambda)]^2}\delta_{m,n} \tag{C1}$$

where $Re(\lambda) > -1/2$ with $\lambda \neq 0$ and that $C_0^\alpha(x) = 1$. Then, we obtain for the integral $J_1$ the following expression:

$$
\begin{aligned}
J_1 &= \sum_{n=0}^{\infty}(2n+d-2)\,R\left(-\frac{1}{2}\right)_n 2^{d-2}\,\pi^{-1/2} \\
&\frac{\Gamma(\frac{d}{2}-1)\Gamma(\frac{d}{2})}{\Gamma(d+n-\frac{1}{2})}\int C_n^{\frac{d}{2}-1}(\cos\theta_{12})\,d\Omega_1 d\Omega_2 \\
&= \int d\Omega_1 \sum_{n=0}^{\infty}(2n+d-2)\,R\left(-\frac{1}{2}\right)_n 2^{d-2} \\
&\pi^{-1/2}\frac{\Gamma(\frac{d}{2}-1)\Gamma(\frac{d}{2})}{\Gamma(d+n-\frac{1}{2})}\int C_n^{\frac{d}{2}-1}(\cos\theta_{12})\,d\Omega_{12} \\
&= \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})}\sum_{n=0}^{\infty}(2n+d-2)\,R\left(-\frac{1}{2}\right)_n 2^{d-2} \\
&\pi^{-1/2}\frac{\Gamma(\frac{d}{2}-1)\Gamma(\frac{d}{2})}{\Gamma(d+n-\frac{1}{2})} \\
&\times\int C_n^{\frac{d}{2}-1}(\cos\theta_{12})\,C_0^{\frac{d}{2}-1}(\cos\theta_{12}) \\
&\qquad\qquad \times[\sin\theta_{j=1}^{(12)}]^{d-2}\,d\Omega_{j=1}^{(12)} \\
&\times\prod_{j=2}^{d-2}\int_0^{\pi}[\sin\theta_j^{(12)}]^{d-j-1}\,d\theta_j^{(12)}\int_0^{2\pi}d\phi^{(12)}
\end{aligned}
$$

Now we do change of integration variables,

$$
\begin{aligned}
t &= \cos\theta_{j=1}^{(12)}, && \text{(C2)} \\
dt &= -\sin\theta_{j=1}^{(12)}\,d\theta_{j=1}^{(12)} && \text{(C3)} \\
&= -(1-t^2)^{1/2}\,d\theta_{j=1}^{(12)},
\end{aligned}
$$

obtaining the following expression

$$
\begin{aligned}
J_1 &= \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \sum_{n=0}^{\infty}(2n+d-2)\, R \left(-\frac{1}{2}\right)_n 2^{d-2} \\
&\quad \pi^{-1/2} \frac{\Gamma(\frac{d}{2}-1)\Gamma(\frac{d}{2})}{\Gamma(d+n-\frac{1}{2})} \\
&\times \int C_n^{\frac{d}{2}-1}(t)\, C_0^{\frac{d}{2}-1}(t)(1-t^2)^{(\frac{d}{2}-1)-\frac{1}{2}}\, dt \\
&\quad (2\pi) \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma(\frac{d-j}{2})}{\Gamma(\frac{d-j+1}{2})} \\
&= \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \sum_{n=0}^{\infty}(2n+d-2)\, R \left(-\frac{1}{2}\right)_n 2^{d-2} \\
&\quad \pi^{-1/2} \frac{\Gamma(\frac{d}{2}-1)\Gamma(\frac{d}{2})}{\Gamma(d+n-\frac{1}{2})} (2\pi)\delta_{n,0} \\
&\times \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma(\frac{d-j}{2})}{\Gamma(\frac{d-j+1}{2})} \frac{\pi\, 2^{3-d}\Gamma(n+d-2)}{n!(n+\frac{d}{2}-1)\Gamma(\frac{d}{2}-1)^2} \\
&= \frac{2^{d+1}\pi^{\frac{d}{2}+1}\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(d-\frac{1}{2}\right)} R \\
&\quad \times \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma(\frac{d-j}{2})}{\Gamma(\frac{d-j+1}{2})} \\
&= \frac{2^{d+1}\pi^{d-\frac{1}{2}}}{\Gamma\left(d-\frac{1}{2}\right)} R
\end{aligned}
\tag{C4}
$$

for the integral $J_1$ which is equal to the wanted value (29). Operating in a similar way we obtain

$$
\begin{aligned}
J_2 &= \int d\Omega_1 \int r_{12}^2\, d\Omega_{12} \\
&= \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \int \Bigg( 2\, R^2\, C_0^{\frac{d}{2}-1}(\cos\theta_{12}) \\
&\quad - \frac{2\, R^2}{d-2} C_1^{\frac{d}{2}-1}(\cos\theta_{12}) \Bigg)\, d\Omega_{12} \\
&= \frac{8\pi^{\frac{d+3}{2}}\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)^2} R^2 \\
&\quad \times \prod_{j=2}^{d-2} \sqrt{\pi} \frac{\Gamma(\frac{d-j}{2})}{\Gamma(\frac{d-j+1}{2})} \\
&= \frac{8\pi^d}{\Gamma\left(\frac{d}{2}\right)^2} R^2
\end{aligned}
\tag{C5}
$$

which is equal to the wanted value (30). Finally, by performing the sum in (21) with $J_0, J_1$ and $J_2$, we arrive at final expression (31) for the normalization, $N_1$.
It is worth to say that it is possible to compute the normalizaton of an arbitrary $s$-state of the $d$-dimensional spherium by means of the integral $J_0$ and the general one-center integral

$$
\int r_{12}^q\, d\Omega_1 d\Omega_2 = \frac{2^{d+q}\pi^{d-\frac{1}{2}}\Gamma\left(\frac{d+q-1}{2}\right)}{\Gamma\left(\frac{d}{2}\right)\Gamma\left(d+\frac{q}{2}-1\right)} R^q \tag{C6}
$$

with $q \geq 1$.

*Derivation of the values (39)-(43) for the multicenter integrals $I_i, i = 0-4$ defined by Eqs. (34)-(38), which are involved in the entanglement of the s-states of the d-dimensional spherium.* These values are characterized by the parameter $n$, which determines the radius $R_n$ of the sphere on which the particles are confined. For this issue we have first determined the following general expressions

$$\begin{aligned}\int r_{12}^{q_1} r_{12'}^{q_2} r_{1'2}^{q_3} r_{1'2'}^{q_4}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'} \;&=\; \pi^{2d-2} 2^{4d+q_1+q_2+q_3+q_4-7} \\ &\times \frac{\Gamma\left(\frac{d+q_1-1}{2}\right)\Gamma\left(\frac{d+q_2-1}{2}\right)}{\Gamma(d-1)\Gamma\left(d+\frac{q_1}{2}-1\right)\Gamma\left(d+\frac{q_1}{2}\right)\Gamma\left(d+\frac{q_2}{2}-1\right)\Gamma\left(d+\frac{q_2}{2}\right)} \\ &\times \frac{\Gamma\left(\frac{1}{2}(d+q_3-1)\right)\Gamma\left(\frac{1}{2}(d+q_4-1)\right)}{\Gamma\left(d+\frac{q_3}{2}-1\right)\Gamma\left(d+\frac{q_3}{2}\right)\Gamma\left(d+\frac{q_4}{2}-1\right)\Gamma\left(d+\frac{q_4}{2}\right)} R^{q_1+q_2+q_3+q_4} \\ &\times \Bigg[ 8\Gamma(d-1)\Gamma\left(d+\frac{q_1}{2}\right)\Gamma\left(d+\frac{q_2}{2}\right)\Gamma\left(d+\frac{q_3}{2}\right)\Gamma\left(d+\frac{q_4}{2}\right) \\ &\;{}_5F_4\Big(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},d-2;d+\frac{q_1}{2}-1,d+\frac{q_2}{2}-1, \\ &\qquad\qquad d+\frac{q_3}{2}-1,d+\frac{q_4}{2}-1;1\Big) \\ &+\Gamma(d-1)\Gamma\left(d+\frac{q_1}{2}-1\right)\Gamma\left(d+\frac{q_2}{2}-1\right)\Gamma\left(d+\frac{q_3}{2}-1\right)\Gamma\left(d+\frac{q_4}{2}-1\right) \\ &\;{}_5F_4\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},d-1;d+\frac{q_1}{2},d+\frac{q_2}{2},d+\frac{q_3}{2},d+\frac{q_4}{2};1\right)\Bigg]\end{aligned} \tag{C7}$$

for four-center integrals,

$$\begin{aligned}&\int r_{ij}^{q_1} r_{ik'}^{q_2} r_{pk}^{q_3}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'} = \\ &2^{3d-3+q_1+q_2+q_3}\pi^{\frac{3}{2}(d-1)} R^{q_1+q_2+q_3} \\ &\frac{\Gamma(\frac{d+q_1-1}{2})\Gamma(\frac{d+q_2-1}{2})\Gamma(\frac{d+q_3-1}{2})}{\Gamma(d-1+\frac{q_1}{2})\Gamma(d-1+\frac{q_2}{2})\Gamma(d-1+\frac{q_3}{2})}\frac{2\pi^{d/2}}{\Gamma(d/2)}.\end{aligned} \tag{C8}$$

for three-center integrals,

$$\begin{aligned}&\int r_{ij}^{q_1} r_{pk'}^{q_2}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'} = \\ &2^{2d-2+q_1+q_2}\pi^{d-1} R^{q_1+q_2} \\ &\frac{\Gamma(\frac{d+q_1-1}{2})\Gamma(\frac{d+q_2-1}{2})}{\Gamma(d-1+\frac{q_1}{2})\Gamma(d-1+\frac{q_2}{2})}\left(\frac{2\pi^{d/2}}{\Gamma(d/2)}\right)^2.\end{aligned} \tag{C9}$$

for two-center integrals, and

$$\begin{aligned}\int r_{ij}^{q_1}\, d\Omega_1 d\Omega_2 d\Omega_{1'} d\Omega_{2'} &= \frac{2^{d-1+q_1}\pi^{\frac{d-1}{2}} R^{q_1}\Gamma(\frac{d+q_1-1}{2})}{\Gamma(d-1+\frac{q_1}{2})} \\ &\times \left(\frac{2\pi^{d/2}}{\Gamma(d/2)}\right)^3.\end{aligned} \tag{C10}$$

for one-center integrals, where the parameters $q_i \geq 1$ for $i = 1, \ldots, 4$.
Apart from the value (39) of the integral $I_0$, which is straightforward, these general multicenter integral expressions allow us to calculate not only the values (39)-(43) of the integrals $I_i, i = 1-4$ needed for the entanglement of the ground-state wavefunctions $\Psi_{1,0}(r_{12})$, but also the corresponding integrals involved in the entanglement of the ground-state wavefunctions $\Psi_{n,0}(r_{12})$ with $n \geq 2$, of the $d$-dimensional spherium in an analytical way.

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***J. Phys. A: Math. Theor. 48, 475302 (2015)***

# Conclusions and open problems

> *What we observe is not nature itself, but nature exposed to our method of questioning.*
> **Werner Heisenberg**

Here we gather some conclusions and open problems associated with the contributions of this Thesis to the entropy, complexity and entanglement theory of the harmonic systems of oscillator and Harmonium types, the Coulomb systems of hydrogenic and Spherium types and the blackbody radiation in multidimensional spaces.

Summarizing,

- In *Pauli effects in uncertainty relations, Chem. Phys. Lett. 614, 1-4 (2014):*
  - ✓ We have explicitly shown the combined effects of the spatial and spin dimensionalities in two mathematical formulations of the uncertainty principle, the Heisenberg-like and Fisher-information-based uncertainty relations. Firstly, we have found that for a finite fermion system there exists a delicate balance between both effects: the concomitant lower bound increases(decreases) with respect to the spinless general bound depending on whether the spatial dimensionality is small(large), thus improving or not the accuracy of the uncertainty relation. Second, when the number of constituents of the system increases, the lower bound of the two associated uncertainty products globally increases, thus improving them.
  - ✗ The Pauli(spin) effects in the quantum uncertainty relations based on the Shannon, Rényi or Tsallis entropies remain unknown. To determine them it is necessary to design a *modus operandi* different to the one used in this work. This is basically because it is not yet possible to express their corresponding uncertainty sums in terms of the familiar Heisenberg product based on the standard deviation.
- In *Heisenberg-like and Fisher-information-based uncertainty relations for $N$-electron $d$-dimensional systems, Phys. Rev. A 91, 062122 (2015):*

  - ✓ We have found a general set of Heisenberg-like uncertainty relations based on the radial expectation values of arbitrary order which generalizes the expressions of similar type previously published in the literature. Moreover, its accuracy have been numerically discussed for a large set of many-electron systems: all the neutral and singly ionized atoms of the periodic table and a large diversity of polyatomic molecules.
  - ✓ We have explicitly shown the uncertainty character of the Fisher information product of finite fermion systems by means of the Zumbach inequality-based method. Even more, we have found a lower bound on this product in terms of the number of its constituents.
  - ✗ Although our general bounds are quite accurate for light electronic systems, they are less sharp as the number of electrons increases. So, there is still a lot of space for improvement in heavy $N$-electron systems.
  - ✗ We have to point out that this lower bound in the Fisher information product is not optimal because the Zumbach constant $C_d$ can be improved [174].

- In *Extremum-entropy-based Heisenberg-like uncertainty relations, J. Phys. A: Math. Theor. 49, 025301 (2016):*

  - ✓ We have used three extremization-informational methods to derive various uncertainty inequalities of Heisenberg type which hold for multidimensional systems of $N$ fermions with spin $s$.
  - ✓ We have found that the maximum-Tsallis-entropy method provides relationships with a better accuracy than the maximum-Shannon-entropy method, basically due to the role played by the Tsallis' order parameter $q$. This has been numerically checked for a large variety of neutral atoms from Helium to Xenon.
  - ✗ There is still much space for improving these inequalities due the large gap between our bounds and the corresponding Hartree-Fock values. In this sense, other informational approaches to the uncertainty principle, such as the application of the majorization theory [107] which relies on the partial order on probability vectors to characterize uncertainty, might complement the entropic and variance-based formulations, leading to a deeper knowledge of the fundamental aspects of uncertainty and disorder in quantum theory.

- In *Heisenberg-like uncertainty measures for D-dimensional hydrogenic systems at large D, J. Math. Phys. 57, 082109 (2016):*

  - ✓ The Heisenberg-like uncertainty measures of the high-dimensional Coulomb systems of hydrogenic type are explicitly calculated for all quantum states.

  - ✓ The uncertainty equality-type relations associated to them are determined, finding that they fulfill and saturate the known uncertainty inequality-type relations for both general and central quantum systems.
  - ✓ The position and momentum radial expectation values are used to bound the entropic uncertainty measures of the Shannon, Rényi and Tsallis types at high dimensions.
  - ✗ The analytical determination of these three entropies at the pseudoclassical limit for all quantum high-dimensional hydrogenic states is an open problem, not yet solved. In fact we do have some ideas to tackle this problem which we plan to develop in the near future.

- In *Monotone measures of statistical complexity, Phys. Lett. A 380, 377-380 (2016):*
  - ✓ We have proposed the mathematical notion of monotonicity of the complexity measure of a probability distribution.
  - ✓ We have given a set of general conditions to be satisfied by an informational quantity to be a true statistical complexity.
  - ✓ We have shown that the basic complexity measures of Fisher-Shannon and Crámer-Rao types fulfill them.
  - ✗ It is yet an open problem to show that the LMC complexity measure, and generalizations of the Fisher-Rényi and LMC-Rényi types, also fulfill these conditions.

- In *One-parameter Fisher-Rényi complexity: Notion and hydrogenic applications, Entropy 19(1), 16 (2017):*
  - ✓ To pave the way towards an informational quantity to capture, at least partially, the intuitive notion of complexity of a physical system we have introduced a complexity quantifier, the one-parameter Fisher-Rényi complexity.
  - ✓ We have shown its analytical properties of monotonicity, behavior under replications and universal bounding from below.
  - ✓ We have developed an algorithmic way to calculate analytically its value for all quantum hydrogenic states. Furthermore, we have given the explicit values for all *ns* states and the circular states, which are specially relevant *per se*, because they can be used as reference values for the complexity of all Coulombian systems.
  - ✗ The results tend to conjecture an interesting phenomenon (the existence of two regimes of complexity for the circular states which depend on the complexity order) which may provide a novel complexity-related insight into the internal structure of the system's states. Nevertheless, this conjecture deserves further research before it to be firmly settled down.

- In *Entropy and complexity properties of the d-dimensional blackbody radiation, Eur. Phys. J. D 68, 316 (2014):*

  ✓ We have studied the blackbody radiation in an universe with spatial dimensionality $d \geq 3$ by means of the entropy and complexity measures of its frequency Planck distribution.

  ✓ We have found that its fundamental entropy and complexity quantifiers can be explicitly expressed in terms of the dimensionality $d$ and the temperature $T$.

  ✓ We have found three entropic-dependent characteristic frequencies of the blackbody spectrum which have a dependence on temperature similar to the well-known Wien's law followed by the frequency $\nu_{max}$ at which the spectrum is maximum.

  ✓ We have shown that the three basic measures of complexity (i.e., Crámer-Rao, Fisher-Shannon and LMC) do not depend on the temperature, but only on the universe dimensionality.

  ✗ A possible extension of this work is the inclusion of quantum gravity effects, which will certainly modify the black body spectrum and might open new windows to know deeper the quantum gravitational features of the early universe through study of CMB spectrum.

  ✗ This entropy and complexity analysis should be extended to the nonlinear blackbody radiation laws, which likely takes into account the small deviations from the Planck radiation formula that have been detected in the CMB radiation.

- In *Rényi entropies of the highly-excited states of multidimensional harmonic oscillators by use of strong Laguerre asymptotics, Eur. Phys. J. B 89, 85 (2016):*

  ✓ We have determined in an analytical way the Rényi entropies of all orders for the Rydberg states of a $D$-dimensional harmonic system in position space.

  ✓ We have found that for a given Rydberg state the Rényi entropy has a very fast decreasing behavior as the parameter order is increasing, being the lowest order Rényi entropies the most significant,

  ✓ the second-order Rényi entropy has a Bell-like quasi-Gaussian behavior in terms of $D$, its maximum located at about $D = 12$, and

  ✓ the disequilibrium of the $ns$-Rydberg oscillator states decreases(increases) as a function of the principal hyperquantum number $n$ when the dimensionality $D$ is less(bigger) than 4 and it becomes constant when $D = 4$.

  ✗ It remains open the corresponding issues in momentum space.

  - ✗ These results may be potentially useful in the study of entropic uncertainty relations and relevant in connection with quantitative entanglement indicators, since Rényi entropies have been recently used for this purpose. This is left for future research.

- In *Rényi, Shannon and Tsallis entropies of Rydberg hydrogenic systems, Europhysics Letters (EPL) 113, 48003 (2016):*

  - ✓ We have explicitly calculated the dominant term of the Rényi, Shannon and Tsallis entropies for all Rydberg hydrogenic states in position space in terms of the nuclear charge $Z$ and the quantum numbers. This has been done by using a novel technique based on some ideas extracted from the modern approximation theory, which allows to determine the asymptotics ($n \to \infty$) of the $\mathcal{L}_p$-norm of the Laguerre polynomials.
  - ✓ We have found, e.g., that the $p$th-order Rényi entropy for the Rydberg ($ns$)-states behaves so that (a) it decreases as a function of $p$, being the most relevant quantities those associated with the Shannon entropy and the disequilibrium, (b) it has an increasing character for all Rydberg values of $n$ as the parameter $p$ is increasing due to the fact that the system tends to the classical regime as $n$ grows, and (c) it decreases for all $p$ as the nuclear charge increases when $n$ is fixed.
  - ✗ It remains open the corresponding issues in momentum space.

- In *Entanglement in N-Harmonium: bosons and fermions, J. Phys. B: At. Mol. Opt. Phys. 47, 195503 (2014)*

  - ✓ We have extended to harmonic systems with an arbitrary number of particles the study of the quantum entanglement recently done for various two-electron and helium-like systems as well as for certain quantum networks, with the aim to understand some entanglement features of finite many-particle systems. Indeed, we have analyzed in detail the entanglement of the $N$-boson and $N$-fermion systems of Harmonium type. We have calculated not only the one-body reduced density matrix for bosons and fermions, but also the von Neumann entropy in the bosonic case and linear entropy in the fermionic case for both spatial and spin degrees of freedom in terms of the number of particles and the relative interaction strength.
  - ✓ We have found that for positive coupling (a) the entanglement of the $N$-boson Harmonium decreases as $N$ increases and (b) grows when the positive coupling constant increases. On the other hand, in global terms, (a) the spatial entanglement of the $N$-fermion Harmonium grows when $N$ increases for both negative and sufficiently small positive values of the coupling constant, (b) the entanglement behavior is opposite in the positive strong-coupling regime,

(c) entanglement grows when the coupling constant increases and (d) contribution of the spin degree of freedom to the entanglement is shown to be of positive comparable size to the contribution of the spatial degrees of freedom.

- ✓ As a general trend in both bosonic and fermionic systems we have found that (a) in the repulsive and attractive (for relatively small values of the coupling constant) cases the entanglement grows when the number of particles increases (purity decreases) and (b) in the regime of strong coupling the situation gets inverted as the entanglement decreases (purity increases) when adding particles to the system.

- In *Quantum entanglement in* $(d-1)$*-Spherium, J. Phys. A: Math. Theor. 48, 475302 (2015)*

  - ✓ We have explored the entanglement-related features of a quasi-exactly solvable multidimensional two-electron model, the $(d-1)$-Spherium. We have computed in an exact analytical way the amount of quantum entanglement (measured by the linear entropy of the single-particle reduced density matrix) of the ground state of Spherium for several values of the radius $R$ and of the space dimension $d$. The relation between the radius, the spatial dimensionality and the energy was considered.
  - ✓ We have found that (a) the amount of entanglement of the ground state of Spherium increases with the radius $R$ of the hypersphere (consistent with a general property exhibited by other two-electron systems: entanglement tends to increase when the confinement due to the external common fields acting on both particles decreases), (b) the amount of entanglement decreases with the spatial dimensionality $d$ (also related to the entanglement-confinement connection) and (c) the entanglement tends to increase with energy (similar to what is observed in other two-electron models, such as the Moshinsky, Hooke and Crandall ones).
  - ✗ The characterization of the quantum entanglement for many-electron models (e.g., Calogero-Moser-Sutherland-type [54]) would be a natural continuation of this research, deserving a much further future investigation.

Finally, let us point out some concluding remarks relative to the mathematical methodology based on the theory of orthogonal polynomials and special functions of Applied Mathematics which we have developed to determine the previous physico-informational results.

- In *Entropic functionals of Laguerre and Gegenbauer polynomials with large parameters, J. Phys. A: Math. Theor. 50, 215206 (2017):*

- ✓ We have investigated in a detailed manner the asymptotics of the power and logarithmic integral functionals of Laguerre and Gegenbauer polynomials $I_j(m, \alpha)$, $j = 1 - 4$ when the parameter $\alpha \to \infty$ and the rest of parameters, including the polynomial degree $m$, are fixed.
- ✗ It remains open the determination of the Shannon integral functionals for the particular cases $\mu = \alpha + \sigma, \lambda = 1$ (Laguerre) and $c = d = 1$ (Gegenbauer).
- ✗ Some related issues have not yet been solved such as e.g., the asymptotics of the Laguerre and Gegenbauer polynomials for large values of the degree of the polynomials due to its relevance from both fundamental and applied standpoints. Let us remark that the underlying asymptotic analysis for large degree is essentially more difficult than the large-parameter case and it requires other mathematical tools. Nevertheless, some remarkable results are already known in the Laguerre case [12, 51].

- In *Frequency moments, $L_q$ norms and Rényi entropies of general hypergeometric polynomials, J. Math. Chem. 52, 1372-1385 (2014):*

  - ✓ We have developed a procedure to determine closed expressions for the weighted $L_q$-norms ($q$ positive integer) of the orthogonal hypergeometric polynomials in terms of $q$ and the parameters of the associated weight function.
  - ✓ We have used the extended Laplace method [164] to tackle the asymptotics ($q \to \infty$) of the unweighted $L_q$-norms of the classical orthogonal polynomials of Jacobi type.
  - ✗ It remains as an open problem the determination of the asymptotic behavior of the unweighted $L_q$-norms of Hermite and Laguerre polynomials.
  - ✗ The investigation of further analytical properties of these quantities and, most interesting, the determination of these functional norms for any real positive number $q$, which requires a completely different approach than the one used here, are still missing in the literature.

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