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MEDIDAS ENTRÓPICAS Y DE COMPLEJIDAD
DE
FUNCIONES ESPECIALES Y SISTEMAS CUÁNTICOS

Tesis Doctoral

por

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A mis padres y hermanos.

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Que la presente Memoria titulada "Medidas entrópicas y de complejidad de funciones especiales y sistemas cuánticos", presentada por Ángel Guerrero Martínez para optar al Grado de Doctor en Física y Matemáticas, ha sido realizada bajo nuestra 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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Índice general

Resumen

Esta tesis aborda el estudio teórico-informacional de las funciones especiales de la matemática aplicada y de la física matemática, con especial hincapié en los polinomios ortogonales hipergeométricos y los armónicos hiperesféricos. Los conceptos e ideas clave en este tratamiento son las entropías y longitudes entrópicas, así como las medidas de complejidad de la densidad de Rakhmanov o densidad de probabilidad asociada a tales funciones. En este trabajo, se calculan estas magnitudes matemáticas haciendo uso de las diversas caracterizaciones de las funciones consideradas y se estudia su asintótica. Se desarrollan y utilizan conceptos y técnicas derivados de la teoría de la aproximación, la teoría de funciones especiales y la mecánica cuántica. Además, se aplican los resultados obtenidos en varios sistemas cuánticos concretos (e.g., el rotador rígido) y se analiza la acotación de varios productos de incertidumbre y medidas de complejidad de sistemas cuánticos generales.

La tesis consta de Introducción, cuatro Capítulos, Conclusiones, un Apéndice y Bibliografía. En el Capítulo 1 se definen y se discuten las medidas entrópicas y de complejidad empleadas a lo largo de este trabajo. El Capítulo 2 recoge los elementos y las propiedades básicas de las funciones especiales a las que se aplicarán las medidas de información; a saber, los polinomios ortogonales hipergeométricos y los armónicos hiperesféricos. En el Capítulo 3 se describe brevemente la metodología usada en nuestro trabajo. Finalmente, el Capítulo 4 contiene los resultados obtenidos y las publicaciones asociadas, ordenadas temáticamente.

Los contenidos de esta tesis han dado lugar a cinco publicaciones en revistas de física y matemáticas (Journal of Physics A: Mathematical and Theoretical, Physical Review A, Complex Analysis and Operator Theory, Applied Mathematics and Computation, Journal of Mathematical Chemistry), así como a un manuscrito aceptado en Journal of Computational and Applied Mathematics, y otro más enviado para su publicación.

Publicaciones del autor

A continuación se enumeran las publicaciones que sustentan esta tesis.

Artículos publicados:

1. *Asymptotics of L_p norms of hypergeometric orthogonal polynomials*
   J. S. Dehesa, **A. Guerrero**, J. L. López y P. Sánchez-Moreno
   Journal of Mathematical Chemistry 52 (2014) 283-300
2. *Rényi entropies, L_q norms and linearization of powers of hypergeometric orthogonal polynomials by means of multivariate special functions*
   P. Sánchez-Moreno, J. S. Dehesa, A. Zarzo y **A. Guerrero**
   Applied Mathematics and Computation 223 (2013) 25-33
3. *Information theoretic-based spreading measures of orthogonal polynomials*
   J. S. Dehesa, **A. Guerrero** y P. Sánchez-Moreno
   Complex Analysis and Operator Theory 6 (2012) 585-601
4. *Upper bounds on quantum uncertainty products and complexity measures*
   A. Guerrero, P. Sánchez-Moreno y J. S. Dehesa
   Physical Review A 84 (2011) 042105 (8 páginas)
5. *Information-theoretic lengths of Jacobi polynomials*
   A. Guerrero, P. Sánchez-Moreno y J. S. Dehesa
   Journal of Physics A: Mathematical and Theoretical 43 (2010) 305203 (19 páginas)

Artículos aceptados y enviados para su publicación:

1. *Complexity analysis of hypergeometric orthogonal polynomials*
   J. S. Dehesa, **A. Guerrero** y P. Sánchez-Moreno
   Journal of Computational and Applied Mathematics (2014). Aceptado.
   DOI: 10.1016/j.cam.2014.08.013
2. *Entropy and complexity analysis of the D-dimensional rigid rotator and hyperspherical harmonics*
   J. S. Dehesa, **A. Guerrero** y P. Sánchez-Moreno
   Journal of Mathematical Chemistry (2014). Enviado.

Introducción

Las funciones especiales y los polinomios ortogonales de la matemática aplicada y la física matemática [58, 59, 78] destacan sobre las demás funciones matemáticas por el gran número de propiedades algebraicas simples y elegantes que poseen, lo cual facilita su manipulación analítica y su aplicación para resolver, interpretar y modelizar una gran cantidad de problemas científicos y tecnológicos. No obstante, estas funciones presentan aún muchas incógnitas y cuestiones abiertas cuya solución resulta útil e interesante tanto desde un punto de vista fundamental como aplicado, como ocurre con las propiedades teórico-informacionales y de entrelazamiento.

En esta tesis se lleva a cabo un estudio teórico-informacional de los polinomios ortogonales hipergeométricos [58, 59, 78] y los armónicos hiperesféricos [8–11, 26, 55, 80, 81] por medio de la determinación de varias medidas entrópicas y de complejidad de su densidad de probabilidad asociada (densidad de Rakhmnanov), tales como e.g. la información de Fisher, la entropía de Shannon, las entropías de Rényi y las complejidades de Cramér-Rao, Fisher-Shannon, Fisher-Rényi y LMC. Estas medidas no solo están estrechamente ligadas con magnitudes fundamentales de la teoría de aproximación, como son e.g., las normas L_p, sino que permiten cuantificar distintos aspectos de la distribución o esparcimiento de las funciones especiales (polinomios ortogonales) en su dominio de definición (intervalo de ortogonalidad). Hasta muy recientemente, el interés estaba centrado casi exclusivamente en la varianza y en la entropía de Shannon de los polinomios ortogonales clásicos [6, 34], las funciones de Airy y Bessel [35, 36, 70], los armónicos hiperesféricos [33, 81], las funciones hipergeométricas [82] y los polinomios ortogonales de variable discreta [5, 37]. En este trabajo se extiende este estudio a las medidas entrópicas y de complejidad arriba mencionadas.

Por otra parte, las funciones especiales en general y los polinomios ortogonales en particular se utilizan habitualmente para describir un gran número de fenómenos y propiedades de los sistemas científicos y tecnológicos. Además, de acuerdo a la teoría funcional de la densidad de Hohenberg-Kohn [60], se sabe que las propiedades físicas y químicas de los sistemas cuánticos finitos (átomos, moléculas, núcleos,...) están controladas por su densidad monoparticular. Cuando la ecuación de Schrödinger de tales sistemas es exacta- o cuasi-exactamente resoluble, esta densidad viene dada en términos de la densidad de probabilidad de Rakhmanov [62] de las funciones especiales que controlan las funciones de onda de los estados cuánticos del sistema. En particular, los polinomios ortogonales hipergeométricos y los armónicos hiperesféricos controlan las funciones de onda de numerosos sistemas cuánticos [12, 24, 41, 42, 58], incluyendo el átomo de hidrógeno, el oscilador armónico y el rotador rígido.

Por consiguiente, las propiedades físicas y químicas de los sistemas cuánticos (que son valores esperados de operadores hermíticos y, por ende, funcionales integrales de su densidad monoparticular) dependen esencialmente de distintos cuantificadores de la distribución de las funciones especiales de la matemática aplicada que controlan sus funciones de onda en la región de confinamiento del potencial mecano-cuántico de tales sistemas. Estas magnitudes matemáticas no sólo nos permiten obtener información sobre varios aspectos del desorden interno de los sistemas cuánticos finitos (el cual está conectado con la geometría tridimensional de la distribución monoparticular), sino que también posibilitan la descripción de numerosas magnitudes físicas de gran interés (e.g., densidad electrónica media, energía de interacción entre núcleo y electrón, energías cinéticas, entre otras muchas; ver por ejemplo [3,4,27–29,32]). Estas magnitudes pueden expresarse [52, 53, 56] por medio de medidas teórico-informacionales de la densidad monoparticular, y su determinación para los sistemas cuánticos exacta- o cuasi-exactamente resolubles es una de las aplicaciones fundamentales de la teoría de la información de las funciones especiales.

En esta tesis se utilizan varias medidas de dispersión (los momentos ordinarios y la desviación estándar, y las entropías y longitudes entrópicas de Fisher, Rényi y Shannon) de la densidad de probabilidad de Rakhmanov [62] de los polinomios ortogonales. Cada una cuantifica un aspecto diferente de la distribución $\rho(x)$ de estos polinomios en su intervalo de ortogonalidad. Mientras que los momentos ordinarios y la desviación estándar dependen de un punto específico del intervalo de ortogonalidad (el origen en el primer caso, y el centroide en el segundo), las entropías y longitudes entrópicas de Fisher, Rényi y Shannon no presentan tal dependencia, lo que les permite caracterizar más adecuadamente la noción de incertidumbre o indeterminación cuántica. Además, mientras que los momentos ordinarios son funcionales integrales del tipo $x^k\rho(x)$, las entropías y longitudes entrópicas de Rényi y Shannon son funcionales del tipo $[\rho(x)]^k$ y por tanto están estrechamente relacionados con las normas L_p de los polinomios ortogonales.

La determinación analítica de las normas L_p de los polinomios ortogonales $p_n(x)$ ha sido un problema permanente de la teoría de aproximación, y en general de la Matemática Aplicada, desde Bernstein y Steklov (ver por ejemplo [14, 54, 77, 85]) hasta ahora [20, 50], habiéndose obtenido solamente relaciones de tipo desigualdad. Los valores explícitos de tales normas solo se conocen para los valores más bajos del grado n del polinomio; y para valores grandes de n, se han calculado las normas de los polinomios de Hermite [50]. Sólo muy recientemente se ha desarrollado un método analítico sencillo que permite la determinación de estas normas (y de las longitudes entrópicas asociadas) para polinomios con grado arbitrario n. Este método, que hace uso de los polinomios de Bell de carácter combinatorial, ha sido ilustrado en 2010 para los polinomios de Hermite [66] y en 2011 para los polinomios de Laguerre [68]. En esta tesis se aplica este método a los polinomios de Jacobi [43] (ver también [31]), tal como se describe detalladamente en la Sección 4.1. Además, hemos desarrollado un método alternativo que hace uso de las fórmulas de linealización polinómicas de Srivastava-Niukkanen para la determinación de las normas L_p y de las entropías de Rényi de los polinomios ortogonales hipergeométricos de tipo Hermite generalizado, Laguerre y Jacobi [67], tal como se detalla en la Sección 4.2. Además en este mismo capítulo, usando el teorema de Laplace adecuadamente modificado, se investiga teórico-computacionalmente la asintótica [30] de las normas de tales familias de polinomios ortogonales en términos de su grado y de los parámetros que caracterizan su función peso.

Existe una clase de medidas teórico-informacionales que describen no uno, sino dos o más aspectos de la densidad de probabilidad; son las medidas de complejidad. En esta tesis se consideran las medidas de complejidad de tipo Cramér-Rao, Fisher-Shannon, Fisher-Rényi y LMC. Estas magnitudes, que cuantifican simultáneamente dos aspectos macroscópicos de la densidad de probabilidad que estemos analizando, se aplican en las Secciones 4.3 y 4.4 de este trabajo a la densidad de probabilidad de Rakhmanov de los polinomios ortogonales hipergeométricos y los armónicos hiperesféricos tanto analítica como numéricamente y se estudia su asintótica. De esta forma se obtienen propiedades estructurales de nuevo cuño de los polinomios ortogonales hipergeométricos, cuya relación con otras nociones de la teoría de aproximación y teoría de potencial es aún una cuestión abierta. Además, en la Sección 4.4, los resultados obtenidos se aplican a un sistema cuántico prototipo que se utiliza a menudo para la interpretación y predicción de numerosos fenómenos y propiedades moleculares; a saber, el rotador rígido, cuyas funciones de onda mecano-cuánticas están controladas por los armónicos hiperesféricos.

Finalmente, en la Sección 4.5 se muestra explícitamente que las medidas de complejidad de Cramér-Rao, Fisher-Shannon y LMC de sistemas cuánticos generales pueden acotarse superiormente y que los productos de incertidumbre de Shannon y de Rényi pueden acotarse no solo inferiormente (son las conocidas relaciones de indeterminación) sino también superiormente en términos del producto de incertidumbre de Heisenberg-Kennard. Además se determina la mejora de tales cotas para los sistemas cuánticos con simetría esférica, y se aplican los resultados obtenidos para los sistemas Coulombianos y armónicos de tipo oscilador.

Capítulo 1

Medidas teórico-informacionales de una densidad de probabilidad

Claude E. Shannon publicó en 1948 un artículo revolucionario [72] donde proponía un conjunto de postulados que debía satisfacer una medida de incertidumbre, y mostró que estos postulados los verifica la expresión de la entropía que, desde entonces, lleva su nombre. A menudo, la entropía de Shannon recibe el nombre de medida de *información*, de aquí que el trabajo de Shannon haya dado lugar a un campo enteramente nuevo de la ciencia llamado Teoría de la Información. El término *información* es quizás poco afortunado, no porque carezca de connotaciones intuitivas sino porque tiene demasiadas. La noción de información según Shannon es la incertidumbre de un suceso, o del resultado de un experimento, basado en una distribución de probabilidad dada. El desarrollo y generalización de esta forma de cuantificación de la información ha posibilitado la aplicación de la Teoría de la Información en numerosas áreas científicas, tecnológicas y humanistas, que van desde la estadística y la teoría de la probabilidad, la física atómica y molecular, la criptografía y la computación cuánticas hasta la neurobiología, la ecología, la psicología cognitiva y la ingeniería de las telecomunicaciones [25, 38, 73].

En este capítulo describiremos brevemente las medidas teórico-informacionales (i.e., entropías y medidas de complejidad) de cuantificación del esparcimiento o distribución de una densidad de probabilidad $\rho(\vec{r})$, $\vec{r} \in \Delta \subseteq \mathbb{R}^D$, más allá de la noción familiar de varianza dada por

$$V[\rho] = \langle r^2 \rangle - |\langle \vec{r} \rangle|^2 , \tag{1.1}$$

donde $r^2 = |\vec{r}|^2$ y

$$\langle f(\vec{r}) \rangle = \int_\Delta f(\vec{r})\, \rho(\vec{r})\, d^D r, \tag{1.2}$$

es el valor esperado de la cantidad $f(\vec{r})$ o también llamado momento no centrado de orden 1 de la variable en estudio (en este caso una función del vector $\vec{r}$).

Las entropías de carácter global (entropías de Shannon, Rényi y Tsallis) y de carácter local (información de Fisher), así como las medidas de longitud entrópicas asociadas y las medidas de complejidad de tipo Cramér-Rao, Fisher-Shannon y LMC extienden y mejoran la noción de medida de incertidumbre o de información con respecto a la varianza (o su raíz cuadrada, la desviación estándar). Estos cuantificadores del esparcimiento de la probabilidad y las relaciones de incertidumbre que satisfacen son los elementos principales de esta tesis.

1.1. Medidas de incertidumbre entrópicas

La varianza y sus diversas generalizaciones basadas en los momentos ordinarios o valores esperados radiales de la densidad de probabilidad (i.e., las medidas de incertidumbre de tipo Heisenberg) no son especialmente adecuadas para describir la incertidumbre de la densidad (salvo que ésta sea de tipo gaussiano o cuasigaussiano), bien por que no están bien definidas para densidades de probabilidad generales o bien porque dependen de un punto específico del intervalo de definición de la densidad. Por estas y otras razones se suelen utilizar las medidas de incertidumbre entrópicas, que se describen brevemente a continuación, para cuantificar el esparcimiento de densidades de probabilidad generales (sobre todo las densidades de probabilidad de Born de los sistemas cuánticos) y, en definitiva, de la incertidumbre de la posición o el momento de una partícula moviéndose en un espacio de dimensión arbitraria. Estas medidas, en contraste con las medidas de tipo Heisenberg, se definen por medio de los momentos de frecuencia o momentos entrópicos de posiciones

$$W_q[\rho] = \int_\Delta [\rho(\vec{r})]^q d\vec{r}\,; \quad q > 0,$$

y análogamente para las medidas de incertidumbre entrópicas del momento.

Las medidas entrópicas de incertidumbre más relevantes son la entropía de Shannon y sus generalizaciones, las entropías de Rényi y de Tsallis, y la información de Fisher. La entropía de Shannon de la densidad de probabilidad cuántica en el espacio de posiciones es el funcional logarítmico de la densidad $\rho(\vec{r})$ dado [44, 72] por

$$S[\rho] = -\int_\Delta \rho(\vec{r}) \ln[\rho(\vec{r})] d\vec{r}, \tag{1.3}$$

que puede escribirse en términos de los momentos entrópicos W_q como

$$S[\rho] = -\left.\frac{dW_q[\rho]}{dq}\right|_{q=1}.$$

La entropía de Shannon representa la conocida entropía termodinámica en el caso de una colectividad térmica. Vale la pena remarcar que a diferencia de la entropía para una variable discreta $-\sum_i p_i \ln p_i$ (también debida a Shannon), $S[\rho]$ puede tomar cualquier valor real e incluso puede no estar definida. Cualquier pico en la densidad $\rho(\vec{r})$ tiende a hacer $S[\rho]$ negativo mientras que los valores positivos de $S[\rho]$ son provocados por un decaimiento suave; por lo tanto la entropía de Shannon es una medida que cuantifica el grado de localización de la densidad $\rho(\vec{r})$.
Las entropías de Rényi [63] y Tsallis [79], que dependen de un parámetro q, se definen por medio de las expresiones

$$R_q[\rho] = \frac{1}{1-q} \ln\left(\int_\Delta [\rho(\vec{r})]^q d\vec{r}\right); \quad q > 0,\, q \neq 1, \tag{1.4}$$

y

$$T_q[\rho] = \frac{1}{q-1}\left(1 - \int_\Delta [\rho(\vec{r})]^q d\vec{r}\right); \quad q > 0,\, q \neq 1, \tag{1.5}$$

respectivamente. Nótese que cuando q tiende a la unidad, tanto la entropía de Rényi como la de entropía de Tsallis tienden a la entropía de Shannon $S[\rho]$. Además, la entropía de Tsallis es una linealización de la entropía de Rényi con respecto a $W_q[\rho]$, por tanto ambas tienen varias propiedades comunes más allá de la que acabamos de comentar. En particular, ambas son funcionales de potencias de la densidad $\rho(\vec{r})$ por lo que pueden ser interpretadas como medidas globales de esparcimiento espacial de dicha probabilidad. Por otra parte, mientras que las entropías de Rényi son aditivas, las entropías de Tsallis son pseudoaditivas, i.e., satisfacen la relación

$$T_q\left[\rho_1 \otimes \rho_2\right] = T_q\left[\rho_1\right] + T_q\left[\rho_2\right] + (1-q) T_q\left[\rho_1\right] T_q\left[\rho_2\right]$$

para cualquier par de densidades de posición. Las entropías monoparamétricas de Rényi y de Tsallis han sido ampliamente usadas en el estudio de los sistemas cuánticos. En particular, en el análisis del entrelazamiento cuántico, los protocolos de comunicación cuántica, las correlaciones cuánticas, la medida cuántica, la decoherencia, la producción multiparticular en las colisiones de alta energía, la mecánica estadística clásica y cuántica, las propiedades de localización de los estados Rydberg y los sistemas de spin, entre otros muchos fenómenos y sistemas [16, 17].

Finalmente, se define la información de Fisher [39, 40] en el espacio de posiciones por medio del siguiente funcional del gradiente de la densidad de posición $\rho(\vec{r})$:

$$F[\rho] = \int_\Delta \frac{|\nabla_D \rho(\vec{r})|^2}{\rho(\vec{r})} d\vec{r}. \tag{1.6}$$

A diferencia de las entropías de Shannon, Rényi y Tsallis, la información de Fisher es una medida local del esparcimiento de la densidad $\rho(\vec{r})$ debido a la presencia del gradiente, lo cual la hace ser muy sensible a las fluctuaciones de la densidad. Cuanto mayor es su valor, más localizada está la densidad, menor es la incertidumbre y mayor es la precisión en la predicción de la posición de la partícula.

Ahora bien, las medidas entrópicas de una densidad de probabilidad $\rho(\vec{r})$, al tener distintas unidades, no pueden compararse entre sí ni con la desviación estándar de dicha densidad dada por

$$\Delta\vec{r} = \sqrt{V[\rho]} = \sqrt{\langle r^2\rangle - |\langle\vec{r}\rangle|^2}. \tag{1.7}$$

Por ello se han definido otras magnitudes relacionadas del mismo carácter que no presentan este problema y, sin embargo están relacionadas directamente con tales medidas: son las denominadas *longitudes entrópicas* de la densidad, cuya definición y significado enumeramos a continuación. Estas magnitudes, junto con la desviación estándar (también llamada *longitud de Heisenberg* $L_H = \Delta\vec{r}$), tienen una serie de propiedades comunes de gran interés: (a) todas tienen las mismas unidades que la variable de la que depende la densidad de probabilidad, (b) son invariantes bajo traslaciones y reflexiones, y reescalan linealmente con la variable. En particular la *longitud entrópica de Shannon* se define por

$$L_S = \exp\left(S\left[\rho\right]\right). \tag{1.8}$$

y la *longitud entrópica de Rényi* por

$$L_R^{(q)}[\rho] = \exp\left(R^{(q)}\left[\rho\right]\right). \tag{1.9}$$

Nótese que esta magnitud contiene un número infinito de candidatos para una medida directa de incertidumbre; en particular, la longitud de Shannon corresponde al límite $q \to 1$ de la longitud de Rényi. Y, en términos de la entropía de Fisher, se define la *longitud entrópica de Fisher*

$$L_F = \frac{1}{\sqrt{F\left[\rho\right]}}. \tag{1.10}$$

Es interesante destacar que todas las longitudes entrópicas, al tener las mismas unidades, pueden compararse entre sí; de hecho verifican las siguientes relaciones de tipo desigualdad

$$L_F \leq L_H,$$

$$(2\pi e)^{1/2} L_F \leq L_S \leq (2\pi e)^{1/2} L_H,$$

donde las igualdades se alcanzan para la distribución gaussiana. Digamos también que la desigualdad que liga L_S y L_H corresponde a la conocida propiedad de maximización de la entropía de Shannon de la densidad de probabilidad con desviación estándar dada. Y la desigualdad entre L_S y L_F puede obtenerse de la identidad teórico-informacional de de Bruijn e incluso de la desigualdad logarítmica de Sobolev. Más detalles sobre el significado y propiedades de las longitudes entrópicas se dan en la Sección 4.1 de esta tesis.

1.2. Medidas de complejidad

Recientemente se han introducido medidas teórico-informacionales de una densidad de probabilidad que son esencialmente productos de dos de las medidas de esparcimiento anteriormente mencionadas (varianza $V[\rho]$, entropía de Shannon $S[\rho]$, información de Fisher $F[\rho]$). Estas medidas reciben el nombre de medidas de complejidad, porque cuantifican más de un aspecto macroscópico de la densidad. Son las medidas de Cramér-Rao, Fisher-Shannon, y López-Ruiz-Mancini-Calvet (medida LMC de ahora en adelante), que se definen por medio de las expresiones

$$C_{CR}[\rho] = F[\rho] V[\rho], \tag{1.11}$$

$$C_{FS}[\rho] = \frac{1}{2\pi e} F[\rho] \exp\left(\frac{2}{D} S[\rho]\right), \tag{1.12}$$

$$C_{LMC}[\rho] = W_2[\rho] \exp(S[\rho]), \tag{1.13}$$

respectivamente, donde $W_2[\rho]$ es el desequilibrio, que no es más que el valor esperado de la distribución ρ; esto es,

$$W_2[\rho] = \langle\rho\rangle = \int_\Delta [\rho(\vec{r})]^2 \, d\vec{r}. \tag{1.14}$$

Cada una de estas medidas de complejidad cuantifica el balance combinado de dos facetas de la densidad de probabilidad. La medida de Cramér-Rao cuantifica el contenido de gradiente de la densidad junto con el esparcimiento de la probabilidad alrededor de su centroide. La medida de complejidad de Fisher-Shannon cuantifica el balance combinado del contenido de gradiente de la densidad y su esparcimiento total en el dominio soporte. La medida de complejidad LMC cuantifica la altura media de la densidad de probabilidad (tal como viene dada por el desequilibrio) y su esparcimiento total (tal como viene dado por la potencia entrópica de Shannon). Además puede probarse que estas tres medidas de complejidad tienen una serie de propiedades comunes altamente interesantes: son adimensionales, están acotadas inferiormente por la unidad, y toman valores mínimos en el caso extremo de menor complejidad; a saber, el caso de máximo desorden (asociado a una distribución uniforme monodimensional, o a un gas tridimensional). Finalmente, vale la pena hacer notar que las tres medidas de complejidad satisfacen también las propiedades de invariancia bajo replicación, translación y transformaciones de escala. Más detalles sobre el significado y utilización de estas medidas en ambos contextos de teoría de funciones especiales y mecánica cuántica pueden verse en la Sección 4.3 de esta tesis.

1.3. Relaciones de incertidumbre entrópicas

Análogamente a la relación de incertidumbre de Heisenberg $\Delta x \cdot \triangle p \geq \frac{\hbar}{2}$, que satisfacen las desviaciones estándar de posición y momento, también las medidas de incertidumbre entrópicas de Shannon, Rényi y Fisher satisfacen las llamadas relaciones de incertidumbre entrópicas del mismo nombre. Estas relaciones son formulaciones alternativas del principio de incertidumbre de la mecánica cuántica más rigurosas que la relación de Heisenberg anteriormente mencionada.

Las entropías Shannon de posiciones y momentos, que se denotan por $S\,[\rho]$ y $S\,[\gamma]$ respectivamente, satisfacen la siguiente relación de incertidumbre entrópica

$$S\,[\rho] + S\,[\gamma] \geq D\,(1 + \ln\pi)\,. \tag{1.15}$$

donde $\gamma = \gamma(p)$ denota la densidad de momentos o densidad del sistema en el espacio conjugado o espacio de momentos. Esta relación fue obtenida en primer lugar por Hirschman [46] y más tarde demostrada independientemente por Beckner [13] y Bialynicki-Birula y Mycielski en 1975 [18]. Esta expresión indica que la incertidumbre total en el conocimiento de la posición y el momento de la partícula es necesariamente mayor que $D\,(1 + \ln\pi)$.

Análogamente, Bialynicki-Birula e independientemente Zozor y Vignat han demostrado que las entropías de Rényi de posición y momento satisfacen la siguiente relación de incertidumbre entrópica

$$R_q[\rho] + R_p[\gamma] \geq D\ln\left(2\pi(2q)^{\frac{1}{2q-2}}(2p)^{\frac{1}{2p-2}}\right); \quad \frac{1}{q} + \frac{1}{p} = 2 \tag{1.16}$$

para $q > p$. Esta relación fue encontrada en el caso unidimensional de forma independiente por Bialinicki-Birula [15], y Zozor y Vignat [84], siendo generalizada al caso D dimensional por Zozor, Portesi y Vignat en 2009 [83].

Una relación análoga fue obtenida por Rajagopal [61] para las entropías de Tsallis de posiciones y momentos:

$$\{1 + (1-p)T_p[\rho]\}^{\frac{-1}{2p}}\,\{1 + (1-q)T_q[\gamma]\}^{\frac{1}{2q}} \geq \left(\frac{q}{\pi}\right)^{\frac{D}{4q}}\left(\frac{p}{\pi}\right)^{\frac{-D}{4p}}; \quad \frac{1}{q} + \frac{1}{p} = 2. \tag{1.17}$$

Es importante hacer notar que en el límite de (p, q) yendo a la unidad, ambas relaciones de incertidumbre entrópicas se reducen a la relación entrópica de incertidumbre (1.15) basada en la entropía de Shannon.

Las informaciones de Fisher de posiciones y momentos, $F[\rho]$ y $F[\gamma]$ respectivamente, satisfacen la siguiente relación de incertidumbre:

$$F[\rho]F[\gamma] \geq 4D^2. \tag{1.18}$$

Esta relación es válida para cualquier densidad de probabilidad cuántica monodimensional. Para los sistemas D-dimensionales, con $D > 1$, solamente es válida para los estados cuánticos caracterizados por funciones de onda que sean reales bien en el espacio de posiciones o en el espacio de momentos. Para un estudio detallado de esta relación, véase la referencia [69].
Una revisión exhaustiva de las relaciones de incertidumbre cuánticas ha sido hecha recientemente [19, 32] donde se pone de manifiesto el interés científico-tecnológico de tales relaciones.

Capítulo 2

Medidas de esparcimiento de funciones especiales y sistemas cuánticos

2.1. Densidad de Rakhmanov

Las medidas de esparcimiento o distribución de los polinomios ortogonales hipergeométricos $y_n(x)$ que satisfacen la condición (ver Apéndice A)

$$\int_a^b y_n(x)\, y_m(x)\, \omega(x)\, dx = d_n^2\, \delta_{nm},$$

son, por definición, las medidas de esparcimiento de su densidad de probabilidad de Rakhmanov asociada dada por

$$\rho_n(x) = \frac{1}{d_n^2}\, y_n^2(x)\, \omega(x). \tag{2.1}$$

Nótese que efectivamente se verifica $\int_a^b \rho_n(x)\, dx = 1$, dado que la condición de ortogonalidad implica que

$$\int_a^b \frac{1}{d_n^2}\, y_n^2(x)\, \omega(x)\, dx = 1. \tag{2.2}$$

Esta función densidad, que fue introducida por primera vez por Evgeni Rakhmanov [62] en 1977 para describir la asintótica del cociente de dos polinomios de grados consecutivos, juega un papel central en esta tesis. En efecto, es la función que nos permite estudiar los polinomios ortogonales desde el punto de vista de la teoría de la información.

Por extensión, se define de forma análoga la densidad de probabilidad de Rakhmanov de cualquier otra función especial de la matemática aplicada. Veamos cómo se procede para los armónicos esféricos, que juegan un papel importante en nuestro trabajo. Los armónicos hiperesféricos son funciones especiales D-dimensionales [9–11, 80, 81] que pueden definirse por la expresión

$$Y_{l,\{\mu\}}(\Omega_D) = \frac{1}{\sqrt{2\pi}} e^{i\mu_{D-1}\theta_{D-1}} \prod_{j=1}^{D-2} \hat{C}_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}}, \tag{2.3}$$

donde $\Omega_D \equiv (\theta_1, \theta_2, \cdots, \theta_{D-1})$ representa las $D-1$ coordenadas angulares medidas en un espacio de D dimensiones. Los rangos de valores que pueden tomar son $0 \leq \theta_j \leq \pi$ para $j = 1, \ldots, D-2$

y $0 \leq \theta_{D-1} \leq 2\pi$. Los $D-1$ números enteros $l \equiv \mu_1$ y $\{\mu_2, \ldots, \mu_{D-1} \equiv m\} \equiv \{\mu\}$ tienen los valores $l = 0, 1, 2, \ldots$ y $\mu_1 \geq \mu_2 \geq \cdots \geq |\mu_{D-1}| \geq 0$. El parámetro $\alpha_j = (D-j-1)/2$ y la función $\hat{C}_n^\lambda(x)$, $\lambda > -\frac{1}{2}$, denota el polinomio ortonormal de Gegenbauer de grado n y parámetro λ. Los polinomios de Gegenbauer satisfacen la relación de ortogonalidad siguiente

$$\int_{-1}^{+1} \hat{C}_n^\lambda(x)\hat{C}_m^\lambda(x)\omega_\lambda(x)dx = \delta_{mn}, \tag{2.4}$$

donde la función peso viene dada por

$$\omega_\lambda(x) = (1-x^2)^{\lambda-\frac{1}{2}}. \tag{2.5}$$

Las propiedades de los armónicos hiperesféricos han sido ampliamente estudiadas [9, 11, 45, 57]. En particular verifican la condición de ortogonalidad:

$$\int_{S_{D-1}} Y^*_{l,\{\mu\}}(\Omega_D) Y_{l',\{\mu'\}}(\Omega_D) d\Omega_D = \delta_{ll'}\delta_{\{\mu\},\{\mu'\}}, \tag{2.6}$$

donde el elemento de ángulo sólido viene dado por

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

En base a esta condición de ortogonalidad, se define la densidad de probabilidad de Rakhmanov asociada a los armónicos hiperesféricos así:

$$\rho_{l,\{\mu\}}(\Omega_D) = \left| Y_{l,\{\mu\}}(\Omega_D) \right|^2. \tag{2.7}$$

Esta función densidad constituye el punto de partida del estudio de los armónicos hiperesféricos en el marco de la teoría de la información.

2.2. Densidad de probabilidad cuántica

En esta sección se pone de manifiesto que la determinación de las medidas teórico-informacionales de los sistemas cuánticos (que caracterizan sus propiedades físicas y químicas) se reduce en última instancia al cálculo de las correspondientes medidas entrópicas y de complejidad de las funciones especiales y polinomios ortogonales que controlan las funciones de onda de los estados mecano-cuánticos permitidos de dichos sistema físicos. Ello se debe a que la densidad de probabilidad de Born de los sistemas cuánticos puede expresarse en términos de la densidad de probabilidad de Rakhmanov de tales funciones especiales, al menos en aquellos sistemas para los que su ecuación de Schrödinger es exacta- o cuasi-exactamente resoluble. En efecto, sea la ecuación de Schrödinger de una partícula moviéndose en el potencial $V(\vec{r}, t)$:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}, t) + V(\vec{r}, t)\Psi(\vec{r}, t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r}, t). \tag{2.8}$$

La densidad de probabilidad de la partícula viene dada, según los postulados de la mecánica cuántica, por el cuadrado de la función de onda o sea de la solución física $\Psi(\vec{r}, t)$ de esta ecuación de Schrödinger; esto es,

$$P(\vec{r}, t) = |\Psi(\vec{r}, t)|^2. \tag{2.9}$$

Para ilustrar la conexión entre esta densidad de probabilidad cuántica y la densidad de Rakhmanov de los polinomios ortogonales hipergeométricos y la densidad de Rakhmanov de los armónicos hiperesféricos, consideraremos que la partícula se mueve en un potencial tridimensional esféricamente simétrico e independiente del tiempo $V(\vec{r},t) = V(r)$. En tal caso, los estados cuánticos estacionarios del sistema monoparticular pueden describirse por las funciones de onda

$$\psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\theta,\phi) \tag{2.10}$$

con los números cuánticos $n = 0,1,2,\ldots$, $l = 0,1,2,\ldots$, y $m = -l, -l+1\ldots, l$. La parte angular viene dada por los armónicos esféricos tridimensionales

$$Y_{lm}(\theta,\phi) = \frac{1}{\sqrt{2\pi}} C_{l-m}^{l+m}(\cos\theta)(\sin\theta)^m e^{im\phi} \tag{2.11}$$

con $0 \leq \theta \leq \pi$ y $0 \leq \phi \leq 2\pi$, y $C_k^{\alpha}(x)$ denota los polinomios de Gegenbauer o ultraesféricos familiares. La parte radial de la función de onda $R_{nl}(r)$ se puede expresar en términos $\omega^{1/2}(r) y_n(r)$, donde $\{y_n(r)\}$ denota un sistema de polinomios hipergeométricos ortogonales con respecto a la función peso $\omega(r)$. Entonces, la probabilidad de encontrar a la partícula entre $\vec{r}$ y $\vec{r}+d\vec{r}$ viene dada por

$$\rho_{nlm}(\vec{r})d\vec{r} = |\psi_{nlm}(\vec{r},t)|^2 d\vec{r} = D_{nl}(r) r^2 dr \times \Pi_{lm}(\Omega) d\Omega, \tag{2.12}$$

donde el elemento de volumen $d\vec{r} = r^2 dr \sin\theta d\theta d\phi \equiv r^2 dr d\Omega$, y las densidades de probabilidad radial y angular toman la expresión

$$D_{nl}(r) = |R_{nl}(r)|^2 = A(r)\omega(r)\left[y_n(r)\right]^2, \tag{2.13}$$

donde $A(r)$ es una función no negativa, y

$$\Pi_{lm}(\Omega) = |Y_{lm}(\theta,\phi)|^2 = \left[C_{l-m}^{l+m}(\cos\theta)\right]^2 [\sin\theta]^{2m} \tag{2.14}$$

respectivamente. La primera densidad da la probabilidad por intervalo radial de encontrar a la partícula en $(r, r+dr)$, y la segunda describe el perfil espacial del sistema que estamos considerando.

La teoría de la información basada en estas densidades de probabilidad permite cuantificar la aleatoriedad intrínseca (incertidumbre) y el perfil geométrico del sistema cuántico por medio de las distintas medidas teórico-informacionales antes mencionadas de las densidades radial y angular, respectivamente. Mas allá de la varianza, que viene dada por

$$V[\rho_{nlm}] = \int_0^{\infty} r^4 |R_{nl}(r)|^2 dr \tag{2.15}$$

la información de Fisher, por ejemplo, puede expresarse como

$$F[\rho_{nlm}] = F[R_{nl}] + \langle r^{-2}\rangle F[Y_{lm}], \tag{2.16}$$

donde $F[R_{nl}]$ y $F[Y_{lm}]$ son los funcionales de Fisher de la parte radial $R_{nl}(r)$ y el armónico esférico $Y_{lm}(\Omega)$, respectivamente. Por otra parte, la entropía de Shannon resulta ser igual a la suma de los correspondientes funcionales entrópicos $E[R_{nl}]$ y $E[Y_{lm}]$, dados por

$$E[R_{nl}] = -\int_0^{\infty} |R_{nl}(r)|^2 \ln |R_{nl}(r)|^2 dr \tag{2.17}$$

y

$$E[Y_{lm}] = -\int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\phi |Y_{lm}(\theta,\phi)|^2 \ln |Y_{lm}(\theta,\phi)|^2. \tag{2.18}$$

Las correspondientes medidas de complejidad de tipo Cramér-Rao, Fisher-Shannon y LMC pueden obtenerse subsiguientemente a partir de las definiciones ya expuestas en el capítulo anterior, como productos de dos funcionales de polinomios ortogonales de tipo potencia, de tipo gradiente y de tipo logarítmico.

Para determinar numéricamente las medidas de esparcimiento del sistema, hemos de conocer la forma analítica del potencial central; por ejemplo si el potencial es de tipo coulombiano, de tipo oscilador o de tipo rotador rígido, en cuyo caso ya podríamos especificar el tipo de polinomio ortogonal y/o de función especial que controlan las funciones de onda de los estados cuánticos estacionarios del sistema en consideración.

Capítulo 3

Metodología

En este capítulo se describen brevemente algunas técnicas y métodos que se han empleado en esta tesis.

3.1. Cálculo de momentos ordinarios de polinomios ortogonales

El momento ordinario o momento alrededor del origen de orden k, $\langle x^k \rangle$, de la densidad de Rakhmanov de los polinomios ortogonales $y_n(x)$ viene dado por

$$\langle x^k \rangle = \int_a^b x^k \, \rho_n(x) \, dx = \frac{1}{d_n^2} \int_a^b x^k \, \omega(x) \, y_n(x) \, y_n(x) \, dx,$$

donde d_n^2 denota la constante de normalización de los polinomios ya mencionada en el capítulo anterior. Haciendo uso del desarrollo de potencias $y_n(x) = \sum_{m=0}^{n} a_{nm} \, x^m$ y de la relación de ortogonalidad, se obtiene que

$$\langle x^k \rangle = \frac{1}{d_n^2} \sum_{m=n-k}^{n} a_{nm} \left(\int_a^b x^{k+m} \, y_n(x) \, \omega(x) \, dx \right).$$

Ahora el desarrollo de una potencia arbitraria de x en términos de polinomios ortogonales $x^{k+m} = \sum_{p=0}^{k+m} c_{k+m,p} \, y_p(x)$ [71] junto con la relación de ortogonalidad permite obtener finalmente la expresión

$$\langle x^k \rangle = \frac{1}{d_n^2} \sum_{m=n-k}^{n} a_{nm} \, c_{k+m,n} \, d_n^2 = \sum_{m=n-k}^{n} a_{nm} \, c_{k+m,n} \tag{3.1}$$

para los momentos ordinarios de la distribución de los polinomios ortogonales $y_n(x)$ a lo largo de su intervalo de definición. Esta técnica se utiliza en la Sección 4.1 para la determinación de los momentos de los polinomios ortogonales hipergeométricos.

3.2. Método de Laplace

El método de Laplace se ha empleado para calcular el comportamiento asintótico de los funcionales integrales que aparecen a la hora de determinar la asintótica de las normas L_p y las entropías de Rényi de los polinomios ortogonales. En este método se parte de las funciones reales de variable real f y g definidas en un intervalo $[a, b] \subset \mathbb{R} \cup \{-\infty, +\infty\}$ de manera que la siguiente expresión integral de Riemann tenga sentido:

$$I(\lambda) = \int_a^b f(t) e^{pg(t)} \, dt. \tag{3.2}$$

Para calcular el comportamiento asintótico de $I(\lambda)$ cuando $p \to +\infty$ el método considera que las funciones f y g tengan la regularidad necesaria para poder sustituirlas por su correspondiente desarrollo de Taylor. Se distinguen los dos casos siguientes:

- *Caso 1*: Supongamos que g tiene un máximo estricto en $c \in (a,b)$, y que $g'(c) = 0$, $g''(c) < 0$ y $f(c) \neq 0$. Entonces se verifica que

$$I(\lambda) = \int_a^b f(t)e^{pg(t)}\,dt \sim e^{pg(c)} f(c)\sqrt{\frac{2\pi}{-pg''(c)}} \quad \text{si} \quad p \to +\infty.$$

- *Caso 2*: Supongamos que el máximo estricto sea uno de los extremos del intervalo, que el mínimo está en a, y que $g'(a) = 0$ y $g''(a) < 0$. Entonces se verifica que

$$I(\lambda) = \int_a^b f(t)e^{pg(t)}\,dt \sim e^{pg(a)} f(a)\sqrt{\frac{2\pi}{-2pg''(c)}} \quad \text{si} \quad p \to +\infty.$$

Este método se emplea en la Sección 4.2 para el cálculo de los comportamientos asintóticos de las normas L_p y de las entropías de Rényi de los polinomios ortogonales.

3.3. Desarrollo de la potencia de un polinomio en serie de potencias simples mediante los polinomios de Bell

En la Sección 4.1 se demuestra y se utiliza para el cálculo de las normas L_p y de las entropías de Rényi de los polinomios ortogonales el siguiente resultado matemático.

El desarrollo en serie de potencias de la potencia de un polinomio $y_n(x)$ de grado n se puede expresar como

$$[y_n(x)]^p = \left[\sum_{k=0}^{n} c_k x^k\right]^p = \sum_{k=0}^{np} \frac{p!}{(k+p)!} B_{k+p,p}\left(c_0, 2!c_1, \ldots, (k+1)!c_k\right) x^k, \tag{3.3}$$

donde $B_{m,l}$ son los polinomios de Bell multivariados que son muy útiles en Combinatoria [23,64], y que se definen como

$$B_{m,l}\left(c_1, c_2, \ldots, c_{m-l+1}\right) = \\ = \sum_{\hat{\pi}(m,l)} \frac{m!}{j_1! j_2! \cdots j_{m-l+1}!} \left(\frac{c_1}{1!}\right)^{j_1} \left(\frac{c_2}{2!}\right)^{j_2} \cdots \left(\frac{c_{m-l+1}}{(m-l+1)!}\right)^{j_{m-l+1}}, \tag{3.4}$$

donde $c_i \in \mathbb{R}$, $\forall i = 1, \ldots, m-l+1$, $j_i \in \mathbb{N}$ y $m \geq l$ con $m, l \in \mathbb{N}$. Nótese que el número de variables del polinomio depende del valor de los números naturales m, l. La suma que aparece en la definición se extiende a todos los valores de j_i que verifican las dos condiciones $\hat{\pi}(m,l)$ siguientes:

- $j_1 + j_2 + \cdots + j_{m-l+1} = l$.
- $j_1 + 2j_2 + \cdots + (m-l+1)j_{m-l+1} = m$.

3.4. Cálculo de extremales

Sea el funcional

$$I = \int_{x_1}^{x_2} f\left(x, y(x), y'(x)\right)\, dx, \tag{3.5}$$

donde y es una función de la variable x en el intervalo $[x_1, x_2] \in \mathbb{R}$. f hace referencia a un funcional dependiente de la variable x, la función y y su derivada. La función extremal $y(x)$ que hace mínimo o máximo el valor de I viene dada por la ecuación de Euler, que es una ecuación diferencial con la forma siguiente:

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) = 0.$$

Este resultado sólo da el extremal, pero no indica que sea máximo o mínimo. Hay que acudir a otros argumentos para determinarlo. También podemos señalar que cuando el funcional f depende de más de una función, por ejemplo n funciones, se tiene el siguiente grupo de ecuaciones para llegar a la solución:

$$\frac{\partial f}{\partial y_i} - \frac{d}{dx}\left(\frac{\partial f}{\partial y_i'}\right) = 0 \quad i = 1, 2, \ldots, n.$$

En muchas ocasiones pueden encontrarse restricciones de la forma $\phi_i(x, y, y') = 0, \quad i = 0, 1, \ldots, n$. Entonces se define

$$f^*(x, y, y') = f(x, y, y') + \sum_{i=0}^{n} \lambda_i \phi_i(x, y, y'), \tag{3.6}$$

y las nuevas ecuaciones que permiten llegar a resolver el mismo problema son

$$\begin{aligned} &\frac{\partial f^*}{\partial y} - \frac{d}{dx}\left(\frac{\partial f^*}{\partial y'}\right) = 0, \\ &\phi_i(x, y, y') = 0, \quad i = 0, 1, \ldots, n. \end{aligned}$$

La generalización para el caso de varias funciones $y_i, \quad i = 0, 1, \ldots, n$ puede formularse también directamente si tenemos las restricciones $\phi_i(x, y_1, y_1', \ldots, y_n, y_n') = 0 \quad i = 0, 1, \ldots, m$. Definiendo

$$f^*(x, y_1, y_1', \ldots, y_n, y_n') = f(x, y_1, y_1', \ldots, y_n, y_n') + \sum_{i=0}^{m} \lambda_i \phi_i(x, y_1, y_1', \ldots, y_n, y_n'), \tag{3.7}$$

se obtiene para el caso más general posible:

$$\begin{aligned} &\frac{\partial f^*}{\partial y_i} - \frac{d}{dx}\left(\frac{\partial f^*}{\partial y_i'}\right) = 0 \quad i = 0, 1, \ldots, n, \\ &\phi_i(x, y_1, y_1', \ldots, y_n, y_n') = 0 \quad i = 0, 1, \ldots, m. \end{aligned}$$

Este método se ha empleado en la Sección 4.2 para el cálculo de extremales de medidas de información, como es el caso de la entropía de Shannon cuando $f(x, \rho(x)) = -\rho(x) \ln \rho(x)$ y $\phi(x, \rho(x)) = \rho(x)$.

3.5. Técnica de linealización de Srivastava-Niukkanen

Esta técnica [74, 76] consiste en obtener la expresión del producto de una potencia de la variable independiente por una potencia de un polinomio ortogonal $y_n(x)$ como una serie donde los términos son, a su vez, polinomios de la misma familia que $y_n(x)$:

$$x^{\mu}\left[y_n(tx)\right]^r = \sum_{i=0}^{\infty} c_i(\mu, r, t, n) y_i(x), \tag{3.8}$$

donde los coeficientes c_i se expresan en términos de funciones hipergeométricas generalizadas de varias variables de tipo Lauricella. En particular, a modo de ilustración, digamos que para los polinomios de Laguerre se tiene:

$$x^{\mu}\left[L_n^{(\alpha)}(tx)\right]^r = \sum_{i=0}^{\infty} c_i(\mu, r, t, n, \alpha, \gamma) L_i^{(\gamma)}(x), \tag{3.9}$$

con los coeficientes

$$c_i(\mu, r, t, n, \alpha, \gamma) = (\gamma+1)_{\mu} \binom{n+\alpha}{n}^r F_A^{(r+1)}\left(\begin{array}{c} \gamma+\mu+1; \overbrace{-n, \ldots, -n}^{r}, -i \\ \underbrace{\alpha+1, \ldots, \alpha+1}_{r}, \gamma+1 \end{array} ; \overbrace{t, \ldots, t}^{r}, 1 \right), \tag{3.10}$$

donde $F_A^{(r+1)}(x_1, \ldots, x_{r+1})$ denota la función hipergeométrica generalizada de Lauricella de tipo A de $r+1$ variables y $2r+3$ parámetros definida [75] como

$$F_A^{(s)}\left(\begin{array}{c} a; b_1, \ldots, b_s \\ c_1, \ldots, c_s \end{array} ; x_1, \ldots, x_s \right) = \sum_{j_1, \ldots, j_s=0}^{\infty} \frac{(a)_{j_1+\cdots+j_s}(b_1)_{j_1} \cdots (b_s)_{j_s}}{(c_1)_{j_1} \cdots (c_s)_{j_s}} \frac{x_1^{j_1} \cdots x_s^{j_s}}{j_1! \cdots j_s!}. \tag{3.11}$$

Este método se emplea en la Sección 4.2 para el cálculo de las normas L_p y las entropías de Rényi de los polinomios ortogonales.

Capítulo 4

Resultados

A continuación se presenta una descripción de cada uno de los artículos incluidos en esta tesis ordenados temáticamente:

4.1. Longitudes entrópicas de los polinomios ortogonales

Esta sección contiene los dos artículos siguientes que tratan el cálculo de medidas entrópicas de polinomios ortogonales.

1. **Information-theoretic lengths of Jacobi polynomials.**
   A. Guerrero, P. Sánchez-Moreno y J. S. Dehesa.
   Journal of Physics A: Mathematical and Theoretical 43 (2010) 305203 (19 páginas)

2. **Information theoretic-based spreading measures of orthogonal polynomials.**
   J. S. Dehesa, **A. Guerrero** y P. Sánchez-Moreno.
   Complex Analysis and Operator Theory 6 (2012) 585-601

En el primer artículo se estudian los polinomios de Jacobi $P_n^{(\alpha,\beta)}(x)$, con $\alpha, \beta > -1$, desde el punto de vista de la teoría de la información. Para ello se considera la densidad de probabilidad de Rakhmanov de tales polinomios y se determina su esparcimiento en su intervalo de ortogonalidad no solo por medio de los momentos ordinarios alrededor del origen, sino también a través de las siguientes medidas teórico-informacionales: entropías de Shannon y Rényi, y la información de Fisher. Estas magnitudes son complementarias en el sentido que describen distintos aspectos de la distribución de los polinomios que no son comparables entre sí.

Entre los resultados obtenidos cabe mencionar los siguientes: (a) determinación analítica de los momentos ordinarios y la información de Fisher, así como la desviación estándar y la longitud entrópica de Fisher de la densidad de Rakhmanov de estos polinomios, (b) cálculo de la entropía de Rényi en función del grado n del polinomio y de sus parámetros característicos haciendo uso de los polinomios combinatoriales de Bell, (c) estudio de las cotas superiores de la entropía de Shannon para densidades generales en el intervalo compacto $[-1, 1]$ mediante técnicas variacionales, aplicándose después al caso de los polinomios de Jacobi, y (d) análisis numérico exhaustivo de tales cotas.

En el segundo artículo se hace una discusión teórico-computacional comparativa del esparcimiento o distribución de las tres familias canónicas de polinomios ortogonales hipergeométricas (Hermite, Laguerre y Jacobi) en su correspondiente intervalo de ortogonalidad, haciendo uso no solo de la desviación estándar sino también de las tres longitudes entrópicas principales de su densidad de probabilidad de Rakhmanov asociada; a saber, las longitudes de Fisher, Rényi y Shannon. Y se discute su comportamiento asintótico relativo, observándose en particular que la longitud entrópica de Shannon y la desviación estándar están asintóticamente relacionadas de forma lineal en las tres familias hipergeométricas clásicas. Cabe preguntarse sobre si esta propiedad puede cumplirse para otros polinomios ortogonales de tipo Favard.

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Information-theoretic lengths of Jacobi polynomials

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Abstract

The information-theoretic lengths of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, which are information-theoretic measures (Renyi, Shannon and Fisher) of their associated Rakhmanov probability density, are investigated. They quantify the spreading of the polynomials along the orthogonality interval $[-1, 1]$ in a complementary but different way as the root-mean-square or standard deviation because, contrary to this measure, they do not refer to any specific point of the interval. The explicit expressions of the Fisher length are given. The Renyi lengths are found by the use of the combinatorial multivariable Bell polynomials in terms of the polynomial degree n and the parameters (α, β). The Shannon length, which cannot be exactly calculated because of its logarithmic functional form, is bounded from below by using sharp upper bounds to general densities on $[-1, +1]$ given in terms of various expectation values; moreover, its asymptotics is also pointed out. Finally, several computational issues relative to these three quantities are carefully analyzed.

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1. Introduction

The Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, $(\alpha, \beta > -1)$, are the real hypergeometric orthogonal polynomials with respect to the weight function

$$\omega_{\alpha,\beta}(x) = (1-x)^{\alpha}(1+x)^{\beta}$$

in the interval $[-1, 1]$. These polynomials (or some subclasses of them, such as the Chebyshev and Gegenbauer polynomials) play a fundamental role not only in applied mathematics [1–4] and mathematical physics [5–10] but also in numerous scientific and technological fields such as e.g. atomic physics [11–14], classical [15] and quantum [16] optics, information theory [17–21], molecular physics [22–24], non-relativistic [6, 25, 26] and relativistic [27–33] quantum physics, many-body spin physics [34, 35], physics of the Calogero–Moser and Ruijsenaars–Schneieder systems [36], polymer physics [37], QCD analysis of the polarized quark distribution [38], quantum algebras and groups [39–43], quantum walk [44], Rydberg physics [45, 46] and supersymmetric quantum mechanics [22, 47–49]. Let us highlight that the Jacobi polynomials control the angular part of the position wavefunctions of the quantum states of any spherically symmetric quantum-mechanical potential in arbitrary dimensions; it is well known, for example, that central potentials are able to explain a great deal of natural phenomena such as periodicity in the periodic table of elements and numerous macroscopic and spectroscopic properties of atomic and molecular systems. Moreover, the Jacobi polynomials also control the radial part of the momentum wavefunctions of the hydrogenic systems [50], the explicit expression of the representation functions of certain quantum groups [39–41] and some coupling coefficients of angular momenta [42].

Although many algebraic properties (orthogonality, three-term recurrence relation, ladder relations, second-order differential equation, etc) of these polynomials are well known [1–3, 5, 6], this is not the case for their spreading measures beyond the root-mean-square or the standard deviation. These quantities measure the distribution of the Rakhmanov probability density of the Jacobi polynomials (and so, of the polynomials themselves) defined by [51]

$$\rho_{n,\alpha,\beta}(x) = \left[\widetilde{P}_n^{(\alpha,\beta)}(x)\right]^2 \omega_{\alpha,\beta}(x) \qquad (1)$$

along the orthogonality interval $[-1, 1]$ in various complementary ways, where $\widetilde{P}_n^{(\alpha,\beta)}(x)$ are the orthonormal Jacobi polynomials. Physically, this function characterizes the quantum-mechanical density of the stationary states of numerous physical systems [24–27, 47, 52]. In this work we investigate the direct spreading measures of the Rakhmanov density (1) with emphasis on those of information-theoretic origin. The direct spreading measures [53] of a probability density defined in a finite interval share the same properties as the standard deviation: same units as the variable x, reflection invariance and vanishing when the density tends to a Dirac delta. To this family of measures belongs not only the standard deviation but also the information-theoretic lengths of Fisher, Renyi and Shannon types [53, 54], whose definition and meaning for the Rakhmanov density (1), together with the basic properties of the Jacobi polynomials, will be given in section 2. It is interesting to remark that, contrary to the standard deviation which measures the concentration of the probability cloud around a particular point (the centroid) of the orthogonality interval, the information-theoretic lengths do not refer to any specific point of that interval.

This is a reason why the information-theoretic lengths are physically much more appropriate uncertainty measures than the standard deviation in quantum systems. Moreover, they have finite values for probability distributions where the standard deviation does not exist [53]. These lengths are much more convenient measures of the probability distribution than (more conventional) quantifiers such as the associated Shannon entropy, Fisher information and Renyi entropy because, contrarily to these quantities, all the information-theoretic lengths mentioned above have the same dimensions as the variable x, so, allowing a natural comparison among them and with the standard deviation. For explicit physical applications to various quantum mechanical potentials, see [55, 56].

The structure of the paper is as follows. In section 2, the notion and meaning of the spreading measures of a probability density are briefly described for the sake of clarity and to fix notations. In section 3 we give the explicit values of the moments with respect to the origin $\langle x^k\rangle$, $k \in \mathbb{Z}$, the standard deviation Δx and the Fisher length of the polynomials. Then, in section 4, we compute the Renyi lengths in terms of the polynomial degree n and the parameters (α, β) by the use of an error-free approach based on the multivariable Bell polynomials of Combinatorics [57]. The Shannon length of the Jacobi polynomials cannot be calculated in an exact manner because of its logarithmic-functional form; so, it seems natural to try to obtain sharp bounds and to study its asymptotics. Keeping in mind this purpose, we first obtain in section 5 some upper bounds to the Shannon entropy for general probability densities with support $[-1, +1]$ in terms of various power and logarithmic expectation values and then, in section 6, we determine the asymptotics and some upper bounds for the Shannon length of the Jacobi polynomials. In section 7 three computational issues are tackled: (i) the identification of the pairs (α, β) for which the Shannon length is maximal for a given degree n, (ii) the determination of the numerical accuracy of the upper bounds previously mentioned and (iii) the mutual comparison of the isodimensional or direct spreading quantities (standard deviation and information theoretic lengths) of the Jacobi polynomials. Finally, some open problems are posed and conclusions are given.

2. Basics on spreading measures

In this section we gather the notion and meaning of the spreading measures of a probability density. For a probability density $\rho(x)$, $x \in [-1, 1]$, corresponding to some random variable X, there exist two main classes of measures which quantify the distribution or the spread of X along its interval of definition $[-1, 1]$: the moments with respect to the origin $\langle x^k \rangle$, $k \in \mathbb{Z}$, and the frequency or entropic moments $\langle [\rho(x)]^k \rangle$ (see e.g. [58]). Heretoforth, the symbol $\langle f(x) \rangle$ denotes the expectation value of $f(x)$ with respect to the density $\rho(x)$ as

$$\langle f(x) \rangle := \int_{-1}^{1} f(x)\rho(x)\, \mathrm{d}x. \tag{2}$$

The complete knowledge of each set of moments determines the probability density $\rho(x)$ under certain conditions as the ordinary [59] and the entropic [60] Hausdorff moment problems state.

Often, it is more convenient to use instead some related quantities such as the central moments (or moments around the centroid $\langle x \rangle$) given by the expectation values $\langle (x - \langle x \rangle)^k \rangle$, the Renyi entropies [61] defined by

$$R_q[\rho] := \frac{1}{1-q} \ln \langle [\rho(x)]^{q-1} \rangle; \qquad q > 0, \qquad q \neq 1, \tag{3}$$

and the Tsallis entropies [62] given by

$$T_q[\rho] := \frac{1}{q-1}[1 - \langle [\rho(x)]^{q-1} \rangle]; \qquad q > 0, \qquad q \neq 1,$$

together with their $q \to 1$ limit, the Shannon entropy

$$S[\rho] := -\int_{-1}^{1} \rho(x) \ln(\rho(x))\, \mathrm{d}x. \tag{4}$$

These quantities, however, are not direct measures of spreading [53] of $\rho_n(x)$ in the sense that they do not have the same units as x. The most well-known direct measure of spreading are the root-mean-square or standard deviation

$$\Delta x := \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \tag{5}$$

and, in a less sense, the Onicescu–Heller length [63, 64] (also called inverse participation ratio [63, 64], disequilibrium [65], linear entropy [66] and Brükner–Zeilinger entropy [67] in other contexts)

$$L[\rho] := \frac{1}{\langle \rho(x) \rangle}.$$

Recently, other direct measures of spreading related to the entropic moments have been introduced: the Renyi and Shannon lengths [53] defined by

$$L_q^R[\rho] := \exp(R_q[\rho]), \tag{6}$$

and

$$N[\rho] := \lim_{q\to 1} L_q^R[\rho] = \exp(S[\rho]), \tag{7}$$

respectively. Remark that $L_2^R[\rho] = L[\rho]$. It is worth noting that

- the standard deviation and the Renyi and Shannon lengths are global spreading measures because they are powerlike (standard deviation and Renyi lengths) or logarithmic (Shannon length) functionals of the density,
- the standard deviation is a measure of separation of the probability cloud from a particular point of the support interval of the density (namely the mean value or centroid) and
- the Renyi and Shannon lengths are measures of the extent to which the density is in fact concentrated.

In addition, there is another direct measure of spreading which is qualitatively different from the previous one. It is the Fisher length [68], defined by

$$\delta x := \frac{1}{\sqrt{F[\rho]}}, \tag{8}$$

where $F[\rho(x)]$ denotes the Fisher information of the density $\rho(x)$ given by

$$F[\rho] := \left\langle \left[\frac{\mathrm{d}}{\mathrm{d}x}\ln\rho(x)\right]\right\rangle = \int_{-1}^{1}\frac{[\rho'(x)]^2}{\rho(x)}\,\mathrm{d}x. \tag{9}$$

The Fisher length, then, is a functional of the derivative of the density; so, it is very sensitive to the fluctuations of the density in contrast to the global direct measures of spreading mentioned previously. This local quantity measures the pointwise probability concentration of the density along its support interval.

The four direct spreading measures (standard deviation and the Renyi, Shannon and Fisher lengths) defined in a finite interval, besides the properties mentioned in the previous section, enjoy an uncertainty property; see [53] for the standard deviation, Renyi and Shannon cases, and [69, 70] for the Fisher case.

3. Moments, standard deviation and Fisher length

In this section we show the values of the ordinary moments $\langle x^k\rangle_{n,\alpha,\beta}$, the standard deviation $(\Delta x)_{n,\alpha,\beta}$ and the Fisher length $(\delta x)_{n,\alpha,\beta}$ of the Rakhmanov probability density $\rho_{n,\alpha,\beta}(x)$ of the Jacobi polynomials given by equation (1). The Jacobi polynomials $\widetilde{P}_n^{(\alpha,\beta)}(x)$ are known to satisfy the orthonormality relation

$$\int_{-1}^{1}\widetilde{P}_n^{(\alpha,\beta)}(x)\widetilde{P}_m^{(\alpha,\beta)}(x)\omega_{\alpha,\beta}(x)\,\mathrm{d}x = \delta_{nm}, \tag{10}$$

for $\alpha, \beta > -1$, so that $P_n^{(\alpha,\beta)}(x) = d_{n,\alpha,\beta}\widetilde{P}_n^{(\alpha,\beta)}(x)$ gives the relation between the orthonormal and orthogonal polynomials, where the constant

$$d_{n,\alpha,\beta}^2 = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)}.$$

The moments around the origin $\langle x^k\rangle_{n,\alpha,\beta}$ of the Jacobi polynomials, according to equation (2), are defined by

$$\langle x^k\rangle_{n,\alpha,\beta} := \int_{-1}^{+1} x^k \rho_{n,\alpha,\beta}(x)\,\mathrm{d}x = \int_{-1}^{+1} x^k \left[\widetilde{P}_n^{(\alpha,\beta)}(x)\right]^2 \omega_{\alpha,\beta}(x)\,\mathrm{d}x.$$

The use of the expansion of $x^k P_n^{(\alpha,\beta)}(x)$ in series of orthogonal polynomials [71] together with the orthogonality relation (10) has allowed us to obtain that

$$\langle x^k\rangle_{n,\alpha,\beta} = \sum_{m=0}^{n} a_{m,n}^{(\alpha,\beta)} \sum_{l=n-k}^{n} \binom{m}{l} (-1)^{m-l} b_{k+l,n}^{(\alpha,\beta)}, \tag{11}$$

where the coefficients $a_{m,n}^{(\alpha,\beta)}$ and $b_{k+l,n}^{(\alpha,\beta)}$ are given by

$$a_{m,n}^{(\alpha,\beta)} = \binom{n}{m} \frac{\Gamma(\alpha+n+1)\Gamma(\alpha+\beta+n+m+1)}{n!2^m\Gamma(\alpha+\beta+n+1)\Gamma(\alpha+m+1)}, \tag{12}$$

and

$$b_{k+l,n}^{(\alpha,\beta)} = \frac{(k+l)!(-1)^{k+l-n}2^n\Gamma(n+\alpha+\beta+1)}{(k+l-n)!\Gamma(2n+\alpha+\beta+1)}\, {}_2F_1\left(\begin{matrix} n-k-l, n+\beta+1 \\ 2n+\alpha+\beta+2 \end{matrix}; 2\right), \tag{13}$$

respectively. For $k = 1$ and $k = 2$, equations (11)–(13) provide the following values

$$\langle x\rangle_{n,\alpha,\beta} = \frac{\beta^2-\alpha^2}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)}, \tag{14}$$

and

$$\langle x^2\rangle_{n,\alpha,\beta} = \frac{4(n+1)(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2(2n+\alpha+\beta+3)} + \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)} + \langle x\rangle^2, \tag{15}$$

for the first and second moments. Then, the standard deviation of the Jacobi polynomials is, according to equations (1) and (5), the expression

$$(\Delta x)_{n,\alpha,\beta} := \left(\langle x^2\rangle_{n,\alpha,\beta} - \langle x\rangle_{n,\alpha,\beta}^2\right)^{\frac{1}{2}},$$

which together with equations (14) and (15) provides the value

$$(\Delta x)_{n,\alpha,\beta} = \left[\frac{4(n+1)(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2(2n+\alpha+\beta+3)} + \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)}\right]^{1/2},$$

in agreement with the expression recently obtained by other means [72]. Remark that

$$(\Delta x)_{n,\alpha,\beta} \approx \frac{1}{\sqrt{2}}, \qquad n \to +\infty. \tag{16}$$

Moreover, the Fisher length can be obtained by the use of equations (1), (8) and (9) as

$$(\delta x)_{n,\alpha,\beta} = \frac{1}{\sqrt{F[\rho_{n,\alpha,\beta}]}},$$

where the Fisher information $F[\rho_{n,\alpha,\beta}]$ has the expression [73]

$$F[\rho_{n,\alpha,\beta}] = \begin{cases} \frac{2n+\alpha+\beta+1}{4(n+\alpha+\beta-1)}\left[n(n+\alpha+\beta-1)\left(\frac{n+\alpha}{\beta+1}+2+\frac{n+\beta}{\alpha+1}\right)\right. \\ \left. \quad +\,(n+1)(n+\alpha+\beta)\left(\frac{n+\alpha}{\beta-1}+2+\frac{n+\beta}{\alpha-1}\right)\right], & \alpha,\beta > 1, \\ \frac{2n+\beta+1}{4}\left[\frac{n^2}{\beta+1}+n+(4n+1)(n+\beta+1)+\frac{(n+1)^2}{\beta-1}\right], & \alpha = 0, \beta > 1, \\ 2n(n+1)(2n+1), & \alpha,\beta = 0, \\ \infty, & \text{otherwise} \end{cases}$$

for the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ with $\alpha, \beta > -1$ and $n = 0, 1, 2, \ldots$; keep in mind, additionally, that $F[\rho_{n,\alpha,\beta}(x)] = F[\rho_{n,\beta,\alpha}(x)]$ due to the (α, β)-symmetry of Jacobi polynomials. Let us highlight, in particular, that the Cramer–Rao inequality $\delta x \leqslant \Delta x$, valid for continuous densities on the whole real line, is satisfied by the Rakhmanov densities $\rho_{n,\alpha,\beta}(x)$, with support on $[-1, +1]$, when $\alpha, \beta > 1$. This is because these densities have zeros at $x = \pm 1$ and they can be considered as continuous densities on the $(-\infty, +\infty)$ interval.

4. Renyi's lengths

In this section we compute the Renyi lengths $L_q^R[\rho_{n,\alpha,\beta}(x)]$ of the Jacobi polynomials by means of an algebraic methodology which uses the explicit expression of the polynomials and the multivariable Bell polynomials of Combinatorics [57]. According to equations (1), (3) and (6), these quantities are given by

$$L_q^R[\rho_{n,\alpha,\beta}] = \{W_q[\rho_{n,\alpha,\beta}]\}^{-\frac{1}{q-1}}; \qquad q > 0, \qquad q \neq 1,$$

where

$$\begin{aligned} W_q[\rho_{n,\alpha,\beta}] &:= \langle [\rho_{n,\alpha,\beta}(x)]^{q-1} \rangle = \int_{-1}^{+1} [\rho_{n,\alpha,\beta}(x)]^q \, \mathrm{d}x \\ &= \int_{-1}^{+1} \left[\widetilde{P}_n^{(\alpha,\beta)}(x)\right]^{2q} [\omega_{\alpha\beta}(x)]^q \, \mathrm{d}x \end{aligned} \tag{17}$$

are the frequency or entropic moments of the Rakhmanov density (1) of the Jacobi polynomials. To calculate this functional we begin with the explicit expression of the Jacobi polynomials, which can be formulated as the following power series:

$$\widetilde{P}_n^{(\alpha,\beta)}(x) = \sum_{k=0}^{n} c_k x^k, \tag{18}$$

where the expansion coefficients have the values

$$\begin{aligned} c_k = &\sqrt{\frac{\Gamma(\alpha+n+1)(2n+\alpha+\beta+1)}{n!2^(\alpha+\beta+1)\Gamma(\alpha+\beta+n+1)\Gamma(n+\beta+1}} \\ &\times \sum_{i=k}^{n} (-1)^{i-k} \binom{n}{i} \binom{i}{k} \frac{\Gamma(\alpha+\beta+n+i+1)}{2^i \Gamma(\alpha+i+1)}. \end{aligned} \tag{19}$$

Recently it has been found (see the appendix of [54]) that a finite power of a polynomial can be expressed by means of the multivariable Bell polynomials of Combinatorics [57]. This result applied to Jacobi polynomials (18) gives

$$\left[\widetilde{P}_n^{(\alpha,\beta)}(x)\right]^p = \left[\sum_{k=0}^{n} c_k x^k\right]^p = \sum_{k=0}^{np} \frac{p!}{(k+p)!} B_{k+p,p}(c_0, 2!c_1, \ldots, (k+1)!c_k) x^k, \tag{20}$$

with $c_i = 0$ for $i > n$, and the remaining coefficients are given by equation (19). Moreover the Bell polynomials are given by

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

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

$$j_1 + j_2 + \cdots + j_{m-l+1} = l, \qquad \text{and} \qquad j_1 + 2j_2 + \cdots + (m-l+1) j_{m-l+1} = m.$$

The substitution of expression (20) with $p = 2q$ into equation (17) yields the value

$$W_q[\rho_{n,\alpha,\beta}] = \sum_{k=0}^{2nq} \frac{(2q)!}{(k+2q)!} B_{k+2q,2q}(c_0, 2!c_1, \ldots, (k+1)!c_k)\mathcal{I}(k,q,\alpha,\beta), \quad (21)$$

where

$$\mathcal{I}(k,q,\alpha,\beta) = \int_{-1}^{+1} x^k (1-x)^{\alpha q}(1+x)^{\beta q}\,\mathrm{d}x$$
$$= \frac{(-1)^k 2^{1+\alpha q+\beta q}\Gamma(\alpha q+1)\Gamma(\beta q+1)}{\Gamma(\alpha q+\beta q+2)}\, {}_2F_1\left(\begin{matrix}-k, 1+\beta q\\ 2+(\alpha+\beta)q\end{matrix}; 2\right).$$

For the sake of checking we first note that for $q = 1$

$$W_1[\rho_{n,\alpha,\beta}] = \int_{-1}^{+1} \rho_{n,\alpha,\beta}(x)\,\mathrm{d}x = 1,$$

and for $q = 2$,

$$W_2[\rho_{n,\alpha,\beta}] = \int_{-1}^{+1} [\rho_{n,\alpha,\beta}(x)]^2\,\mathrm{d}x$$
$$= \sum_{k=0}^{4n} \frac{4!}{(k+4)!} B_{k+4,4}(c_0, 2!c_1, \ldots, (k+1)!c_k)\mathcal{I}(k,2,\alpha,\beta),$$

which immediately produces the Onicescu–Heller length $L[\rho_{n,\alpha,\beta}]$ of the Jacobi polynomials, since $L[\rho_{n,\alpha,\beta}] = \langle\rho_{n,\alpha,\beta}(x)\rangle^{-1} = \left\{W_2[\rho_{n,\alpha,\beta}]\right\}^{-1}$. The Renyi lengths of these polynomials can be obtained from (6) and (21), obtaining the expression

$$L_q^R[\rho_{n,\alpha,\beta}] = \{W_q[\rho_{n,\alpha,\beta}]\}^{-\frac{1}{q-1}}$$
$$= \left(\sum_{k=0}^{2nq} \frac{(2q)!}{(k+2q)!} B_{k+2q,2q}(c_0, 2!c_1, \ldots, (k+1)!c_k)\mathcal{I}(k,q,\alpha,\beta)\right)^{-\frac{1}{q-1}},$$

with $q = 2, 3, \ldots$. For the two Jacobi polynomials with lowest degrees one has, then, the values

$$L_q^R[\rho_{0,\alpha,\beta}] = \left[\left(\frac{\Gamma(\alpha+\beta+2)}{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}\right)^2 \frac{2^{1+\alpha q+\beta q}\Gamma(\alpha q+1)\Gamma(\beta q+1)}{\Gamma(\alpha q+\beta q+2)}\right]^{-\frac{1}{q-1}},$$

$$L_q^R[\rho_{1,\alpha,\beta}] = \left[\sum_{k=0}^{2q}\binom{2q}{n} c_0^{2q-k} c_1^k \mathcal{I}(k,q,\alpha,\beta)\right]^{-\frac{1}{q-1}},$$

for the Renyi lengths, respectively, and the values

$$L[\rho_{0,\alpha,\beta}] = \left[\left(\frac{\Gamma(\alpha+\beta+2)}{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}\right)^q \frac{2^{1+2\alpha+2\beta}\Gamma(2\alpha+1)\Gamma(2\beta+1)}{\Gamma(2\alpha+2\beta+2)}\right]^{-1},$$

$$L[\rho_{1,\alpha,\beta}] = \left[\sum_{k=0}^{4}\binom{4}{n} c_0^{4-k} c_1^k \mathcal{I}(k,2,\alpha,\beta)\right]^{-1},$$

for the Onicescu–Heller length of the polynomials $P_n^{(\alpha,\beta)}(x)$ with $n = 0, 1$ respectively.

5. Upper bounds to the Shannon entropy for general densities on [−1, +1]

Before starting the study of the Shannon length of the Jacobi polynomials, in the next section we find here several general upper bounds to the Shannon entropy $S[\rho]$ and the Shannon length $N[\rho]$ for any density $\rho(x)$ in the $[-1, +1]$ interval, with different constraints in the form of expectation values.

First, we find the well-known maximum value of this information measure for any normalized density by considering the following Lagrangian:

$$\mathcal{L} = -\int_{-1}^{1} \rho(x) \ln \rho(x)\, \mathrm{d}x - \lambda \left(\int_{-1}^{1} \rho(x)\, \mathrm{d}x - 1 \right).$$

The associated Euler–Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial \mathcal{L}}{\partial \rho'} - \frac{\partial \mathcal{L}}{\partial \rho} = 0,$$

yields

$$\ln \rho_{\max}(x) + 1 + \lambda = 0.$$

So $\rho_{\max}(x)$ is a constant distribution that, once normalized to unity and obtained the value of λ, becomes $\rho_{\max}(x) = 1/2$. The maximum Shannon entropy is $S[\rho_{\max}] = \ln 2$, so we have the well-known general upper bound

$$S[\rho] \leqslant \ln 2,$$

and taking into account equation (7), we obtain

$$N[\rho] \leqslant 2. \tag{22}$$

Now let us find the variational bounds to the Shannon entropy of a general probability density subject not only to the normalization to unity but also to the known expectation value $\langle f(x) \rangle$ of an arbitrary (but given) function $f(x)$. Working similarly as before, we start with the Lagrangian associated with this problem:

$$\mathcal{L} = -\int_{-1}^{1} \rho(x) \ln \rho(x)\, \mathrm{d}x - \lambda_1 \left(\int_{-1}^{1} \rho(x)\, \mathrm{d}x - 1 \right) - \lambda_2 \left(\int_{-1}^{1} f(x)\rho(x)\, \mathrm{d}x - \langle f \rangle \right).$$

Then the corresponding Euler–Lagrange equation yields

$$\rho_{\max}(x) = \mathrm{e}^{-1-\lambda_1}\, \mathrm{e}^{-\lambda_2 f(x)}.$$

The Lagrange multipliers λ_1 and λ_2 are obtained by imposing the two conditions

$$\int_{-1}^{1} \rho_{\max}(x)\, \mathrm{d}x = 1, \tag{23}$$

and

$$\int_{-1}^{1} f(x)\rho_{\max}(x)\, \mathrm{d}x = \langle f \rangle. \tag{24}$$

The analytical determination of the upper bound $S[\rho_{\max}]$ to the Shannon entropy $S[\rho]$ will depend on the explicit form of $f(x)$. In the following we give the upper bounds associated with different choices of $f(x)$.

- Bound in terms of the expectation value $\langle \ln(x^2) \rangle$. In this case we have

$$\rho_{\max}(x) = \mathrm{e}^{-1-\lambda_1}\, \mathrm{e}^{-\lambda_2 \ln(x^2)} = \mathrm{e}^{-1-\lambda_1} |x|^{-2\lambda_2}.$$

Then, condition (23) yields

$$\int_{-1}^{1} \rho_{\max}(x)\,\mathrm{d}x = \mathrm{e}^{-1-\lambda_1} \int_{-1}^{1} |x|^{-2\lambda_2}\,\mathrm{d}x = \mathrm{e}^{-1-\lambda_1} \frac{2}{1-2\lambda_2} = 1, \qquad \text{if} \quad \lambda_2 < \frac{1}{2}.$$

so, λ_1 can be expressed in terms of λ_2 and $\rho_{\max}$ becomes

$$\rho_{\max}(x) = \frac{1-2\lambda_2}{2} |x|^{-2\lambda_2}.$$

The second condition (24) yields

$$\int_{-1}^{1} \ln(x^2)\rho_{\max}(x)\,\mathrm{d}x = \frac{1-2\lambda_2}{2} \int_{-1}^{1} \ln(x^2)|x|^{-2\lambda_2}\,\mathrm{d}x$$
$$= \frac{2}{2\lambda_2 - 1} = \langle \ln(x^2)\rangle, \qquad \text{if} \quad \lambda_2 < \frac{1}{2}.$$

Thus, λ_2 is expressed in terms of $\langle \ln(x^2)\rangle$ as $\lambda_2 = 1/\langle \ln(x^2)\rangle + 1/2$, so the condition $\lambda_2 < 1/2$ is satisfied; and $\rho_{\max}$ is finally written as

$$\rho_{\max}(x) = -\frac{1}{\langle \ln(x^2)\rangle} |x|^{-\frac{2}{\langle \ln(x^2)\rangle} - 1}.$$

The corresponding value of the Shannon entropy for this density is

$$S[\rho_{\max}] = -\int_{-1}^{1} \rho_{\max}(x) \ln \rho_{\max}(x)\mathrm{d}x = 1 + \frac{\langle \ln(x^2)\rangle}{2} + \ln(-\langle \ln(x^2)\rangle).$$

Then, the variational upper bound to the Shannon entropy, with the constraint $\langle \ln(x^2)\rangle$, is given by

$$S[\rho] \leqslant 1 + \frac{\langle \ln(x^2)\rangle}{2} + \ln(-\langle \ln(x^2)\rangle). \tag{25}$$

- Bound in terms of the expectation value $\langle \ln(1-x)\rangle$. Working similarly, we have that

$$\rho_{\max}(x) = \frac{2^{\frac{-1}{\ln 2 - \langle \ln(1-x)\rangle}}}{\ln 2 - \langle \ln(1-x)\rangle} (1-x)^{\frac{1}{\ln 2 - \langle \ln(1-x)\rangle} - 1},$$

and the corresponding upper bound to the Shannon entropy of any distribution with support $[-1, +1]$ and constraint $\langle \ln(1-x)\rangle$ is given by

$$S[\rho] \leqslant 1 + \langle \ln(1-x)\rangle + \ln(\ln 2 - \langle \ln(1-x)\rangle). \tag{26}$$

- Bound in terms of the expectation value $\langle \ln(1+x)\rangle$. In this case we obtain that

$$\rho_{\max}(x) = \frac{2^{\frac{-1}{\ln 2 - \langle \ln(1+x)\rangle}}}{\ln 2 - \langle \ln(1+x)\rangle} (1+x)^{\frac{1}{\ln 2 - \langle \ln(1+x)\rangle} - 1},$$

and the upper bound

$$S[\rho] \leqslant 1 + \langle \ln(1+x)\rangle + \ln(\ln 2 - \langle \ln(1+x)\rangle). \tag{27}$$

- Bound in terms of the expectation value $\langle \ln(1-x^2)\rangle$. In this case the expression of $\langle \ln(1-x^2)\rangle$ in terms of the Lagrange multiplier λ_2 is not invertible, so that we obtain

$$\rho_{\max}(x) = \frac{\Gamma\left(\frac{3}{2} - \lambda_2\right)}{\sqrt{\pi}\,\Gamma(1-\lambda_2)} (1-x^2)^{-\lambda_2},$$

and the upper bound

$$S[\rho] \leqslant -\ln \frac{\Gamma\left(\frac{3}{2} - \lambda_2\right)}{\sqrt{\pi}\,\Gamma(1-\lambda_2)} + \lambda_2 \left(\psi(1-\lambda_2) - \psi\left(\frac{3}{2} - \lambda_2\right)\right), \tag{28}$$

where $\psi(x)$ is the digamma function, with the implicit relation

$$\psi(1-\lambda_2) - \psi\left(\frac{3}{2} - \lambda_2\right) = \langle \ln(1-x^2)\rangle \tag{29}$$

that must be solved numerically for every value of $\langle \ln(1-x^2)\rangle$.

- Bound in terms of the expectation value $\langle x\rangle$. As in the previous case, we have

$$\rho_{\max}(x) = \frac{\lambda_2}{2\sinh(\lambda_2)}\,\mathrm{e}^{-\lambda_2 x},$$

and the upper bound

$$S[\rho] \leqslant -\ln\frac{\lambda_2}{2\sinh(\lambda_2)} - \lambda_2\coth(\lambda_2) - 1, \tag{30}$$

with the implicit relation

$$\frac{1}{\lambda_2} - \coth(\lambda_2) = \langle x\rangle. \tag{31}$$

- Bound in terms of the expectation value $\langle x^2\rangle$. As in the two previous cases, we have

$$\rho_{\max}(x) = \sqrt{\frac{\lambda_2}{\pi}}\frac{1}{\mathrm{erf}(\sqrt{\lambda_2})}\,\mathrm{e}^{-\lambda_2 x^2},$$

and the upper bound

$$S[\rho] \leqslant \frac{1}{2} - \ln\left(\sqrt{\frac{\lambda_2}{\pi}}\frac{1}{\mathrm{erf}(\sqrt{\lambda_2})}\right) - \sqrt{\frac{\lambda_2}{\pi}}\frac{\mathrm{e}^{-\lambda_2}}{\mathrm{erf}(\sqrt{\lambda_2})}, \tag{32}$$

where $\mathrm{erf}(x)$ is the error function, with the implicit relation

$$\frac{1}{\lambda_2} - \frac{\mathrm{e}^{-\lambda_2}}{\sqrt{\lambda_2\pi}\,\mathrm{erf}(\sqrt{\lambda_2})} = \langle x^2\rangle. \tag{33}$$

Finally, let us point out that the combination of equation (7) with each of the bounds (25)–(30) and (32) provides the corresponding upper bounds to the Shannon length of any probability density with the support $[-1, +1]$.

6. The Shannon length

The purpose of this section is twofold. First, to fix the asymptotics of the Shannon length $N[\rho_{n,\alpha,\beta}]$ of the Jacobi polynomials $P_n^{(\alpha,\beta)}$ and its relation to the standard deviation. Second, to determine sharp upper bounds to $N[\rho_{n,\alpha,\beta}]$ by using the results of the previous section. With respect to the first purpose let us start writing that, according to equations (4) and (7),

$$N[\rho_{n,\alpha,\beta}(x)] = \exp\{S[\rho_{n,\alpha,\beta}(x)]\}, \tag{34}$$

with

$$\begin{aligned} S[\rho_{n,\alpha,\beta}] &= -\int_{-1}^{+1} \omega_{\alpha\beta}(x)\big[\widetilde{P}_n^{(\alpha,\beta)}(x)\big]^2 \ln\left\{\omega_{\alpha\beta}(x)\big[\widetilde{P}_n^{(\alpha,\beta)}(x)\big]^2\right\}\mathrm{d}x \\ &= E\big[\widetilde{P}_n^{(\alpha,\beta)}\big] + I\big[\widetilde{P}_n^{(\alpha,\beta)}\big], \end{aligned}$$

with the entropic functionals [70, 74]

$$\begin{aligned} E\big[\widetilde{P}_n^{(\alpha,\beta)}\big] &= -\int_{-1}^{+1} \omega_{\alpha,\beta}(x)\big[\widetilde{P}_n^{(\alpha,\beta)}(x)\big]^2 \ln\big[\widetilde{P}_n^{(\alpha,\beta)}(x)\big]^2\,\mathrm{d}x \\ &= \ln\pi - 1 - (\alpha+\beta)\ln 2 + o(1), \end{aligned} \tag{35}$$

and

$$I\left[\widetilde{P}_n^{(\alpha,\beta)}\right] = -\int_{-1}^{+1} \omega_{\alpha,\beta}(x)\left[\widetilde{P}_n^{(\alpha,\beta)}(x)\right]^2 \ln \omega_{\alpha,\beta}(x)$$
$$= -\alpha\psi(n+\alpha+1) - \beta\psi(n+\beta+1) + (\alpha+\beta)$$
$$\times \left[-\ln 2 + \frac{1}{2n+\alpha+\beta+1} + 2\psi(2n+\alpha+\beta+1) - \psi(n+\alpha+\beta+1)\right].$$

The logarithmic functional $E\left[\widetilde{P}_n^{(\alpha,\beta)}\right]$ cannot be exactly calculated, but its asymptotics has been fully determined by means of the L_p-method of Aptekarev *et al* [75]. Taking into account this result (given by equation (35)) together with the fact that $\lim_{n\to\infty} I\left[\widetilde{P}_n^{(\alpha,\beta)}\right] = (\alpha+\beta)\ln 2$ one has that

$$S[\rho_{n,\alpha,\beta}] = \ln\pi - 1 + o(1); \qquad n \to +\infty,$$

for the Shannon entropy, and with equation (34)

$$N[\rho_{n,\alpha,\beta}] \approx \frac{\pi}{e}; \qquad n \to \infty, \tag{36}$$

for the Shannon length of the Jacobi polynomials. Moreover, from equations (16) and (36) we find the asymptotical relation

$$N[\rho_{n,\alpha,\beta}] \approx \frac{\pi\sqrt{2}}{e}(\Delta x)_{n,\alpha,\beta} \approx 1.6389\,(\Delta x)_{n,\alpha,\beta}; \qquad n \to \infty \tag{37}$$

between the Shannon length and the standard deviation of the Jacobi polynomials. It is interesting to highlight that this asymptotical linear correlation between these two quantities has exactly the same form as for Hermite [54, 76] and Laguerre polynomials [76, 77].

In order to obtain upper bounds for the Shannon length, we can use the variational bounds found in the previous section for the Shannon entropy. Then, from equation (22) we would obtain the general upper bound

$$N[\rho_{n,\alpha,\beta}] \leqslant 2.$$

Imposing now the different constraints based on the expectation values considered before, we obtain the following upper bounds in a straightforward manner:

- Bound with the constraint $\langle \ln(x^2)\rangle$:

$$N[\rho_{n,\alpha,\beta}] \leqslant -\langle \ln(x^2)\rangle \exp\left(1 + \frac{\langle \ln(x^2)\rangle}{2}\right). \tag{38}$$

- Bound with the constraint $\langle \ln(1\pm x)\rangle$:

$$N[\rho_{n,\alpha,\beta}] \leqslant (\ln 2 - \langle \ln(1\pm x)\rangle)\exp(1 + \langle \ln(1\pm x)\rangle). \tag{39}$$

- Bound with the constraint $\langle \ln(1-x^2)\rangle$:

$$N[\rho_{n,\alpha,\beta}] \leqslant \frac{\sqrt{\pi}\,\Gamma(1-\lambda_2)}{\Gamma\left(\frac{3}{2}-\lambda_2\right)} \exp\left[\lambda_2\left(\psi(1-\lambda_2) - \psi\left(\frac{3}{2}-\lambda_2\right)\right)\right], \tag{40}$$

  where λ_2 is related to $\langle \ln(1-x^2)\rangle$ through equation (29).
- Bound with the constraint $\langle x\rangle$:

$$N[\rho_{n,\alpha,\beta}] \leqslant \frac{2\sinh(\lambda_2)}{\lambda_2}\exp(-1 - \lambda_2\coth(\lambda_2)), \tag{41}$$

  where λ_2 is given in terms of $\langle x\rangle$ by equation (31), and $\langle x\rangle$ is given explicitly by equation (14) in terms of (n, α, β).

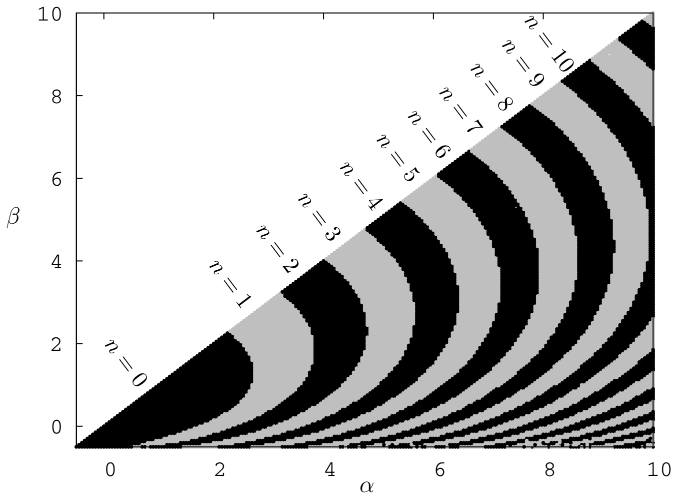

Figure 1. Numerical study of the maximal Shannon length of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$. Regions in the plane (α, β) where the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ have maximal Shannon lengths. Note that the degree n varies from a region to the following.

- Bound with the constraint $\langle x^2 \rangle$:

$$N[\rho_{n,\alpha,\beta}] \leqslant \sqrt{\frac{\pi}{\lambda_2}}\mathrm{erf}(\sqrt{\lambda_2}) \exp\left(\frac{1}{2} - \sqrt{\frac{\lambda_2}{\pi}}\frac{\mathrm{e}^{-\lambda_2}}{\mathrm{erf}(\sqrt{\lambda_2})}\right), \tag{42}$$

where λ_2 is given in term of $\langle x^2 \rangle$ by equation (33), and $\langle x^2 \rangle$ is given by equation (15) in terms of (n, α, β).

The accuracy of these bounds is numerically studied in the next section.

7. Some computational issues

In this numerical section, we first investigate the regions in the plane (α, β) where the Shannon spreading length of the Jacobi polynomials is maximal for various degrees n. Then, we analyze the accuracy of the upper bounds to the Shannon length obtained in the previous section and finally we study the mutual comparison of the four direct spreading lengths considered in this paper, namely the standard deviation and the Fisher, Renyi and Shannon lengths.

In figure 1, we show the regions where the maximal Shannon length of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ in the plane (α, β) is obtained for various degrees n going from 0 to 10. Only half of the plane is shown because the Shannon length is invariant under the exchange of α and β. We observe a rich structure of successive black and gray regions, which is an open analytical problem. All points lying down in a certain region correspond to obtaining the maximum value of the Shannon length for the same degree n. Note the region for $n = 0$, indicating that the maximum Shannon length is $N[\rho_{0,\alpha,\beta}]$. This region is surrounded by other regions where the maximum is sequentially achieved for polynomials with increasing degree, as is shown in the figure.

In figures 2–4 we study numerically the variational bounds (38)–(42) to the Shannon length of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ obtained in the previous section with respect to its exact value $N[\rho_{n,\alpha,\beta}]$ for n going from 0 to 20 and the parameters (α, β) are equal to

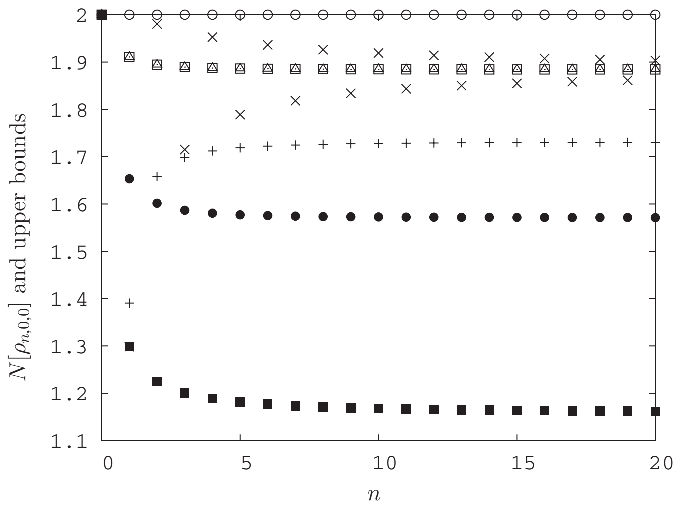

Figure 2. Numerical study of the Shannon length $N[\rho_{n,\alpha,\beta}]$ (■) and its upper bounds in terms of the expectation values $\langle \ln(x^2)\rangle$ (×), $\langle \ln(1-x)\rangle$ (⊡), $\langle \ln(1+x)\rangle$ (△), $\langle \ln(1-x^2)\rangle$ (●), $\langle x\rangle$ (○), $\langle x^2\rangle$ (+), as a function of n for $(\alpha, \beta) = (0, 0)$.

$(0, 0)$, $\left(-\frac{1}{3}, -\frac{1}{3}\right)$ and $(2, 5)$, respectively. The bounds are controlled by the expectation values $\langle \ln(x^2)\rangle$, $\langle \ln(1-x)\rangle$, $\langle \ln(1+x)\rangle$, $\langle \ln(1-x^2)\rangle$, $\langle x\rangle$, $\langle x^2\rangle$, respectively. Several observations can be done. First, all the bounds lie above, or equal in the case $n = \alpha = \beta = 0$, to the exact value; moreover all of them improve the trivial bound 2, except the one controlled by $\langle x\rangle$ in the cases when $\alpha = \beta$, where the density is even and $\langle x\rangle = 0$. Second, expression (40) controlled by the expectation value $\langle \ln(1-x^2)\rangle$ provides the best upper bound in both figures 2 and 3, except for $n = 1$, but that is not true in figure 4. Third, there is still plenty of space for the improvement of the upper bounds in the three figures.

In figures 5 and 6 we make a similar study of the previous bounds to the Shannon length of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ as a function of the parameter α when the pair of values (n, β) is equal to $(0, 2)$ and $(1, 0)$, respectively. It is found that, at times, some upper bounds are equal or very close to the exact value of the Shannon length; this occurs, e.g., for the bounds depending on the expectation values $\langle \ln(1-x)\rangle$ and $\langle \ln(1-x^2)\rangle$ in figure 5, and for the bound depending on $\langle \ln(x^2)\rangle$ in figure 6. Nevertheless, none of the expectation values chosen as constraint supply a sufficiently good upper bound for the whole interval considered.

Finally, in figure 7 we compare the four direct spreading measures of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ among themselves for $(\alpha, \beta) = (2, 2)$ and n going from 0 to 80: the Shannon length $N[\rho_{n,\alpha,\beta}]$, the Renyi lengths $R_q[\rho_{n,\alpha,\beta}]$ with $q = 2$, 5 and 10, the Fisher length $(\delta x)_{n,\alpha,\beta}$ and the standard deviation $(\Delta x)_{n,\alpha,\beta}$. This is possible because all of them have the same dimensions. It is observed that (i) the Fisher length is smaller than the remaining spreading measures, mainly because of its locality property, and it tends toward zero for large values of the polynomial degree n, (ii) the Shannon length is bigger than the rest of spreading measures and, together with the standard deviation, tends asymptotically (i.e. for large n) to constant values, which are mutually related by equation (37) and (iii) the three Renyi lengths considered in the figure, contrary to the two previous global quantities, asymptotically vanish because the power functionals of the densities decrease along the support interval when the polynomial degree is increasing.

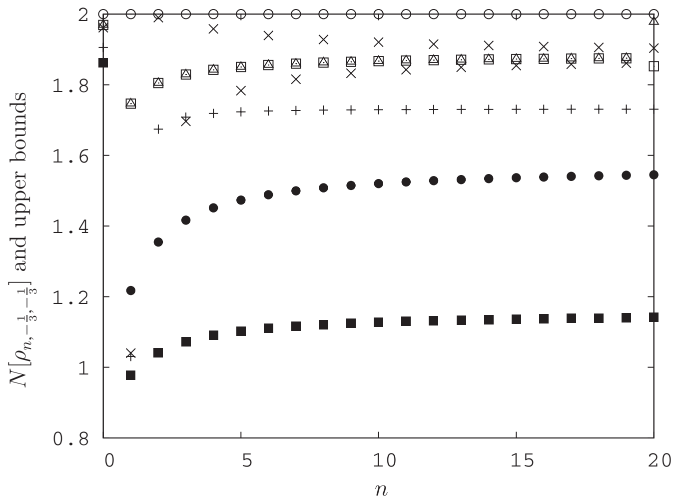

Figure 3. Numerical study of the Shannon length $N[\rho_{n,\alpha,\beta}]$ (■) and its upper bounds in terms of the expectation values $\langle \ln(x^2)\rangle$ (×), $\langle \ln(1-x)\rangle$ (⊡), $\langle \ln(1+x)\rangle$ (△), $\langle \ln(1-x^2)\rangle$ (•), $\langle x\rangle$ (○), $\langle x^2\rangle$ (+), as a function of n for $(\alpha, \beta) = (-1/3, -1/3)$.

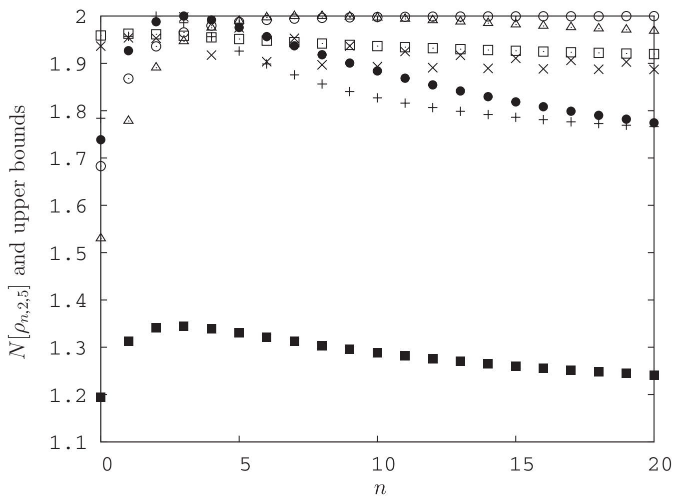

Figure 4. Numerical study of the Shannon length $N[\rho_{n,\alpha,\beta}]$ (■) and its upper bounds in terms of the expectation values $\langle \ln(x^2)\rangle$ (×), $\langle \ln(1-x)\rangle$ (⊡), $\langle \ln(1+x)\rangle$ (△), $\langle \ln(1-x^2)\rangle$ (•), $\langle x\rangle$ (○), $\langle x^2\rangle$ (+), as a function of n for $(\alpha, \beta) = (2, 5)$.

8. Open problems and conclusions

In this work we first give the moments-around-the-origin $\langle x^k\rangle$, the standard deviation Δx and the Fisher length δx of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ in terms of the degree n and the parameters (α, β). Second, we calculate the Renyi lengths of these mathematical objects by means of the Bell polynomials, so much used in Combinatorics.

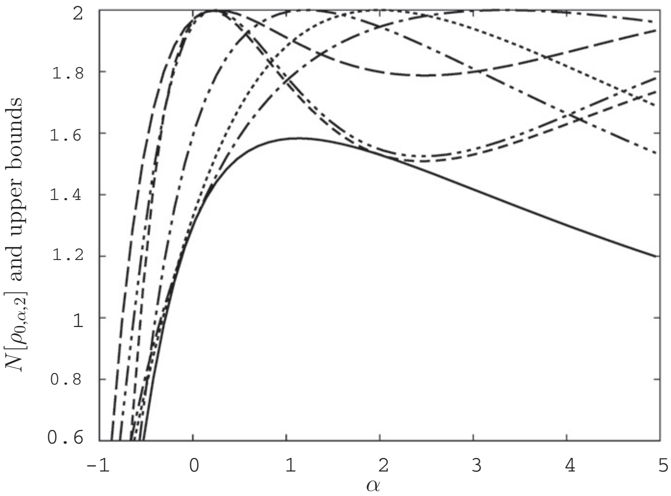

Figure 5. Numerical study of the Shannon length $N[\rho_{n,\alpha,\beta}]$ (■) and its upper bounds in terms of the expectation values $\langle \ln(x^2) \rangle$ (long dashed line), $\langle \ln(1-x) \rangle$ (dash-dotted line), $\langle \ln(1+x) \rangle$ (dash-dot-dotted line), $\langle \ln(1-x^2) \rangle$ (short dashed line), $\langle x \rangle$ (dotted line), $\langle x^2 \rangle$ (dash-dot-dot-dotted line), as a function of α for $(n, \beta) = (0, 2)$.

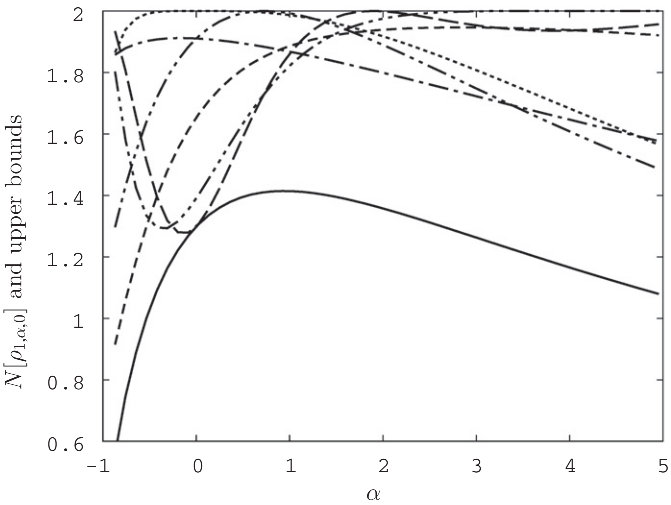

Figure 6. Numerical study of the Shannon length $N[\rho_{n,\alpha,\beta}]$ (■) and its upper bounds in terms of the expectation values $\langle \ln(x^2) \rangle$ (long dashed line), $\langle \ln(1-x) \rangle$ (dash-dotted line), $\langle \ln(1+x) \rangle$ (dash-dot-dotted line), $\langle \ln(1-x^2) \rangle$ (short dashed line), $\langle x \rangle$ (dotted line), $\langle x^2 \rangle$ (dash-dot-dot-dotted line), as a function of α for $(n, \beta) = (1, 0)$.

Then, since the analytical determination of the Shannon length N is a formidable task, we calculate upper bounds of variational type to the Shannon entropy $S[\rho]$ of general densities $\rho(x), x \in [-1, +1]$. These results are subsequently used to yield upper bounds to the Shannon length of the Jacobi polynomials, $N[\rho_{n,\alpha,\beta}]$, via some power and logarithmic expectation values which can be, at times, analytically calculated. Moreover, the accuracy of these bounds is numerically computed and discussed for various polynomial degrees and pairs of parameters (α, β).

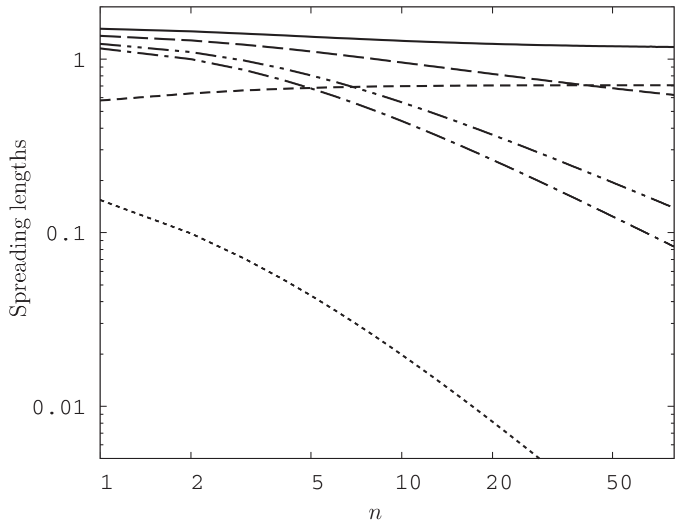

Figure 7. $N[\rho_{n,\alpha,\beta}]$ (solid line), $R_2[\rho_{n,\alpha,\beta}]$ (long dashed line), $R_5[\rho_{n,\alpha,\beta}]$ (dash-dotted line), $R_{10}[\rho_{n,\alpha,\beta}]$ (dash-dotted line), $(\Delta x)_{n,\alpha,\beta}$ (short dashed line) and $(\delta x)_{n,\alpha,\beta}$ (dotted line), as a function of n, for $(\alpha, \beta) = (2, 2)$.

Finally, the mutual comparison of the global (standard deviation, Renyi and Shannon lengths) and local (Fisher length) spreading measures of a Jacobi polynomial is computationally performed since all of them have the same dimensions as the variable x. They grasp various aspects of the polynomial, quantifying its distribution all over the support in different ways.

There are a number of open information-theoretic issues which deserve to be considered for a deeper understanding of the spread of Jacobi polynomials along its support interval. Beyond the exact calculation of the Shannon entropy of the Jacobi polynomials (which is a formidable open task because of its logarithmic functional form), it is interesting from both theoretical and applied points of view to find the asymptotics of the Renyi lengths $L_q^R[\rho_{n,\alpha,\beta}]$ and the entropic moments $W_q[\rho_{n,\alpha,\beta}]$ in the following three following cases: (i) $n \to +\infty$ and (q, α, β) fixed, (ii) $q \to +\infty$ and (n, α, β) fixed and (iii) α and β large but (n, q) fixed. A further open problem is the determination of the analytical boundaries of the regions of the maximal Shannon length in the plane (α, β).

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Complex Analysis and Operator Theory

Information-Theoretic-Based Spreading Measures of Orthogonal Polynomials

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Abstract The macroscopic properties of a quantum system strongly depend on the spreading of the physical eigenfunctions (wavefunctions) of its Hamiltonian operador over its confined domain. The wavefunctions are often controlled by classical or hypergeometric-type orthogonal polynomials (Hermite, Laguerre and Jacobi). Here we discuss the spreading of these polynomials over its orthogonality interval by means of various information-theoretic quantities which grasp some facets of the polynomial distribution not yet analyzed. We consider the information-theoretic lengths closely related to the Fisher information and Rényi and Shannon entropies, which quantify the polynomial spreading far beyond the celebrated standard deviation.

Keywords Classical orthogonal polynomials · Hermite polynomials · Laguerre polynomials · Jacobi polynomials · Information-theoretic lengths · Fisher length · Rényi length · Shannon length

Mathematics Subject Classification (2000) 33C45 · 94A17 · 62B10 · 65C60

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1 Introduction

The special functions of applied mathematics and mathematical physics [1–3] tower above the jungle of mathematical functions for its numerous, simple and elegant algebraic properties, what has facilitated their analytical manipulation and application to solve and interpret a great deal of scientific and technological problems. Nevertheless there are still many open problems related to them whose solution would be very useful and interesting from both fundamental and applied standpoints. This is particularly the case for the information-theoretic properties, whose knowledge for the classical orthogonal polynomials in a real continuous variable has been reviewed in [4] up to 2001 and their asymptotics in [5] up to 2010. The information theory of the discrete orthogonal polynomials and the special functions other than orthogonal polynomials is still in its infancy despite a few efforts on Airy and Bessel functions [6–8], hyperspherical harmonics [9,10], hypergeometric functions [11] and on orthogonal polynomials in a discrete variable [12,13].

According to the Hohenberg–Kohn density functional theory [14], the physical and chemical properties of a quantum system are controlled by the distribution of the single-particle density of the system over its confined domain. This quantum-mechanical density is given by the Rakhmanov probability density of the special function which controls the single-particle wavefunction. Consequently, the physics and chemistry of the quantum systems essentially depend on the spreading of the special functions of applied mathematics over its domain of definition, which is usually fixed by the confining limits of the system. To identify and compute the most appropriate measures of the various facets of this spreading far beyond the celebrated root-mean-square or standard deviation is a main goal of the emerging theory of information of the special functions.

In this paper we are going to discuss the class of direct spreading measures (the standard deviation and the information-theoretic lengths of Fisher, Rényi and Shannon types) of the Rakhmanov probability density [15] of the orthogonal polynomials and to compute them for the Hermite, Laguerre and Jacobi polynomials. They have been shown to best quantify different aspects of the spreading of these polynomials all over its orthogonality interval. It is well known that these classical orthogonal polynomials controls the wavefunctions of numerous quantum systems [1,16–19], including the hydrogenic and oscillator-like systems, and they are very frequently used in modeling a great deal of scientific and technological phenomena.

The structure of this review paper is the following. In Sect. 2 we define the direct spreading measures of the orthogonal polynomials recently introduced [20–26] and we fix the notations which will be used in the rest of the paper. In Sects. 3, 4 and 5 we give the values of the standard deviation and the Fisher length, and the Rényi and Shannon information-theoretic lengths, respectively, as well as the corresponding methodology to calculate them. Then, in Sect. 6 the numerical analysis of these quantities is done for some particular polynomials. Finally, some conclusions are given and various open problems are posed.

2 Direct Spreading Measures of Orthogonal Polynomials

Let us here describe the direct spreading measures of the real hypergeometric-type orthonormal polynomials, i.e. the polynomials which satisfy the orthogonality relation

$$\int_{\Delta} p_n(x) p_m(x) \omega(x) dx = \delta_{n,m}, \quad m, n \in \mathbb{N}, \tag{1}$$

where the weight function $\omega(x)$ has the expressions

$$\begin{aligned} \omega_H(x) &= e^{-x^2}, \\ \omega_L(x) &= x^\alpha e^{-x}, \quad (\alpha > -1) \\ \omega_J(x) &= (1-x)^\alpha (1+x)^\beta, \quad (\alpha, \beta > -1) \end{aligned} \tag{2}$$

for the three canonical families of Hermite $H_n(x)$, Laguerre $L_n^{(\alpha)}(x)$ and Jacobi $P_n^{(\alpha,\beta)}(x)$, respectively. The spreading measures which quantify the different facets of the distribution of these polynomials all over the orthogonality interval are given by the corresponding measures of their associated Rakhmanov probability density, which is defined by

$$\rho_n(x) = p_n^2(x) \omega(x), \tag{3}$$

as defined by this mathematician [15], who first discovered that this density governs the asymptotic ($n \to +\infty$) behavior of the ratio of two polynomials with consecutive orders. It is worth saying here that this normalized-to-unity probability density characterizes the stationary states of a large family of quantum-mechanical potentials [1, 16–19].

The class of direct spreading measures of a probability density [20–22] include the standard deviation and the information-theoretic lengths of Fisher, Rényi and Shannon types. The standard deviation of the polynomial $p_n(x)$ is given by the following root-mean-square

$$(\Delta x)_n = \left(\langle x^2 \rangle_n - \langle x \rangle_n^2 \right)^{\frac{1}{2}}, \tag{4}$$

where the expectation value of a function $f(x)$ is defined by

$$\langle f(x) \rangle_n = \int_{\Delta} f(x) \rho_n(x) dx. \tag{5}$$

The Rényi information-theoretic lengths [22] of the (Rakhmanov density associated to) the polynomial $p_n(x)$ is defined as

$$\mathcal{L}_q^R[\rho_n] = \left\langle [\rho_n(x)]^{q-1} \right\rangle^{-\frac{1}{q-1}} = \left\{ \int_\Delta [\rho_n(x)]^q \, dx \right\}^{-\frac{1}{q-1}}, \quad q > 0, q \neq 1, \tag{6}$$

where $R_q[\rho_n]$ denotes the qth-order Rényi entropy [27]. Let us highlight the case $q = 2$, which corresponds to the Onicescu–Heller length (closely related to the notions of disequilibrium, inverse participation ratio, Brükner–Zeilinger entropy and quantum entanglement in various contexts) given by

$$\mathcal{L}_2^R[\rho_n] = \langle [\rho_n(x)] \rangle^{-1} = \left\{ \int_\Delta [\rho_n(x)]^2 \, dx \right\}^{-1}, \tag{7}$$

and the Shannon length [22], which corresponds to the limiting case $q \to 1$:

$$N[\rho_n] = \lim_{q \to 1} \mathcal{L}_q^R[\rho_n] = \exp(S[\rho_n]) = \exp\left\{ -\int_\Delta \rho_n(x) \ln \rho_n(x) dx \right\}, \tag{8}$$

where $S[\rho_n]$ denotes the Shannon information entropy [28].

Now let us consider a direct spreading measure which is qualitatively different from the previous ones, the Fisher length [20,21]; it is defined by

$$(\delta x)_n \equiv \frac{1}{\sqrt{F[\rho_n]}} \equiv \left\langle \left[\frac{d}{dx} \ln \rho_n(x) \right]^2 \right\rangle^{-\frac{1}{2}} = \left\{ \int_\Delta dx \frac{[\rho_n'(x)]^2}{\rho_n(x)} \right\}^{-\frac{1}{2}}, \tag{9}$$

where $F[\rho_n]$ denotes the Fisher information [29] of the polynomial p_n. It is interesting to remark that this quantity is a functional of the derivative of the Rakhmanov density of the polynomial. So, the Fisher length is very sensitive to the polynomial oscillations. It is a local quantity in the sense that it measures the pointwise concentration of the probability over the orthogonality interval, and it quantifies the gradient content of the Rakhmanov density providing (i) a quantitative estimation of the oscillatory character of the density and the polynomials, and (ii) the bias to particular points of the interval, so that it measures the degree of local disorder.

In contrast, the standard deviation and the Rényi and Shannon lengths are global spreading measures because they are power-like (standard deviation and Rényi lengths) and logarithmic (Shannon length) functionals of the density. Moreover, the standard deviation is a measure of separation of the probability cloud from a particular point of the support interval (namely, the mean value or centroid) while the Rényi and Shannon lengths are measures of the extent to which the density (so, the polynomial) is in fact concentrated.

Finally, let us mention that all the four direct spreding measures share the following properties [20–22]: same units as the random variable, translation and reflection invariance and linear scaling under adequate boundary conditions, and vanishing when the density tends to a delta function. Moreover they fulfil an uncertainty property [30–33] and the Cramér–Rao [20] and Shannon [28] inequalities given by

$$(\delta x)_n \le (\Delta x)_n, \quad \text{and} \quad N[\rho_n] \le (2\pi e)^{\frac{1}{2}} (\Delta x)_n, \tag{10}$$

respectively.

3 Standard Deviation and Fisher's Length of Classical Orthogonal Polynomials

In this Section we give the values of the standard deviation and the Fisher length of the Hermite, Laguerre and Jacobi polynomials in terms of their degree and the characterizing parameters, as well as the methodology used for their analytical calculation.

First let us show that the standard deviation Δx, given by (4), has the value

$$(\Delta x)_n = \sqrt{n + \frac{1}{2}}, \tag{11}$$

for the Hermite polynomials $H_n(x)$,

$$(\Delta x)_{n,\alpha} = \sqrt{2n^2 + 2(\alpha+1)n + \alpha + 1}, \tag{12}$$

for the Laguerre polynomials $L_n^{(\alpha)}(x)$, $\alpha > -1$, and

$$(\Delta x)_{n,\alpha,\beta} = \left[\frac{4(n+1)(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2(2n+\alpha+\beta+3)} + \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)} \right]^{1/2}, \tag{13}$$

for the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, with $\alpha, \beta > -1$. These results can be obtained from Eqs. (4) and (5) and the three-term recurrence relation of the polynomials [23] (see also [24–26] for an alternative proof of the Hermite, Laguerre and Jacobi cases, respectively).

On the other hand, the Fisher information-theoretic length δx, defined by (9), has the value

$$(\delta x)_n = \frac{1}{\sqrt{4n+2}}, \tag{14}$$

for Hermite polynomials $H_n(x)$,

$$(\delta x)_{n,\alpha} = \begin{cases} \frac{1}{\sqrt{4n+1}}; & \alpha = 0, \\ \sqrt{\frac{\alpha^2-1}{(2n+1)\alpha+1}}; & \alpha > 1, \\ 0; & \alpha \in (-1,+1], \alpha \neq 0. \end{cases} \tag{15}$$

for Laguerre polynomials $L_n^{(\alpha)}(x)$, $\alpha > -1$, and

$$(\delta x)_{n,\alpha,\beta} = \frac{1}{\sqrt{F\left[\rho_{n,\alpha,\beta}\right]}}, \tag{16}$$

where the Fisher information $F\left[\rho_{n,\alpha,\beta}\right]$ has the expression

$$F\left[\rho_{n,\alpha,\beta}\right] = \begin{cases} 2n(n+1)(2n+1), & \alpha,\beta = 0, \\ \frac{2n+\beta+1}{4}\left[\frac{n^2}{\beta+1} + n + (4n+1)(n+\beta+1) + \frac{(n+1)^2}{\beta-1}\right], & \alpha = 0, \beta > 1, \\ \frac{2n+\alpha+\beta+1}{4(n+\alpha+\beta-1)}\left[n(n+\alpha+\beta-1)\left(\frac{n+\alpha}{\beta+1} + 2 + \frac{n+\beta}{\alpha+1}\right)\right. & \\ \left. +\,(n+1)(n+\alpha+\beta)\left(\frac{n+\alpha}{\beta-1} + 2 + \frac{n+\beta}{\alpha-1}\right)\right], & \alpha,\beta > 1, \\ \infty, & \text{otherwise,} \end{cases}$$

for Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, with $\alpha, \beta > -1$. These expressions follow from Eq. (9) and the algebraic determination of the Fisher information of the classical orthogonal polynomials [11,34].

The comparison of Eqs. (11)–(13) and (14)–(16) allows us to point out that the Cramér–Rao inequality $\delta x \leq \Delta x$, valid for all continuous probability densities on the whole real line, is indeed fulfilled not only in the Hermite case but also in the Laguerre and Jacobi cases. It is easy to verify that the Cramér–Rao inequality is satisfied for $\alpha = 0$, and for $\alpha = \beta = 0$ and $\alpha = 0, \beta > 0$, respectively. And the corresponding Rakhmanov densities for $\alpha > 1$ and $\alpha, \beta > 1$, with supports $[0, +\infty)$ and $[-1, +1]$, respectively, vanish at $x = 0$ and $x = \pm 1$, so that they can be considered as continuous on the whole real line. Moreover, the Cramér–Rao product $(\delta x)_n(\Delta x)_n = \frac{1}{2}$ for Hermite polynomials. Finally, it is worth noting that the asymptotic ($n \to +\infty$) behaviour of this product is

$$(\delta x)_{n,\alpha}(\Delta x)_{n,\alpha} \simeq \begin{cases} \sqrt{\frac{n}{2}}; & \alpha = 0, \\ \sqrt{\frac{\alpha^2-1}{\alpha}n}; & \alpha > 1, \\ 0; & \alpha \in (-1,+1], \alpha \neq 0. \end{cases}$$

for the Laguerre polynomials $L_n^{(\alpha)}(x)$, and

$$(\delta x)_{n,\alpha,\beta}(\Delta x)_{n,\alpha,\beta} \simeq \begin{cases} (2n)^{-\frac{3}{2}}; & \alpha, \beta = 0, \\ \left(\frac{1}{\beta+1} + \frac{1}{\beta-1} + 4\right)^{-\frac{1}{2}} n^{-\frac{3}{2}}; & \alpha = 0, \beta > 1, \\ \left(\frac{1}{\beta+1} + \frac{1}{\beta-1} + \frac{1}{\alpha+1} + \frac{1}{\alpha-1}\right)^{-\frac{1}{2}} n^{-\frac{3}{2}}; & \alpha > 1, \beta > 1, \\ 0; & \text{otherwise}, \end{cases}$$

for the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$.

4 Rényi's Lengths of Classical Orthogonal Polynomials

In this Section we show the value of the Rényi lengths $\mathcal{L}_q^R[\rho_n]$, with half-integer order q, of Hermite, Laguerre and Jacobi polynomials obtained by a combinatorial methodology based on the use of the multivariate Bell polynomials [35], and the values of these quantities obtained for the Laguerre polynomials by means of an algebraic methodology based on the linearization relation of Srivastava and Niukkanen [36] and the use of Lauricella functions [37].

4.1 Combinatorial Approach

This approach is based on the following lemma

Lemma 4.1 (Ref. [24]) *The p th power of the polynomial*

$$y_n(x) = \sum_{t=0}^{n} c_t x^t \tag{17}$$

is given by

$$[y_n(x)]^p = \sum_{t=0}^{np} \frac{p!}{(t+p)!} B_{t+p,p}(c_0, 2!c_1, \ldots, (t+1)!c_t) x^t, \tag{18}$$

with $c_i = 0$ for $i > n$. The B-symbols denote the Bell polynomials of Combinatorics [35] which are given by

$$B_{m,l}(c_1, c_2, \ldots, c_{m-l+1}) = \sum_{\hat{\pi}(m,l)} \frac{m!}{j_1! j_2! \cdots j_{m-l+1}!} \left(\frac{c_1}{1!}\right)^{j_1} \left(\frac{c_2}{2!}\right)^{j_2} \cdots \left(\frac{c_{m-l+1}}{(m-l+1)!}\right)^{j_{m-l+1}} \tag{19}$$

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

$$j_1+j_2+\cdots+j_{m-l+1}=l, \quad \textit{and} \quad j_1+2j_2+\cdots+(m-l+1)j_{m-l+1}=m. \tag{20}$$

From the definition (6) of the Rényi length of the Rakhmanov density (3) of the classical orthogonal polynomials, the explicit expressions (17) of these polynomials and this lemma, we obtain the following $\mathcal{L}_q^R[\rho_n]$ values for $2q \in \mathbb{N}, q > 2$:

(i) Hermite polynomials $H_n(x)$ [24]

$$\mathcal{L}_q^R[\rho_n] = \left\{W_q[\rho_n]\right\}^{-\frac{1}{q-1}}$$
$$= \left(\sum_{j=0}^{nq} \frac{\Gamma\left(j+\frac{1}{2}\right)}{q^{j+\frac{1}{2}}} \frac{(2q)!}{(2j+2q)!} \times B_{2j+2q,2q}(c_0^{(n)}, 2!c_1^{(n)}, \ldots, (2j+1)!c_{2j}^{(n)})\right)^{-\frac{1}{q-1}}, \tag{21}$$

where the expansion coefficients c_t are given by

$$c_t^{(n)} = \frac{(-1)^{\frac{3n-t}{2}} n!}{\left(2^n n!\sqrt{\pi}\right)^{\frac{1}{2}}} \frac{2^t}{\left(\frac{n-t}{2}\right)!t!} \frac{(-1)^t + (-1)^n}{2}, \tag{22}$$

(ii) Laguerre polynomials $L_n^{(\alpha)}(x)$ [25]

$$\mathcal{L}_q^R\left[\rho_{n,\alpha}\right] = \left[\sum_{k=0}^{2nq} \frac{\Gamma(\alpha q+k+1)}{q^{\alpha q+k+1}} \frac{(2q)!}{(k+2q)!} B_{k+2q,2q}\left(c_0^{(n,\alpha)}, 2!c_1^{(n,\alpha)}, \ldots, (k+1)!c_k^{(n,\alpha)}\right)\right]^{-\frac{1}{q-1}}, \tag{23}$$

with the Laguerre expansion coefficients

$$c_t^{(n,\alpha)} = \sqrt{\frac{\Gamma(n+\alpha+1)}{n!}} \frac{(-1)^t}{\Gamma(\alpha+t+1)} \binom{n}{t}, \tag{24}$$

(iii) Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ [26]

$$\mathcal{L}_q^R\left[\rho_{n,\alpha,\beta}\right] = \left(\sum_{k=0}^{2nq} \frac{(2q)!}{(k+2q)!} \times B_{k+2q,2q}\left(c_0^{(n,\alpha,\beta)}, 2!c_1^{(n,\alpha,\beta)}, \ldots, (k+1)!c_k^{(n,\alpha,\beta)}\right) \mathcal{I}(k,q,\alpha,\beta)\right)^{-\frac{1}{q-1}}, \tag{25}$$

where

$$\mathcal{I}(k,q,\alpha,\beta)=\frac{(-1)^k 2^{1+\alpha q+\beta q}\Gamma(\alpha q+1)\Gamma(\beta q+1)}{\Gamma(\alpha q+\beta q+2)}\,{}_2F_1\left(\begin{matrix}-k,\,1+\beta q\\ 2+(\alpha+\beta)q\end{matrix};2\right).$$

and with the Jacobi expansion coefficients

$$c_t^{(n,\alpha,\beta)}=\sqrt{\frac{\Gamma(\alpha+n+1)(2n+\alpha+\beta+1)}{n!2(\alpha+\beta+1)\Gamma(\alpha+\beta+n+1)\Gamma(n+\beta+1)}}\times\sum_{i=t}^{n}(-1)^{i-t}\binom{n}{i}\binom{i}{t}\frac{\Gamma(\alpha+\beta+n+i+1)}{2^i\Gamma(\alpha+i+1)}. \tag{26}$$

From relations (21)–(25) we can obtain all the Rényi lengths $\mathcal{L}_q^R[\rho]$ with $2q\in\mathbb{N}$ of the three real classical orthogonal polynomials. In particular, for $q=2$ we obtain the following values for the Onicescu–Heller information-theoretic length $\mathcal{L}_2^R[\rho_n]$ [see Eq. (7)]:

$$\mathcal{L}_2^R[\rho_0]=\sqrt{2\pi},\quad \mathcal{L}_2^R[\rho_1]=\frac{4}{3}\sqrt{2\pi},\quad \mathcal{L}_2^R[\rho_2]=\frac{64}{41}\sqrt{2\pi}$$

of the first few Hermite polynomials with degrees $n=0,1,2$,

$$\mathcal{L}_2^R[\rho_{0,\alpha}]=\left(\frac{2^{2\alpha+1}\,(\Gamma(\alpha+1))^2}{\Gamma(2\alpha+1)}\right)^{\frac{1}{2}}, \tag{27}$$

$$\mathcal{L}_2^R[\rho_{1,\alpha}]=\left(\frac{2^{2\alpha+3}\,(\Gamma(\alpha+2))^2}{(1+\alpha)(2+3\alpha)\Gamma(2\alpha+1)}\right)^{\frac{1}{2}} \tag{28}$$

of the Laguerre polynomials $L_n^{(\alpha)}(x)$ with $n=0,1$, and

$$\mathcal{L}_2^R[\rho_{0,\alpha,\beta}]=\left[\left(\frac{\Gamma(\alpha+\beta+2)}{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}\right)^q\frac{2^{1+2\alpha+2\beta}\Gamma(2\alpha+1)\Gamma(2\beta+1)}{\Gamma(2\alpha+2\beta+2)}\right]^{-1}, \tag{29}$$

$$\mathcal{L}_2^R[\rho_{1,\alpha,\beta}]=\left[\sum_{k=0}^{4}\binom{4}{n}c_0^{4-k}c_1^k\mathcal{I}(k,2,\alpha,\beta)\right]^{-1}, \tag{30}$$

of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ with $n=0$ and 1.

4.2 Algebraic Approach

This approach is based on the linearization relation of an arbitrary product of classical orthogonal polynomials of the same type which would allow us to express the

qth-power of the polynomials in terms of the polynomials themselves, so that the power functional involved in the Rényi lengths (6) of the associated Rakhmanov density would be solvable by using the orthogonality relation. Such a linearization relation is known only for Laguerre polynomials [25,36], to the best of our knowledge. Indeed, the linearization relations found by the Srivastava and Niukkanen for arbitrary products of Laguerre polynomials [36] have allowed us to find [25] the expansion relation

$$(qt)^{2q}\left[L_n^{(\alpha)}(t)\right]^{2q}=\sum_{k=0}^{\infty}\Theta_k\left(\alpha q,0,2q,\{n\},\{\alpha\},\left\{\frac{1}{q}\right\}\right)L_k^{(0)}(qt), \tag{31}$$

with the Θ_k-coefficients given by

$$\begin{aligned}\Theta_k\left(\alpha q,0,2q,\{n\},\{\alpha\},\left\{\frac{1}{q}\right\}\right)&=\Gamma(\alpha q+1)\binom{n+\alpha}{n}^{2q}\\ &\times F_A^{(2q+1)}\left(\alpha q+1;-n,\ldots,-n;-k;\alpha+1\cdots,\alpha+1,1;\frac{1}{q},\ldots,\frac{1}{q},1\right).\end{aligned} \tag{32}$$

where $F_A^{(r+1)}$ denotes a Lauricella's hypergeometric function of $r+1$ variables [37]. The combination of Eqs. (3), (6), (31) and (32) yields the following value for the qth-order Rényi length of the Laguerre polynomial

$$\begin{aligned}\mathcal{L}_q^R\left[\rho_{n,\alpha}\right]=\Bigg[&\left(\frac{n!}{\Gamma(\alpha+n+1)}\right)^q\frac{1}{q^{\alpha q+1}}\Gamma(\alpha q+1)\binom{n+\alpha}{n}^{2q}\\ &\times F_A^{(2q+1)}\left(\alpha q+1,-n,\ldots,-n,0;\alpha+1,\ldots,\alpha+1,1;\frac{1}{q},\ldots,\frac{1}{q},1\right)\Bigg]^{-\frac{1}{q-1}},\end{aligned} \tag{33}$$

for every $q>0$ such that $2q\in\mathbb{N}$. As particular cases, this expression gives the value

$$\mathcal{L}_q^R[\rho_{0,\alpha}]=\left[\frac{1}{\Gamma(\alpha+1)^q}\frac{\Gamma(\alpha q+1)}{q^{\alpha q+1}}\right]^{-\frac{1}{q-1}}, \tag{34}$$

and

$$\mathcal{L}_q^R\left[\rho_{1,\alpha}\right]=\left[\frac{\Gamma(\alpha q+1)(1+\alpha)^{2q}}{(\Gamma(\alpha+2))^q q^{\alpha q+1}}\,{}_2F_0\left(\begin{matrix}-2q,\alpha q+1\\ -\end{matrix};\frac{1}{q(\alpha+1)}\right)\right]^{-\frac{1}{q-1}}. \tag{35}$$

for the Laguerre polynomials $L_n^{(\alpha)}(x)$ with lowest degrees $n=0,1$. It is worth remarking that Eqs. (34) and (35) with $q=2$ boil down to the previous values (27) and (28), respectively, of the Onicescu–Heller lengths.

5 Shannon's Length of Classical Orthogonal Polynomials

The Shannon length (8) of the Rakhmanov density (3) of the classical orthogonal polynomials of the classical orthogonal polynomials $N[\rho_n] = \exp(S[\rho_n])$ have not yet been analytically calculated in terms of the degree n and the characterizing parameters, mainly because it is a logarithmic functional of the polynomials. Here, we show "only" its asymptotic ($n \to +\infty$) behaviour and the common linear asymptotical relation with the standard deviation. Moreover, we also give sharp bounds to $N[\rho_n]$ in terms of various expectation values $\langle f(x) \rangle$.

5.1 Asymptotics

In a series of works initiated in 1994 and recently summarized in [5], Aptekarev et al. have studied the asymptotic behaviour of the Shannon entropy

$$S[\rho_n] = -\int \omega(x)\rho_n(x) \log \rho_n(x) dx$$

of the Rakhmanov density $\rho_n(x)$ defined by Eq. (3) for the classical orthogonal polynomials given by Eqs. (1) and (2). They have found the values

$$S[\rho_n] = \log \sqrt{2n} + \log \pi - 1 + o(1),$$
$$S[\rho_{n,\alpha}] = (\alpha + 1) \log n - \alpha \psi(\alpha + n + 1) - 1 + \log(2\pi) + o(1),$$

and

$$S[\rho_{n,\alpha,\beta}] = \log \pi - 1 + o(1)$$

for the Hermite, Laguerre and Jacobi polynomials, respectively, by use of powerful, highbrow concepts and techniques of approximation theory [38]. Taking these results into (8), we obtain the following asymptotical values

$$N[\rho_n] \simeq \frac{\pi\sqrt{2n}}{e} \tag{36}$$

$$N[\rho_{n,\alpha}] \simeq \frac{2\pi n}{e} \tag{37}$$

and

$$N[\rho_{n,\alpha,\beta}] \simeq \frac{\pi}{e} \tag{38}$$

for the Shannon length of Hermite, Laguerre and Jacobi polynomials, respectively.

The comparison of Eqs. (36)–(38) with the asymptotical values of the standard deviation Δx given by Eqs. (11)–(13) for Hermite, Laguerre and Jacobi polynomials, respectively, yields the following linear relation

$$N[\rho] \simeq \frac{\pi\sqrt{2}}{e}\Delta x \simeq 1.6389\Delta x, \tag{39}$$

which is common for all three cases [39] (see also [24–26]). It is interesting to mention here that this relation also holds for the whole class of Bernstein–Szegö polynomials [39] but it is not true for arbitrary orthogonal polynomials, since e.g. it is violated for Freud polynomials. Indeed, the Shannon length and the standard deviation has a quadratic relation in the Freud case [39].

5.2 Upper Bounds

Since the exact value of the Shannon length $N[\rho_n]$ of the classical orthogonal polynomials cannot be calculated in terms of the degree n and the characterizing parameters, it is natural to look for analytical upper bounds to this quantity as simple and accurate as possible. This has been done in 2010 [24–26] in terms of expectation values $\langle x^k\rangle_n$ of the associated Rakhmanov density given by (3).

In the Hermite and Laguerre cases [24,25] we have used an optimized information-theoretic technique based on the non-negativity of the Kullback–Leibler functional of the Rakhmanov density of the polynomial and a probability density of exponentially decreasing type of the form $\exp(-x^k)$. It is found that

$$N[\rho_n] \leq \frac{2(ek)^{\frac{1}{k}}}{k}\Gamma\left(\frac{1}{k}\right)\langle x^k\rangle_n^{\frac{1}{k}}; \quad k = 2, 4, \ldots$$

and

$$N[\rho_{n,\alpha}] \leq \frac{\Gamma\left(\frac{1}{b}\right)(be)^{\frac{1}{b}}}{b}\langle x^b\rangle^{\frac{1}{b}}; \quad b > 0,$$

for the Rényi length of Hermite and Laguerre polynomials, respectively. For completeness we give here the values

$$\langle x^k\rangle_n = \begin{cases} \frac{k!}{2^k\Gamma\left(\frac{k}{2}+1\right)}\, {}_2F_1\left(\begin{matrix}-n, -\frac{k}{2}\\ 1\end{matrix}\middle| 2\right), & \text{even } k \\ 0, & \text{odd } k\end{cases}, \tag{40}$$

and

$$\langle x^k\rangle_{n,\alpha} = \frac{n!\Gamma(k+\alpha+1)}{\Gamma(n+\alpha+1)}\sum_{r=0}^{n}\binom{k}{n-r}^2\binom{k+\alpha+r}{r}, \tag{41}$$

of the ordinary moments of Hermite and Laguerre polynomials, respectively. See [24,25] for further discussion about these bounds. Let us point out here, for completeness, that the results (11) and (12) may be also obtained from Eq. (4) together with Eqs. (40) and (41) with $k = 1$ and 2, respectively.

In the Jacobi case, beyond the general upper bound $N[\rho] \leq 2$ valid for any probability density $\rho(x)$ with the support interval $[-1, +1]$, we [26] have variationally found various upper bounds in terms of the following expectation values: $\langle x \rangle$, $\langle x^2 \rangle$, $\langle \log x^2 \rangle$, $\langle \log(1 \pm x) \rangle$, $\langle \log(1 - x^2) \rangle$. The analytical and numerical analysis of these bounds are discussed in detail in Ref. [26].

6 Numerical Discussion

Here we carry out the numerical comparison of four direct spreading measures (standard deviation, Onicescu length or Renyi length with $q = 2$, Shannon length and Fisher length) of various real classical orthogonal polynomials ($H_n(x)$, $L_n^{(5)}(x)$, $P_n^{(2,2)}(x)$) as a function of the degree n. This is done in Figs. 1, 2 and 3.

In the Hermite and Laguerre cases all the four measures have a similar qualitative behaviour when the polynomial degree increases, as shown in Figs. 1 and 2, respectively for $n = 0, \ldots, 20$. The three global quantities (standard deviation and Onicescu and Shannon lengths) grows when the degree n is increasing, essentially because the polynomials spread more and more. Moreover, they behave so that $\Delta x < \mathcal{L}_2^R < N$, indicating that the spreading rate is weaker with respect to the mean value or centroid of the random variable than in absolute terms. In addition, we observe that the (local) Fisher length δx decreases when the degree n is increasing; this is because the polynomial becomes more and more oscillatory, so making its gradient content bigger. Finally, note that the Fisher length $\delta x < \Delta x$ in the two polynomial cases. It is worth remarking that the rate $\delta x / \Delta x$ fulfils the following characteristics. First, it is less than unity in accordance with the Cramer–Rao inequality (10). Second, it decreases as n^{-1} in the Hermite and as $n^{-\frac{3}{2}}$ in the Laguerre case.

In the Jacobi case $P_n^{(2,2)}(x)$ the results are shown in Fig. 3 when n goes from 0 to 80. The overall behaviour is qualitatively similar to the Hermite and Laguerre cases for

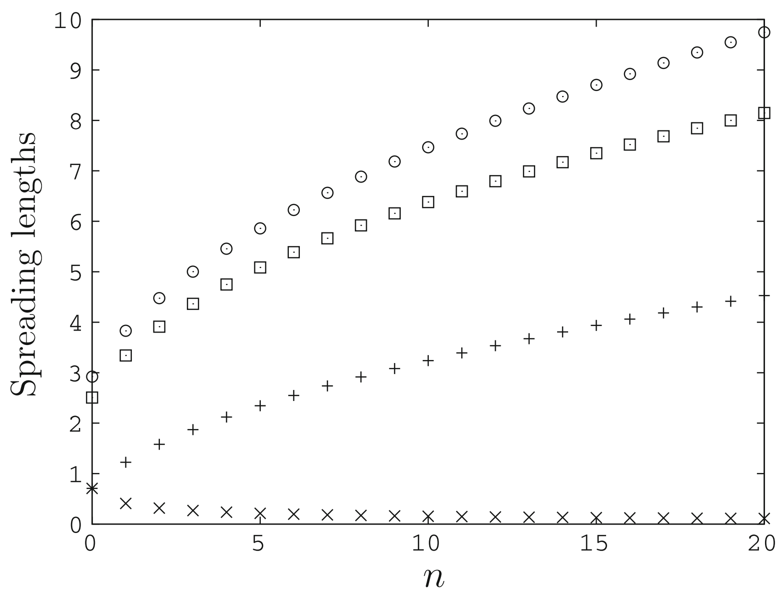

Fig. 1 Standard deviation Δx (+), Fisher length δx (×), Onicescu length $\mathcal{L}_2$ (⊡), and Shannon length N (⊙) of the Hermite polynomial $H_n(x)$ as a function of n

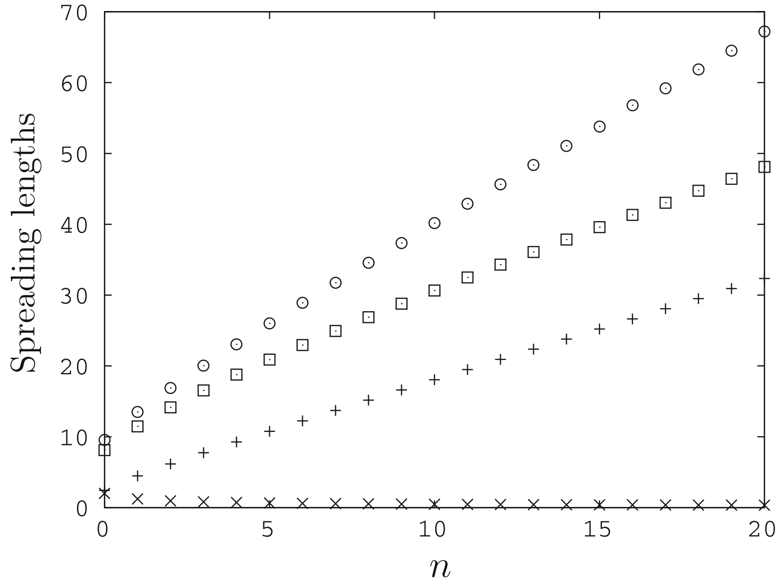

Fig. 2 Standard deviation Δx (+), Fisher length δx (×), Onicescu length $\mathcal{L}_2$ (⊡), and Shannon length N (⊙) of the Laguerre polynomial $L_n^{(5)}(x)$ as a function of n

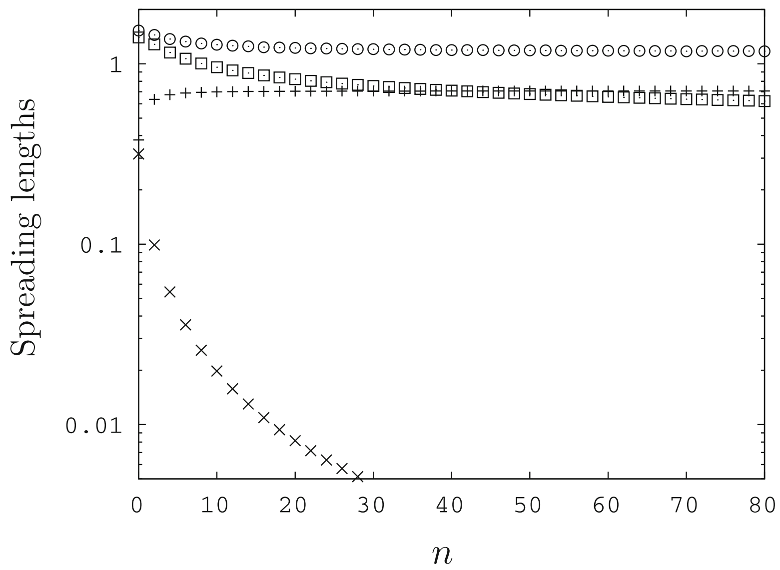

Fig. 3 Standard deviation Δx (+), Fisher length δx (×), Onicescu length $\mathcal{L}_2$ (⊡), and Shannon length N (⊙) of the Jacobi polynomial $P_n^{(2,2)}(x)$ as a function of n

the standard deviation and the Fisher length, while the Shannon and Onicescu lengths decrease in this case as n grows. There are quantitative differences, of course; but there is one quantitative similarity: the rate $\delta x/\Delta x$ decreases as $n^{-\frac{3}{2}}$ like in the Laguerre case. For a more extensive numerical discussion of the various spreading measures of these and other classical orthogonal polynomials, please see Refs. [24–26].

7 Conclusions and Open Problems

We have reviewed the knowledge of the recently introduced information-theoretic lengths of the classical orthogonal polynomials in a real, continuous variable. These measures quantify the spreading of these polynomials over its orthogonality interval in a complementary and more appropriate way than the standard deviation. They do not depend on any specific point of the interval. Moreover, they are direct spreading measures in the sense that they have the same units as the involved random variable and they possess a number of common invariance properties with the standard deviation, what facilitates their use and interpretation.

The standard deviation and the Fisher length can be explicitly given in a simple manner. The Rényi length can be expressed in terms of the degree n and the polynomial parameter(s) via the Bell polynomials in all cases and a Lauricella function in the Laguerre case. The Shannon length has not yet been calculated but its asymptotics has been determined and some bounds have been found either variationally (Jacobi) or by means of an information-theoretic technique. Then, the accuracy of these bounds and the mutual comparision of the four direct spreading measures used in this work have been numerically studied. For completeness let us here mention that interesting but formal and cumbersome expressions between the Shannon entropy and the zeros of some classical orthogonal polynomials have been found in the literature [4,40,41]

Finally let us point out a few open problems whose solution is not only very relevant per se for the algebraic theory of classical orthogonal polynomials but they could also help to improve and extend this work. First, to derive linearization formulas for arbitrary powers of Hermite and Jacobi polynomials; this would help to find alternative expressions to the Rényi lengths of those polynomials. Second, to determine the $\mathcal{L}_q$-norms of the Laguerre and Jacobi polynomials what are not known for all the classical orthogonal polynomials save for the Hermite polynomials [42]. These two problems and their corresponding asymptotics with respect to the degree of the polynomials and the parameter q appear in the study of the Rényi lengths of the polynomials. Third, to find sharp variational bounds to the Shannon length of the orthogonal polynomials mentioned above. Fourth, to identify the largest class of orthogonal polynomials which satisfy the relation (39) fulfilled by three canonical families of classical orthogonal polynomials in a real continuous variable. Fifth, to look for similar correlations among the Fisher and Rényi lengths and standard deviation for Hermite, Laguerre and Jacobi polynomials.

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4.2. Normas L_p y entropías de Rényi de los polinomios ortogonales

Esta sección contiene los dos artículos siguientes que tratan el cálculo de normas L_p y de entropía de Rényi de polinomios ortogonales, y su asintótica.

1. **Rényi entropies, L_q norms and linearization of powers of hypergeometric orthogonal polynomials by means of multivariate special functions.**
   P. Sánchez-Moreno, J. S. Dehesa, A. Zarzo y **A. Guerrero**.
   Applied Mathematics and Computation 223 (2013) 25-33

2. **Asymptotics** $(p \to \infty)$ **of** L_p **norms of hypergeometric orthogonal polynomials.**
   J. S. Dehesa, **A. Guerrero**, J. L. López y P. Sánchez-Moreno.
   Journal of Mathematical Chemistry 52 (2014) 283-300

En el primer artículo se calculan las normas L_p asociadas a los polinomios ortogonales de Laguerre, Hermite generalizados y Jacobi, así como las entropías de Rényi correspondientes R_p, $p \in \mathbb{N}$. Para ello se utilizan las técnicas de linealización polinómica de Srivastava y Niukkanen, escasamente conocidas. Los resultados obtenidos se expresan en términos de funciones hipergeométricas generalizadas de tipo Lauricella (en el caso Hermite y Laguerre) y de Srivastava-Daoust (en el caso de Jacobi) evaluados en algunos valores específicos de las $2p$ variables. Estas funciones dependen de $4p+1$ y $6p+2$ parámetros, respectivamente, que están determinados por el orden p y los parámetros de la función peso correspondiente.

En el segundo artículo se investiga la asintótica ($p \to \infty$, n fijo) de las normas L_p de las densidades de Rakhmanov de los polinomios ortogonales hipergeométricos genéricos $\{y_n(x)\}$ mediante el método de Laplace y la ecuación diferencial de tipo hipergeométrico que tales polinomios satisfacen. De esta forma extendemos los resultados de Larsson-Cohn sobre los polinomios de Hermite [51] a cualquier polinomio ortogonal de carácter hipergeométrico. Además, se analiza y discute críticamente la propiedad de monotonía de esta asintótica y se lleva a cabo un estudio numérico de ella.

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Rényi entropies, L_q norms and linearization of powers of hypergeometric orthogonal polynomials by means of multivariate special functions

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ABSTRACT

The quantification of the spreading of the orthogonal polynomials $p_n(x)$ can be investigated by means of the Rényi entropies $R_q[\rho], q$ being a positive integer number, of the associated Rakhmanov probability densities, $\rho(x) = \omega(x)p_n^2(x)$, where $\omega(x)$ is the corresponding weight function. The Rényi entropies are closely related to the L_q-norms of the polynomials. In this manuscript, the L_q-norms and the associated Rényi entropies of the real hypergeometric orthogonal polynomials (i.e., Hermite, Laguerre, and Jacobi polynomials) and the generalized Hermite polynomials are expressed in an explicit way in terms of some generalized multivariate special functions of Lauricella and Srivastava–Daoust types which are evaluated at some specific values of $2q$ variables. These functions depend on $4q+1$ and $6q+2$ parameters, respectively, which are determined by the order q, the degree n of the polynomial, and the parameters of the orthogonality weight function $\omega(x)$. The key idea is based on some extended linearization formulas for these polynomials. These results open the way to determine the Rényi information entropies of the quantum systems whose wavefunctions are controlled by hypergeometric orthogonal polynomials.

1. Introduction

The theoretical determination of integrals containing products of an arbitrary number of hypergeometric orthogonal polynomials is a long standing, yet generally unsolved, mathematical problem from the times of Erdélyi, Feldheim, Busbridge, Bailey, Carlitz and Titchmarsh (see e.g. [25,17,27,18]) up until now [4,8,1,2,9–11,14,62,33,34,39,42,44–46,52–55,61,65,68,70,71,74,36]. It appears frequently in many scientific and technological domains, ranging from combinatorics [62] and weighted permutation problems [30,26,12,36,29,35], to the theory of angular momentum and mathematical physics for the evaluation of matrix elements of Hermitian operators which describe physical observables of quantum systems (see e.g. [52,68,51] and references therein). Specially relevant from both fundamental and applied standpoints is the calculation of the integrals containing arbitrary (i.e., non-necessarily integer) powers of a certain hypergeometric orthogonal polynomial, because (a) they are closely related to its L_q norm (see e.g. [5,43,6]), to different quantifiers of its spreading all over its orthogonality interval, the information-theoretic lengths [22,32,63,64], and various information-theoretic quantities (Rényi and Tsallis entropies and lengths) of the probability density associated to the polynomial, (b) they admit combinatorial [62,29,42,39,36,35] and entropic [22,32,63,64] interpretations, and (c) they describe the expectation values of some

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quantum observables of the Hilbert space of numerous physical systems (which are the quantum–mechanical predictions of the experimentally accessible physical quantities) [52].

Let us consider the system $\{p_n(x)\}$ of hypergeometric polynomials which are orthonormal with respect to the weight function $\omega(x)$ on the real interval $\Delta = (a, b)$. The probability density associated to these polynomials is given by $\rho_n(x) = \omega(x)p_n^2(x)$, which is to be called Rakhmanov's density, because this author discovered [56] for the first time that it governs the asymptotic $(n \to +\infty)$ behavior of the ratio of two polynomials with consecutive orders. The spreading of the polynomials $p_n(x)$ along its orthogonality interval may be quantified by means of the qth-order frequency moments (also called probability or entropic moments) of its associated probability density, which are the qth-power of the weighted L_q norms of the polynomials, defined by

$$W_q[\rho_n] = \int_\Delta [\rho_n(x)]^q dx = \int_\Delta \left[\omega(x)p_n^2(x)\right]^q dx = \|\rho_n\|_q^q, \tag{1}$$

as well as in terms of the closely related Rényi [58,80] and Tsallis [77,78] entropies of order q, which are given by

$$R_q[\rho_n] = \frac{1}{1-q} \ln W_q[\rho_n]; \quad q > 0, \ q \neq 1, \tag{2}$$

and

$$T_q[\rho_n] = \frac{1}{q-1}(1 - W_q[\rho_n]); \quad q > 0, \ q \neq 1, \tag{3}$$

respectively. The R_q and T_q quantities, which include the celebrated Shannon information entropy $S[\rho_n] = -\int_\Delta \rho_n(x) \log \rho_n(x) dx$ in the limiting case $q \to 1$, grasp different aspects of the distribution of the probability density $\rho_n(x)$ along the interval Δ when the order q is varying. See e.g., the recent review [23].

The goal of this work is the determination of the frequency moments, so the weighted L_q norms and the Rényi and Tsallis entropies, of the three canonical families of real hypergeometric ortogonal polynomials (i.e., Hermite, Laguerre and Jacobi) and the generalized Hermite polynomials in terms of some generalized multivariate hypergeometric functions of Lauricella and Srivastava–Daoust types [69]. These quantities inform us about the distribution of the hypergeometric polynomials along the orthogonality domain in a quantitative manner.

This issue has a manifold motivation. The integer-order frequency moments of a probability density completely characterize the density under certain conditions [41,59]; this is specially interesting in those cases where the ordinary or power moments do not do it properly (see e.g., [60]). The L_q norms has received much attention in approximation theory, the theory of extremal polynomials [49] and the theory of trigonometric series [81], but only recently they have been calculated for the nth-degree real classical ortogonal polynomials in terms of the combinatorics-based multivariate Bell polynomials [32,63,64] (see also the review [22]). This method, however, is not very efficient for high and very high degrees. The asymptotics $(n \to \infty)$ of the L_q norms of the orthogonal polynomials $p_n(x)$ has had its own interest and development since the times of Bernstein and Steklov [49,15,72] up until now [5,6,43] (see also [7] for a review); recently, the leading term of this asymptotics has been fully determined for Hermite polynomials [6], remaining open the Laguerre and Jacobi cases. As well, the asymptotics $(q \to \infty)$ has also been considered by Suetin [72] and Rakhmanov [57] for polynomials orthonormal with respect to a positive weight; recently the leading term of this asymptotics has been calculated for Hermite, Laguerre and Jacobi polynomials [21] and the generalized Hermite polynomials [31].

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 $p_n(x)$ (see e.g. [24] and references therein). Moreover, the physical and chemical properties of a quantum system strongly depend on the distribution of its charge density over the confinement region of the system. This charge density is closely connected with the Rakhmanov density of the hypergeometric orthogonal polynomials or the special functions of mathematical physics which control the wavefunctions of the quantum–mechanically allowed states of the physical system under consideration. The frequency moments of this density (a) allow us to gain insight into the internal disorder of the quantum systems and (b) represent various fundamental and/or experimentally measurable quantities of the systems; e.g., the frequency moments of order $q = 1, \ 2, \ \frac{4}{3}$ and $\frac{5}{3}$ are, at times up to a proportionality factor, the number of constituents, the average electron density, and the Thomas–Fermi and Dirac exchange energies (see e.g. [3,23]), respectively. In addition, they can be used to characterize the macroscopic properties of atoms and molecules which can be represented by functionals of the single-particle density of the physical systems [48,47,50]. On the other hand, let us point out here that the L_q norms of the Hermite polymomials fully determine the frequency moments of the highly-excited (i.e., Rydberg) states of the isotropic harmonic oscillator [6]. The Rényi and Tsallis entropies, which are global measures of the spreading of the density because they are power functionals of $\rho_n(x)$, have been recently used for different purposes in a great variety of fields ranging from finances (see e.g., [13,16]), theory of multifractal systems [38], statistical physics [77–79], to theory of electronic structure and quantum information (see the recent review [66]).

The structure of this paper is the following. First, in Sections 2–4, the Rényi entropies $R_q[\rho_n]$ of the real hypergeometric orthogonal polynomials (i.e., the classical orthogonal polynomials in a real continuous variable) are expressed in terms of the multivariate Lauricella functions $F_A^{(2q)}\left(\frac{1}{q}, \ldots, \frac{1}{q}\right)$ for the Laguerre, Hermite and generalized Hermite cases, and in terms of the Srivastava–Daoust generalized function $F^{1:2;\ldots;2}_{1:1;1\ldots;1}(1, \ldots, 1)$ for the Jacobi case, respectively. Finally, some conclusions and open problems are pointed out.

2. Rényi entropy of Laguerre polynomials $L_n^{(\alpha)}(x)$

In this Section, we calculate the Rényi entropies $R_q[\rho_{n,\alpha}]$ of the Rakhmanov density

$$\rho_{n,\alpha}^L(x) \equiv \rho[L_n^{(\alpha)}] = \frac{1}{d_{n,\alpha}^2} x^\alpha e^{-x} \left[L_n^{(\alpha)}(x)\right]^2 \tag{4}$$

associated to the Laguerre polynomials $L_n^{(\alpha)}(x)$, orthogonal for $\alpha > -1$, with normalization constant $d_{n,\alpha}^2 = \Gamma(n+\alpha+1)/n!$, so that the probability density $\rho_{n,\alpha}^L(x)$ is normalized to unity. They are found to be determined by a Lauricella function $F_A^{(2q)}\left(\frac{1}{q},\ldots,\frac{1}{q}\right)$. The key idea is to use the extended formula of Srivastava–Niukkanen [68,71] which linearizes any positive integer power of Laguerre polynomials.

We begin with the definition (2) for the qth-order Rényi entropy of the Rakhmanov probability density $\rho_{n,\alpha}^L(x)$:

$$R_q[\rho_{n,\alpha}^L] = \frac{1}{1-q} \ln\left[\left(d_{n,\alpha}^2\right)^{-q} \int_0^{+\infty} e^{-qx} x^{\alpha q}\left[\left(L_n^{(\alpha)}(x)\right)^2\right]^q dx\right] = \frac{1}{1-q} \ln\left[\left(d_{n,\alpha}^2\right)^{-q} q^{-\alpha q-1} \int_0^{+\infty} e^{-y} y^{\alpha q}\left[L_n^{(\alpha)}\left(\frac{y}{q}\right)\right]^{2q} dy\right], \tag{5}$$

where we have performed the change of variable $y = qx$. Notice that this expression is valid for $\alpha > -1/q$. The equivalence between the powers of the Laguerre polynomials is valid only for $q \in \mathbb{N}$. We now employ the linearization method of Srivastava–Niukkanen [68,71] for products of various Laguerre polynomials of the form $x^\mu L_{m_1}^{(\alpha_1)}(t_1 x)\cdots L_{m_r}^{(\alpha_r)}(t_r x)$ to obtain the following linearization expression of the integer rth-power of the Laguerre polynomial $L_n^{(\alpha)}(ty)$:

$$y^\mu\left[L_n^{(\alpha)}(ty)\right]^r = \sum_{i=0}^{\infty} c_i(\mu,r,t,n,\alpha,\gamma) L_i^{(\gamma)}(y) \tag{6}$$

with the coefficients

$$c_i(\mu,r,t,n,\alpha,\gamma) = (\gamma+1)_\mu \binom{n+\alpha}{n}^r F_A^{(r+1)}\left(\begin{matrix}\gamma+\mu+1;\overbrace{-n,\ldots,-n}^{r},-i \\ \underbrace{\alpha+1,\ldots,\alpha+1}_{r},\gamma+1\end{matrix};\overbrace{t,\ldots,t}^{r},1\right), \tag{7}$$

where $F_A^{(r+1)}(x_1,\ldots,x_r)$ denotes the Lauricella function of type A of $r+1$ variables and $2r+3$ parameters defined as [69]

$$F_A^{(s)}\left(\begin{matrix}a;b_1,\ldots,b_s \\ c_1,\ldots,c_s\end{matrix};x_1,\ldots,x_s\right) = \sum_{j_1,\ldots,j_s=0}^{\infty} \frac{(a)_{j_1+\cdots+j_s}(b_1)_{j_1}\cdots(b_s)_{j_s}}{(c_1)_{j_1}\cdots(c_s)_{j_s}} \frac{x_1^{j_1}\cdots x_s^{j_s}}{j_1!\cdots j_s!}. \tag{8}$$

Now we linearize the power of Laguerre polynomials in right-hand side of Eq. (5) in terms of the system $\{L_i^{(0)}(y)\}$ by means of the linearization formula (6) for the integer power of the orthogonal polynomials $L_n^{(\alpha)}(ty)$. Taking the values $\mu = \alpha q$, $t = \frac{1}{q}$, $r = 2q$ and $\gamma = 0$ into Eqs. (6) and (7) we obtain

$$y^{\alpha q}\left(L_n^{(\alpha)}\left(\frac{y}{q}\right)\right)^{2q} = \sum_{i=0}^{\infty}\Gamma(\alpha q+1)\binom{n+\alpha}{\alpha}^{2q} F_A^{(2q+1)}\left(\begin{matrix}\alpha q+1;\overbrace{-n,\ldots,-n}^{2q},-i \\ \underbrace{\alpha+1,\ldots,\alpha+1}_{2q},1\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q},1\right) L_i^{(0)}(y). \tag{9}$$

Then, the replacement of this expression into Eq. (2) gives rise to the Rényi entropy

$$R_q[\rho_{n,\alpha}^L] = \frac{1}{1-q} \ln\left[\left(d_{n,\alpha}^2\right)^{-q} q^{-\alpha q-1} \times \int_0^{+\infty} e^{-y} \sum_{i=0}^{\infty}\Gamma(\alpha q+1)\binom{n+\alpha}{\alpha}^{2q} F_A^{(2q+1)}\left(\begin{matrix}\alpha q+1;\overbrace{-n,\ldots,-n}^{2q},-i \\ \underbrace{\alpha+1,\ldots,\alpha+1}_{2q},1\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q},1\right) L_i^{(0)}(y)dy\right]. \tag{10}$$

Using now the orthogonalization condition of the polynomials $\{L_i^{(0)}(y)\}$ we can immediately realize that all the summation terms vanish except the one with $i = 0$, so that

$$\begin{aligned} R_q[\rho_{n,\alpha}] &= \frac{1}{1-q} \ln\left[\left(\frac{n!}{\Gamma(n+\alpha+1)}\right)^q \frac{\Gamma(\alpha q+1)}{q^{\alpha q+1}}\binom{n+\alpha}{\alpha}^{2q} F_A^{(2q+1)}\left(\begin{matrix}\alpha q+1;\overbrace{-n,\ldots,-n}^{2q},0 \\ \underbrace{\alpha+1,\ldots,\alpha+1}_{2q},1\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q},1\right)\right] \\ &= \frac{1}{1-q} \ln\left[\frac{\Gamma(\alpha q+1)}{q^{\alpha q+1}} \frac{(\Gamma(n+\alpha+1))^q}{(n!)^q(\Gamma(\alpha+1))^{2q}} F_A^{(2q)}\left(\begin{matrix}\alpha q+1;\overbrace{-n,\ldots,-n}^{2q} \\ \underbrace{\alpha+1,\ldots,\alpha+1}_{2q}\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q}\right)\right],\end{aligned}$$

which gives the values of the Rényi entropy of the Laguerre polynomials $L_n^{(\alpha)}(x)$ for all integer orders (i.e., when $q \in \mathbb{N}$). Note that the order of the Lauricella function has been reduced to $2q$ in the second equality. Finally, let us realize that the L_q-norm and the associated Rényi entropy depend on the order q, the polynomial degree n and the polynomial parameter α.

3. Rényi entropy of generalized Hermite polynomials $H_n^{(\mu)}(x)$

The generalized Hermite polynomials $H_n^{(\mu)}(x), \mu > -\frac{1}{2}$, are real polynomials orthogonal with respect to the weight $\omega(x) = |x|^{2\mu}e^{-x^2}$. These polynomials, which do not have an hypergeometric character, were introduced by Szegö [73] and extensively studied by Chihara [19], who obtained various algebraic properties beyond orthogonality (e.g., the second-order differential equation, the explicit expression, the Rodrigues formula, a generating function,...). Recently other analytic properties have been found, such as characterization problems, operational rules of Dunkl-type and connection and linearization formulas for the products of two polynomials. Moreover, the generalized Hermite polynomials have been shown to be useful in numerical analysis and various physical fields.

In this Section we determine the Rényi entropies $R_q[\rho_{n,\mu}^H]$ of the Rakhmanov density of the generalized Hermite polynomials

$$\rho_{n,\mu}^H(x) \equiv \rho[H_n^{(\mu)}] = \frac{1}{\tilde{d}_{n,\mu}^2}|x|^{2\mu}e^{-x^2}\left[H_n^{(\mu)}(x)\right]^2 \tag{11}$$

in terms of the Lauricella function $F_A^{(2q)}\left(\frac{1}{q},\ldots,\frac{1}{q}\right)$. The factor

$$\tilde{d}_{n,\mu}^2 = 2^{2n}\left\lfloor\frac{n}{2}\right\rfloor!\,\Gamma\left(\left\lfloor\frac{n+1}{2}\right\rfloor + \mu + \frac{1}{2}\right)$$

is the normalization constant of the polynomials, where $\lfloor x \rfloor$ denotes the integer part of x. We will use a methodology which begins with the definition (2) of Rényi entropy, continues with the relation between the generalized Hermite and Laguerre polynomials and, finally, employs the linearization formula (6) of Srivastava–Niukkanen.

From Eq. (2) the Rényi entropies of the Hermite polynomial $H_n(x)$ is given by

$$\begin{aligned} R_q[\rho_{n,\mu}^H] &= \frac{1}{1-q}\ln\int_{-\infty}^{+\infty}(\tilde{d}_{n,\mu}^2)^{-q}|x|^{2\mu q}e^{-qx^2}\left(\left(H_n^{(\mu)}(x)\right)^2\right)^q dx \\ &= \frac{1}{1-q}\ln\left[(\tilde{d}_{n,\mu}^2)^{-q}q^{-\mu q-\frac{1}{2}}\int_{-\infty}^{+\infty}|y|^{2\mu q}e^{-y^2}\left(H_n\left(\frac{y}{\sqrt{q}}\right)\right)^{2q}dy\right] \end{aligned} \tag{12}$$

for $\mu > -\frac{1}{2q}$ where we have made the change of variable $y = \sqrt{q}x$, and the equivalence between the powers of the generalized Hermite polynomials is valid only for $q \in \mathbb{N}$. To calculate this Hermite functional, we first take into account the following expressions of generalized Hermite polynomials of even and odd orders in terms of Laguerre polynomials

$$H_{2n}^{(\mu)}(x) = (-1)^n 2^{2n} n! L_n^{(\mu-\frac{1}{2})}(x^2), \quad \mu > -\frac{1}{2}, \tag{13}$$

$$H_{2n+1}^{(\mu)}(x) = (-1)^n 2^{2n+1} n! x L_n^{(\mu+\frac{1}{2})}(x^2), \quad \mu > -\frac{1}{2}, \tag{14}$$

so that we have

$$\left[H_n^{(\mu)}\left(\frac{y}{\sqrt{q}}\right)\right]^{2q} = A_{n,q}(\nu)q^{-q\nu}y^{2q\nu}\left[L_{\frac{n-\nu}{2}}^{(\mu+\nu-\frac{1}{2})}\left(\frac{y^2}{q}\right)\right]^{2q} \tag{15}$$

with the constant

$$A_{n,q}(\nu) = 2^{2qn}\left(\Gamma\left(\frac{n-\nu}{2}+1\right)\right)^{2q} \tag{16}$$

and the parameter $\nu = 0$ for even n, and $\nu = 1$ for odd n.

Thus, we can use the formula (6) to linearize the $(2q)$th-power of generalized Hermite polynomials given by Eq. (15) although only when $q \in \mathbb{N}$.

From Eqs. (15), (6) and (7), one has

$$|y|^{2\mu q}\left[H_n^{(\mu)}\left(\frac{y}{\sqrt{q}}\right)\right]^{2q} = A_{n,q}(\nu)q^{-q\nu}\sum_{k=0}^{\infty}c_k\left(q(\mu+\nu), 2q, \frac{1}{q}, \frac{n-\nu}{2}, \mu+\nu-\frac{1}{2}, -\frac{1}{2}\right)L_k^{(-\frac{1}{2})}(y^2) \tag{17}$$

with the linearization coefficients

$$c_k\left(q(\mu+\nu),2q,\frac{1}{q},\frac{n-\nu}{2},\mu+\nu-\frac{1}{2},-\frac{1}{2}\right)=\left(\frac{1}{2}\right)_{q(\mu+\nu)}\begin{pmatrix}\mu+\frac{n+\nu-1}{2}\\ \frac{n-\nu}{2}\end{pmatrix}^{2q}\times F_A^{(2q+1)}\left(\begin{matrix}q(\mu+\nu)+\frac{1}{2};\frac{\nu-n}{2},\ldots,\frac{\nu-n}{2},-k\\ \mu+\nu+\frac{1}{2},\ldots,\mu+\nu+\frac{1}{2},\frac{1}{2}\end{matrix};\frac{1}{q},\ldots,\frac{1}{q},1\right)$$

where $F_A^{(2q+1)}\left(\frac{1}{q},\ldots,\frac{1}{q},1\right)$ is a Lauricella function of $2q+1$ variables (see Eq. (8)). Moreover, using again Eq. (15) in Eq. (17) one obtains the following linearization relation for the $(2q)$th-power of generalized Hermite polynomials

$$|y|^{2\mu q}\left[H_n^{(\mu)}\left(\frac{y}{\sqrt{q}}\right)\right]^{2q}=A_{n,q}(\nu)q^{-q\nu}\sum_{k=0}^{\infty}\left(\frac{1}{2}\right)_{q(\mu+\nu)}\begin{pmatrix}\mu+\frac{n+\nu-1}{2}\\ \frac{n-\nu}{2}\end{pmatrix}^{2q}F_A^{(2q+1)}\left(\begin{matrix}q(\mu+\nu)+\frac{1}{2};\frac{\nu-n}{2},\ldots,\frac{\nu-n}{2},-k\\ \mu+\nu+\frac{1}{2},\ldots,\mu+\nu+\frac{1}{2},\frac{1}{2}\end{matrix};\frac{1}{q},\ldots,\frac{1}{q},1\right)\frac{1}{(-1)^k2^{2k}k!}H_{2k}^{(0)}(y). \quad (18)$$

Now, taking this expression into Eq. (12) and keeping in mind the orthogonalization condition of generalized Hermite polynomials one realizes that the only non-vanishing contribution from the summation is the one with $k=0$; so that we find

$$R_q[\rho_{n,\mu}^H]=\frac{1}{1-q}\ln\left[\left(\tilde{d}_{n,q}\right)^{-q}q^{-\mu q-\frac{1}{2}}A_{n,q}(\nu)q^{-q\nu}\left(\frac{1}{2}\right)_{q(\mu+\nu)}\begin{pmatrix}\mu+\frac{n+\nu-1}{2}\\ \frac{n-\nu}{2}\end{pmatrix}^{2q}F_A^{(2q+1)}\left(\begin{matrix}q(\mu+\nu)+\frac{1}{2};\frac{\nu-n}{2},\ldots,\frac{\nu-n}{2},0\\ \mu+\nu+\frac{1}{2},\ldots,\mu+\nu+\frac{1}{2},\frac{1}{2}\end{matrix};\frac{1}{q},\ldots,\frac{1}{q},1\right)\int_{-\infty}^{+\infty}e^{-y^2}H_0^{(0)}(y)dy\right].$$

Thus, one finally finds the values

$$R_q[\rho_{n,\mu}^H]=\frac{1}{1-q}\ln\left[q^{-(\mu+\nu)q-\frac{1}{2}}\left(\frac{\Gamma\left(\mu+\frac{n+\nu+1}{2}\right)}{\Gamma\left(\frac{n-\nu}{2}+1\right)}\right)^q\left(\Gamma\left(\mu+\nu+\frac{1}{2}\right)\right)^{-2q}\Gamma\left(q(\mu+\nu)+\frac{1}{2}\right)F_A^{(2q+1)}\left(\begin{matrix}q(\mu+\nu)+\frac{1}{2};\overbrace{\frac{\nu-n}{2},\ldots,\frac{\nu-n}{2}}^{2q},0\\ \underbrace{\mu+\nu+\frac{1}{2},\ldots,\mu+\nu+\frac{1}{2}}_{2q},\frac{1}{2}\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q},1\right)\right].$$

Finally, since the last upper parameter of the Lauricella function is $b_{2q+1}=0$ we can reduce it to a Lauricella function $F_A^{(2q)}\left(\frac{1}{q},\ldots,\frac{1}{q}\right)$ as follows

$$R_q[\rho_{n,\mu}^H]=\frac{1}{1-q}\ln\left[q^{-(\mu+\nu)q-\frac{1}{2}}\left(\frac{\Gamma\left(\mu+\frac{n+\nu+1}{2}\right)}{\Gamma\left(\frac{n-\nu}{2}+1\right)}\right)^q\left(\Gamma\left(\mu+\nu+\frac{1}{2}\right)\right)^{-2q}\Gamma\left(q(\mu+\nu)+\frac{1}{2}\right)F_A^{(2q)}\left(\begin{matrix}q(\mu+\nu)+\frac{1}{2};\overbrace{\frac{\nu-n}{2},\ldots,\frac{\nu-n}{2}}^{2q}\\ \underbrace{\mu+\nu+\frac{1}{2},\ldots,\mu+\nu+\frac{1}{2}}_{2q}\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q}\right)\right],$$

for the Rényi entropies of integer order q for generalized Hermite polynomials, $H_n^{(\mu)}(x)$, with $\nu=0$ for even degree and $\nu=1$ for odd degree. Notice that they are expressed in terms of n,μ and q, only.

As a particular case, for $\mu=0$, we obtain the expression of the Rényi entropy of the usual Hermite polynomials:

$$R_q[\rho_{n,0}^H]=\frac{1}{1-q}\ln\left[q^{-\nu q-\frac{1}{2}}\left(\frac{\Gamma\left(\frac{n+\nu+1}{2}\right)}{\Gamma\left(\frac{n-\nu}{2}+1\right)}\right)^q\left(\Gamma\left(\nu+\frac{1}{2}\right)\right)^{-2q}\Gamma\left(q\nu+\frac{1}{2}\right)F_A^{(2q)}\left(\begin{matrix}q\nu+\frac{1}{2};\overbrace{\frac{\nu-n}{2},\ldots,\frac{\nu-n}{2}}^{2q}\\ \underbrace{\nu+\frac{1}{2},\ldots,\nu+\frac{1}{2}}_{2q}\end{matrix};\overbrace{\frac{1}{q},\ldots,\frac{1}{q}}^{2q}\right)\right],$$

which is completely determined by n and q.

4. Rényi entropy of Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$

In this Section we determine the Rényi entropies $R_q[\rho_{n,\alpha,\beta}], q\in\mathbb{N}$, of the Rakhmanov probability density

$$\rho_{n,\alpha,\beta}(x)=\frac{1}{d_{n,\alpha,\beta}^2}(1-x)^\alpha(1+x)^\beta\left(P_n^{(\alpha,\beta)}(x)\right)^2, \quad (19)$$

associated to the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, orthogonal for α and $\beta>-1$, with the normalization constant

$$d_{n,\alpha,\beta}^2=\frac{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{n!(\alpha+\beta+2n+1)\Gamma(\alpha+\beta+n+1)}. \quad (20)$$

These entropic quantities are found to be expressed by means of a Srivastava–Daoust function $F_{1:1;\ldots;1}^{1:2;\ldots;2}(1,\ldots,1)$ of the $2q$ variables $(x_1,\ldots,x_{2q})$ evaluated at $(1,\ldots,1)$, and $2q+1$ parameters, as we will show in the following.

We begin with Eq. (2) which defines the Rényi entropy $R_q[\rho_{n,\alpha,\beta}]$ as

$$R_q[\rho_{n,\alpha,\beta}] = \frac{1}{1-q}\ln\left[\frac{1}{\left(d^2_{n,\alpha,\beta}\right)^q}\int_{-1}^{1}(1-x)^{\alpha q}(1+x)^{\beta q}\left(\left(P_n^{(\alpha,\beta)}(x)\right)^2\right)^q dx\right] \tag{21}$$

for $\alpha,\beta > -1/q$. Now, we linearize the term

$$\left[\left(P_n^{(\alpha,\beta)}(x)\right)^2\right]^q = \left[P_n^{(\alpha,\beta)}(x)\right]^{2q}, \quad \text{for } q\in\mathbb{N}, \tag{22}$$

in terms of the Jacobi system $\{P_i^{(\alpha q,\beta q)}\}$ by means of the following Srivastava's linearization formula [68]

$$x^\mu\left(P_n^{(\alpha,\beta)}(x)\right)^r = \sum_{i=0}^{\infty}\tilde{c}_i(\mu,r,n,\alpha,\beta,\gamma,\delta)P_i^{(\gamma,\delta)}(x), \tag{23}$$

where the expansion coefficients are given by

$$\tilde{c}_i(\mu,r,n,\alpha,\beta,\gamma,\delta) = \binom{n+\alpha}{n}^r(\gamma+1)_\mu\frac{(\gamma+\delta+2i+1)(-\mu)_i}{(\gamma+1)_i(\gamma+\delta+i+1)_{\mu+1}}F^{2:2;\ldots;2}_{2:1;\ldots;1}\left(\begin{matrix}\mu+1,\gamma+\mu+1:\overbrace{-n,\alpha+\beta+n+1;\ldots;-n,\alpha+\beta+n+1}^{r}\\ \mu-i+1,\gamma+\delta+\mu+i+2:\underbrace{\alpha+1;\ldots;\alpha+1}_{r}\end{matrix};\overbrace{1,\ldots,1}^{r}\right). \tag{24}$$

The symbol $F^{2:2;\ldots;2}_{2:1;\ldots;1}(x_1,\ldots,x_r)$ denotes the r-variate Srivastava–Daoust function [68] defined as

$$F^{p_0:p_1;\ldots;p_r}_{q_0:q_1;\ldots;q_r}\left(\begin{matrix}a_0^{(1)},\ldots,a_0^{(p_0)}:a_1^{(1)},\ldots,a_1^{(p_1)};\ldots;a_r^{(1)},\ldots,a_r^{(p_r)}\\ b_0^{(1)},\ldots,b_0^{(q_0)}:b_1^{(1)},\ldots,b_1^{(q_1)};\ldots;b_r^{(1)},\ldots,b_r^{(q_r)}\end{matrix};x_1,\ldots,x_r\right)$$
$$= \sum_{j_1,\ldots,j_r=0}^{n}\frac{(a_0^{(1)})_{j_1+\cdots+j_r}\cdots(a_0^{(p_0)})_{j_1+\cdots+j_r}}{(b_0^{(1)})_{j_1+\cdots+j_r}\cdots(b_0^{(q_0)})_{j_1+\cdots+j_r}}\frac{(a_1^{(1)})_{j_1}\cdots(a_1^{(p_1)})_{j_1}(a_2^{(1)})_{j_2}\cdots(a_2^{(p_2)})_{j_2}\cdots(a_r^{(1)})_{j_r}\cdots(a_r^{(p_r)})_{j_r}}{(b_1^{(1)})_{j_1}\cdots(b_1^{(q_1)})_{j_1}(b_2^{(1)})_{j_2}\cdots(b_2^{(q_2)})_{j_2}\cdots(b_r^{(1)})_{j_r}\cdots(b_r^{(q_r)})_{j_r}}\times\frac{x_1^{j_1}x_2^{j_2}\cdots x_r^{j_r}}{j_1!j_2!\cdots j_r!},$$

which depends on $N=\sum_{i=0}^{r}(p_i+q_i)$ parameters. See [68] for further details and applications. Notice that the Srivastava–Daoust' generalized special function $F^{2:2;\ldots;2}_{2:1;\ldots;1}(1,\ldots,1)$ which appears in Eq. (24), has $N=3r+4$ parameters, presenting the expression

$$F^{2:2;\ldots;2}_{2:1;\ldots;1}\left(\begin{matrix}\mu+1,\gamma+\mu+1:\overbrace{-n,\alpha+\beta+n+1;\ldots;-n,\alpha+\beta+n+1}^{r}\\ \mu-i+1,\gamma+\delta+\mu+i+2:\underbrace{\alpha+1;\ldots;\alpha+1}_{r}\end{matrix};\overbrace{1,\ldots,1}^{r}\right)$$
$$= \sum_{j_1,\ldots,j_r=0}^{n}\frac{(\mu+1)_{j_1+\cdots+j_r}(\gamma+\mu+1)_{j_1+\cdots+j_r}}{(\mu-i+1)_{j_1+\cdots+j_r}(\gamma+\delta+\mu+i+2)_{j_1+\cdots+j_r}}\times\frac{(-n)_{j_1}(\alpha+\beta+n+1)_{j_1}\cdots(-n)_{j_r}(\alpha+\beta+n+1)_{j_r}}{(\alpha+1)_{j_1}\cdots(\alpha+1)_{j_r}j_1!\cdots j_r!}.$$

In order to linearize the term (22) encountered in the expression (21) of the Rényi entropy by means of the Srivastava's formula (23)–(24), we have to consider the case $\mu=0$. For such a case the linearization coefficient

$$\tilde{c}_i(\mu,r,n,\alpha,\beta,\gamma,\delta) = \binom{n+\alpha}{n}^r(\gamma+1)_\mu\frac{(\gamma+\delta+2i+1)(-\mu)_i}{(\gamma+1)_i(\gamma+\delta+i+1)_{\mu+1}}\times\sum_{j_1,\ldots,j_r=0}^{n}\frac{(\mu+1)_{j_1+\cdots+j_r}(\gamma+\mu+1)_{j_1+\cdots+j_r}}{(\mu-i+1)_{j_1+\cdots+j_r}(\gamma+\delta+\mu+i+2)_{j_1+\cdots+j_r}}$$
$$\times\frac{(-n)_{j_1}(\alpha+\beta+n+1)_{j_1}\cdots(-n)_{j_r}(\alpha+\beta+n+1)_{j_r}}{(\alpha+1)_{j_1}\cdots(\alpha+1)_{j_r}j_1!\cdots j_r!}, \tag{25}$$

presents an indetermination problem provoked by the first Pochhammer symbol in the denominator of the summation kernel. This problem can be solved by using the following Slater's formula [67]

$$\frac{(-\mu)_i(\mu+1)_{j_1+\cdots+j_r}}{(\gamma+1)_i(\mu-i+1)_{j_1+\cdots+j_r}} = {}_2F_1\left(\begin{matrix}\gamma+\mu+j_1+\cdots+j_r+1,-i\\ \gamma+1\end{matrix};1\right). \tag{26}$$

Taking the expression (26) into Eq. (25), we have that the coefficient needed in our problem becomes

$$\tilde{c}_i(0,r,n,\alpha,\beta,\gamma,\delta) = \binom{n+\alpha}{n}^r\frac{\gamma+\delta+2i+1}{\gamma+\delta+i+1}\sum_{j_1,\ldots,j_r=0}^{n}\sum_{j_{r+1}=0}^{i}\frac{(\gamma+1)_{j_1+\cdots+j_r+j_{r+1}}}{(\gamma+\delta+i+2)_{j_1+\cdots+j_r}}$$
$$\times\frac{(-n)_{j_1}(\alpha+\beta+n+1)_{j_1}\cdots(-n)_{j_r}(\alpha+\beta+n+1)_{j_r}(-i)_{j_{r+1}}}{(\alpha+1)_{j_1}\cdots(\alpha+1)_{j_r}(\gamma+1)_{j_{r+1}}j_1!\cdots j_r!j_{r+1}!}, \tag{27}$$

so that with $\mu=0, r=2q, \gamma=\alpha q$ and $\delta=\beta q$, the Eq. (23) provides the following linearization formula for even powers of the Jacobi polynomials:

$$\left(P_n^{(\alpha,\beta)}(x)\right)^{2q} = \sum_{i=0}^{\infty}\tilde{c}_i(0,2q,n,\alpha,\beta,\alpha q,\beta q)P_i^{(\alpha q,\beta q)}(x). \tag{28}$$

The replacement of this expression in Eq. (21) allows us to find

$$R_q[\rho_{n,\alpha,\beta}] = \frac{1}{1-q}\ln\left[\frac{1}{\left(d_{n,\alpha,\beta}^2\right)^q}\int_{-1}^{1}(1-x)^{\alpha q}(1+x)^{\beta q}\sum_{i=0}^{\infty}\tilde{c}_i(0,2q,n,\alpha,\beta,\alpha q,\beta q)P_i^{(\alpha q,\beta q)}(x)dx\right]. \tag{29}$$

The use of the orthogonalization condition of the system $\{P_i^{(\alpha q,\beta q)}\}$ allows us to boil down this expression to a single term: the one corresponding to $i=0$. We obtain that

$$R_q[\rho_{n,\alpha,\beta}] = \frac{1}{1-q}\ln\left[\frac{d_{0,\alpha q,\beta q}^2}{\left(d_{n,\alpha,\beta}^2\right)^q}\tilde{c}_0(0,2q,n,\alpha,\beta,\alpha q,\beta q)\right], \tag{30}$$

with

$$\begin{aligned}\tilde{c}_0(0,2q,n,\alpha,\beta,\alpha q,\beta q) &= \binom{n+\alpha}{n}^{2q}\times\sum_{j_1,\ldots,j_{2q}=0}^{n}\frac{(\alpha q+1)_{j_1+\cdots+j_{2q}}}{(\alpha q+\beta q+2)_{j_1+\cdots+j_{2q}}}\frac{(-n)_{j_1}(\alpha+\beta+n+1)_{j_1}\cdots(-n)_{j_{2q}}(\alpha+\beta+n+1)_{j_{2q}}}{(\alpha+1)_{j_1}\cdots(\alpha+1)_{j_{2q}}j_1!\cdots j_{2q}!}\\ &= \binom{n+\alpha}{n}^{2q}F_{1:1;\ldots;1}^{1:2;\ldots;2}\left(\begin{matrix}\alpha q+1:-n,\alpha+\beta+n+1;\ldots;-n,\alpha+\beta+n+1\\ \alpha q+\beta q+2:\alpha+1;\ldots;\alpha+1\end{matrix};1,\ldots,1\right),\end{aligned}$$

where the involved generalized special function is a $2q$-variate Srivastava–Daoust function evaluated at unity; i.e., at $(1,\ldots,1)$. Thus, we have finally found the following expression

$$\begin{aligned}R_q[\rho_{n,\alpha,\beta}] = \frac{1}{1-q}\ln&\left[\frac{2^{\alpha q+\beta q+1}\Gamma(\alpha q+1)\Gamma(\beta q+1)}{\Gamma(\alpha q+\beta q+2)}\left(\frac{n!(\alpha+\beta+2n+1)\Gamma(\alpha+\beta+n+1)}{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}\right)^q\right.\\ &\left.\times\binom{n+\alpha}{n}^{2q}F_{1:1;\ldots;1}^{1:2;\ldots;2}\left(\begin{matrix}\alpha q+1:\overbrace{-n,\alpha+\beta+n+1;\ldots;-n,\alpha+\beta+n+1}^{2q}\\ \alpha q+\beta q+2:\underbrace{\alpha+1;\ldots;\alpha+1}_{2q}\end{matrix};\overbrace{1,\ldots,1}^{2q}\right)\right].\end{aligned}$$

for the Rényi entropy of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ with order $q=2,3,4,\ldots$ It is worth noting that this quantity depends on the order q, the polynomial degree n and parameters α and β.

5. Conclusions and open problems

The L_q-norms and the associated Rényi entropies $R_q, q\in\mathbb{N}$, of the hypergeometric orthogonal polynomials $\{p_n(x)\}$ in a real continuous variable (i.e., Hermite, Laguerre and Jacobi polynomials) and the generalized Hermite polynomials have been expressed in terms of some generalized multivariate special functions of Lauricella type and Srivastava–Daoust types evaluated at some specific values of $2q$ variables. These funcions depend on $4q+1$ and $6q+2$ parameters, respectively, which are determined by the order q, the degree n and the parameters of the corresponding weight function. We have used a methodology based on some non-sufficiently known linearization techniques of Srivastava and Niukkanen. Although the Rényi entropy of the polynomials $p_n(x)$ can be efficiently computed directly from its definition (see Eqs. (1) and (2)) when n is not high enough, our results are relevant from an analytical point of view because they open the way to find interesting properties for the Rényi entropies of the polynomials by using the rich variety of analytical properties provided by the theory of the special functions for the generalized multivariate hypergeometric functions. Moreover, they allow us to study the asymptotics of the L_q norms, the entropic moments and the Rényi entropies of the hypergeometric polynomials when the degree n is high and very high, by means of the determination of the concomitant asymptotics of the generalized hypergeometric functions of Lauricella and Srivastava types: when their characterizing parameters are large and very large. The latter requires to use and extend recent investigations of various authors [75,76,28,20] done for simpler functions where one of the parameters is very large, what lies beyond the scope of this paper.

This theoretical effort is not only mathematically interesting *per se* because it might be an alternative approach to the most sophisticated and fine methods of Riemann–Hilbert and Tulyakov (see e.g. [6]) for the analytical evaluation of the L_q norms, but also physically relevant because it would allows us to e.g., determine the exact values of the macroscopic fundamental and experimentally accesible quantities of the highly-excited (i.e., Rydberg) atomic and molecular systems; indeed, they are controlled by the L_q norms and entropic moments of the Rakhmanov probability density of some hypergeometric orthogonal polynomials. In this sense, this work is a further motivation to foster the present investigations in the largely unexplored field of asymptotics of the generalized multivariate hypergeometric functions in spite of the elegant results which have been done by a number of researchers (see e.g. [75,76,28,20]).

Let us mention that the determination of the L_q norms of the orthogonal polynomials of the Askey tableau [40] other than the classical polynomials considered here is a completely open issue for both continuous and discrete variables. In the latter case the problem is harder because there are no practical procedures of linearization of powers of these polynomials in spite of a few efforts based on the recursion relation [46,14], the difference equation [1], or motivated by some combinatorial problems [62,37].

Finally let us point out that our method to calculate L_q-norms with an integer positive q is related to the explicit expressions of the linearization coefficients (see them in e.g. Chapter 9 of [35] or [40] for the squares of hypergeometric orthogonal polynomials, and [68,71] for higher powers). Thus, it cannot be used to calculate the L_q-norms when q is any positive real number. The latter requires a completely different approach, still unknown at least to the best of our knowledge. Indeed, it would be most interesting to develop such an approach to provide a more general answer to our problem, without the need of the linearization coefficients.

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ORIGINAL PAPER

Asymptotics ($p \to \infty$) of L_p-norms of hypergeometric orthogonal polynomials

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Abstract The determination of the weighted L_p norms of the real orthogonal polynomials of hypergeometric type $\{y_n(x)\}$ is not only a very important problem *per se* in the theory of special functions, but also because of their recent entropic characterization and applications in quantum chemistry, quantum physics and information theory. Indeed, they essentially describe the pth-order Rényi and Tsallis entropies of the numerous quantum systems whose wavefunctions are controlled by these polynomials. Moreover, for different values of p, up to a constant factor, these norms characterize various fundamental and experimentally accessible quantities of many-electron systems. As well, the L_p norms have been used to develop and interpret all energy components in the density-functional theory of the ground-state of atoms and molecules. The asymptotics of these quantities when $n \to \infty$ and $p > 0$ have been recently calculated for Hermite polynomials, although not yet for Laguerre and Jacobi

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polynomials. Here, we determine the asymptotics ($p \to \infty$, n fixed) of the weighted L_p norms for general orthogonal polynomials in terms of the weight function and the coefficients of the second-order hypergeometric differential equation that they satisfy, and we apply it to the three classical families of real orthogonal polynomials. Moreover we analyse and discuss the monotonicity of this asymptotics, and we carry out a detailed numerical study of it.

Keywords Orthogonal polynomials · Quantum chemistry · Quantum physics · Information theory · Hermite polynomials · Laguerre polynomials · Jacobi polynomials · L_p-norms asymptotics

1 Introduction

Let $\{y_n(x)\}$ denote a sequence of real polynomials orthogonal with respect to the weight function $\omega(x)$ on the interval Δ. The probability density of the polynomial $y_n(x)$, to be called Rakhmanov‘s density heretoforth because he found [1] that it governs the asymptotic ($n \to \infty$) behaviour of the ratio y_{n+1}/y_n for general $\omega > 0$ almost everywhere on the finite interval Δ, is given by

$$\rho_n(x) = \frac{1}{d_n^2}\omega(x)y_n^2(x),$$

where d_n^2 is the normalization constant. Physically, $\rho_n(x)$ describes the probability density of the ground and excited states of the physical systems whose non-relativistic quantum-mechanical wavefunctions are controlled by the polynomials $y_n(x)$ (see e.g., [2,3]).

This density distribution can be characterized under certain conditions either by means of the ordinary moments $\mu_k := \int_\Delta x^k \rho_n(x)dx$ [4,5] with integer order k, or via the frequency moments (also called probability moments or entropic moments) of integer order k, $\nu_k := \int_\Delta [\rho_n(x)]^k\, dx$ [5–8]. The latter quantities are the integer-order instances of the weighted L_p norms of the orthonormal polynomials $y_n(x)$, which are set by

$$\|\rho_n\|_p \equiv \left(\int\limits_\Delta [\rho_n(x)]^p\, dx \right)^{\frac{1}{p}} = \frac{1}{d_n^2}\left(\int\limits_\Delta \left[\omega(x)y_n^2(x)\right]^p dx \right)^{\frac{1}{p}}; \;\; p > 0. \qquad (1)$$

They are closely related to not only the pth-order frequency moments $W_p[\rho_n] = \|\rho_n\|_p^p$, but also to various information-theoretic measures such as the Rényi entropies [9] $R_p[\rho_n]$, the Tsallis entropies [10], $T_p[\rho_n]$ and the Rényi spreading lengths [11] $L_p^R[\rho_n]$, which are defined as P

$$R_p[\rho_n] = \frac{1}{1-p}\ln W_p[\rho_n]; \;\; p > 0, p \neq 1,$$

$$T_p[\rho_n] = \frac{1}{p-1}\left(1 - W_p[\rho_n]\right); \; p > 0, p \neq 1,$$

$$L_p^R[\rho_n] = \exp\left(R_p[\rho_n]\right) = \|\rho_n\|_p^{-\frac{p}{p-1}}.$$

respectively. These quantities, which include the Shannon information entropy $S[\rho_n] = -\int_\Delta \rho_n \ln \rho_n dx$ in the limiting case $q \to 1$, grasp different aspects of the distribution of the probability density $\rho_n(x)$ along the interval Δ when the order p is varying (see the recent review [12]).

From a chemical point of view these quantities do not only allow us to grasp various aspects of the internal disorder of many-electron systems (which are closely connected with the rich three-dimensional geometry of their electron distributions), but also they describe up to some constant factors numerous fundamental and experimentally accessible chemical quantities (average electron density, electron-nucleus attraction energy, kinetic and exchange energies, among many others; see e.g., [12–14]) and tightly bound other macroscopic properties of these systems [15–17]. Moreover, it most important that the L_p norms have been used to develop and interpret all energy components in the density-functional theory of the ground-state of atoms and molecules [18–20]. In addition, they have been used as uncertainty measures in chemical and physical quantum systems [21]. For further details, see the recent survey [12].

The analytical determination of these norms has been a long standing problem not only in quantum chemistry but also in the theory of special functions and extremal polynomials itself since the times of Bernstein and Steklov (see e.g., [22–24]) and in the theory of trigonometric series [8]. Recently, they have been calculated for polynomials $y_n(x)$ with arbitrary degree n by means of the combinatorics-based Bell polynomials in the Hermite [25], Laguerre [26] and Jacobi [27] cases; see also [28]. However, this methodology is computationally very demanding and analytically inefficient for high and very high values of n. Recently, extending some previous works of Aptekarev et al. [29] when $p \in \left[0, \frac{4}{3}\right]$, the strong asymptotics ($n \to \infty$ and $p > 0$) of the weighted L_p norms has been fully determined for Hermite polynomials $H_n(x)$ [30] orthogonal with respect to the weight function $\omega_H = e^{-x^2}$. This result has been achieved by means of the Tulyakov method [31] whose initial starting point is the recurrence relation of the polynomials; so, opposite to the matrix Riemann–Hilbert method [28] which begins with the orthogonality weight. We should immediately underline that both weak* [32] and strong [29] asymptotics of Laguerre and Jacobi polynomials are still lacking in spite of some serious efforts [23,33,34].

For completeness, it is worth mentioning here that the pth-power of the (non-weighted) L_p norms defined as $N_n(p;\omega) := \int_\Delta [y_n(x)]^p \, \omega(x)\, dx$ has also been considered and its asymptotics has been determined for $n \to \infty$ in some special cases [29,33,35]. Indeed, the leading term of the asymptotic behavior of the norms $N_n(p;\omega)$ for the polynomials orthogonal with respect to a weight function satisfying either the Bernstein condition or the weaker Szego condition has been calculated, obtaining more refined results for Jacobi polynomials [29,33]. As well, the asymptotic behavior of the Hermite norms $N_n(p;\omega_H^{1/2})$ when $n \to \infty$ has been found and applied by Larsson-Cohn [35] to some extremal problems on Wiener chaos [35]. In the discrete case, the only results found in the literature are the ones of Meixner [36] and Charlier [37] polynomials, which were recently used to determine the asymptotics of generalised derangements.

The aim of this work is the calculation of the complementary asymptotics (i.e., for $p \to \infty$ and n fixed) of the weighted L_p norms of general hypergeometric orthogonal polynomials (i.e., with respect to a general weight function on the real line) and their applications to the systems of orthogonal polynomials of Hermite, Laguerre and Jacobi types. We use the Laplace's asymptotic method, which is much more efficient for this problem than the ones based on linearisation [38–48], combinatorial [49] and integro-differential [50] techniques.

The structure of the paper is the following. In Sect. 2 we determine the asymptotics of the pth-power of the weigthed L_p norms of general orthogonal polynomials for large values of p by means of the Laplace's method [51] together with the second-order hypergeometric differential equation of the polynomials [52]. Then, in Sect. 3, we apply the previous result to Hermite, Laguerre and Jacobi polynomials. In Sect. 4 we analyse the monotonicity behaviour of the asymptotics of the L_p norms of these hypergeometric polynomials. Later, in Sect. 5, we make a numerical study of the weighted L_p norms in some special cases. Finally some conclusions and references are given.

2 Weighted L_p-norms of general orthogonal polynomials: asymptotics ($p \to \infty$)

In this section we determine the asymptotics ($p \to \infty$) of weighted L_p norms of the system of polynomials $\{y_n(x)\}$ orthogonal with respect to the weight function $\omega(x)$ on the interval (a, b) of the real line, not necessarily finite. According to Eq. (1) we have that the pth-power of the weighted L_p norm of the polynomials $y_n(x)$ is given by

$$\int_a^b \left[\omega(x) y_n^2(x)\right]^p \, dx = \int_a^b e^{p\left[\ln \omega(x) + \ln y_n^2(x)\right]} \, dx. \tag{2}$$

To estimate the asymptotic behaviour of this quantity when $p \to \infty$, we use the Laplace's method [51], designed to derive an asymptotic expansion of the functional integral

$$F[f] = \int_a^b e^{pf(x)} \, dx, \quad p > 0, \quad f(x) \text{ real.}$$

Let us suppose that this integral converges absolutely for large enough p. For large p, the dominant contribution of the integrand to the integral occurs around the point $x_0 \in [a, b]$ where $f(x)$ reaches its maximum value, so that the contribution of the integrand to the integral is exponentially damped away from it.

Assume that $f \in \mathcal{C}^3(a, b)$ and has only one simple maximum at $x = x_0$ in (a, b). Then $f'(x_0) = 0$, $f''(x_0) < 0$ and

$$F[f] = e^{pf(x_0)}\left[\sqrt{\frac{2\pi}{-pf''(x_0)}} + \mathcal{O}(p^{-1})\right], \quad p \to \infty. \tag{3}$$

Moreover, if the function $f(x)$ has two or more maxima the dominat contribution to the functional $F[f]$ comes from the absolute maximum x_0 of $f(x)$, mainly because the contribution from a local maximum at x_1 is suppressed by the factor $\exp(f(x_1) - f(x_0))$. Then, the asymptotics of the weighted L_p norm of $y_n(x)$ is basically controlled by the absolute maximum of the function

$$f(x) = \ln\omega(x) + \ln y_n^2(x),$$

whose value $x_0 = x_0(n)$ is the solution of the equation

$$\frac{y_n'(x_0)}{y_n(x_0)} = -\frac{1}{2}\frac{\omega'(x_0)}{\omega(x_0)}. \tag{4}$$

So, from Eqs. (2)–(4) one has that

$$\int_a^b \left[\omega(x)y_n^2(x)\right]^p dx = \left[\omega(x_0)y_n^2(x_0)\right]^p \left[\sqrt{\frac{2\pi}{-pf''(x_0)}} + \mathcal{O}(p^{-1})\right], \; p \to \infty, \tag{5}$$

where

$$f''(x_0) = \frac{\omega''(x_0)}{\omega(x_0)} - \frac{3}{2}\left[\frac{\omega'(x_0)}{\omega(x_0)}\right]^2 + \frac{2y_n''(x_0)}{y_n(x_0)}.$$

Furthermore, since the polynomial $y_n(x)$ satisfies [52] the hypergeometric differential equation

$$\sigma(x)y_n''(x) + \tau(x)y_n'(x) + \lambda_n y_n(x) = 0 \tag{6}$$

(where σ and τ are polynomials of degree 2 and 1, at most, respectively, and λ_n is a scalar), one has that

$$f''(x_0) = \frac{\omega''(x_0)}{\omega(x_0)} - \frac{3}{2}\left[\frac{\omega'(x_0)}{\omega(x_0)}\right]^2 - \frac{2\lambda_n}{\sigma(x_0)} + \frac{\tau(x_0)}{\sigma(x_0)}\frac{\omega'(x_0)}{\omega(x_0)}, \tag{7}$$

where use of the Laplace's condition (4) has been used.

3 Applications

In this section, we apply the general results (5) and (7) obtained in the previous section to determine the pth-power of the L_p norms of the three canonical systems of real orthogonal hypergeometric polynomials [52]; that is, the Hermite, Laguerre

Table 1 Data on classical orthogonal polynomials

	Hermite $H_n(x)$	Laguerre $L_n^{(\alpha)}(x)$ $(\alpha > -1)$	Jacobi $P_n^{(\alpha,\beta)}(x)$ $(\alpha > -1, \beta > -1)$
(a, b)	$(-\infty, +\infty)$	$(0, +\infty)$	$(-1, +1)$
$\omega(x)$	e^{-x^2}	$x^\alpha e^{-x}$	$(1-x)^\alpha(1+x)^\beta$
$\sigma(x)$	1	x	$1-x^2$
$\tau(x)$	$-2x$	$1+\alpha-x$	$-(\alpha+\beta+2)x+\beta-\alpha$
λ_n	$2n$	n	$n(n+\alpha+\beta+1)$
d_n^2	$2^n n!\sqrt{\pi}$	$\frac{\Gamma(n+\alpha+1)}{n!}$	$\frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)}$

and Jacobi polynomials. These polynomials are known to satisfy the orthogonality condition

$$\int_a^b y_n(x)y_m(x)\omega(x)\,dx = d_n^2\delta_{mn},$$

and the second-order differential equation (6), whose coefficients $\sigma(x)$, $\tau(x)$, λ_n, weight function $\omega(x)$, orthogonality interval (a, b), and normalization constant d_n^2 are given in Table 1.

3.1 Hermite polynomials $H_n(x)$

These polynomials are orthogonal with respect to the weight function $\omega_H(x) = e^{-x^2}$ on the whole real line and satisfy the differential equation (6) with the coefficients (see Table 1).

$$\sigma(x) = 1, \quad \tau(x) = -2x, \quad \lambda_n = 2n.$$

According to (4), the absolute maximum $x_0 = x_0(n)$ is given by one solution of the equation

$$x_0 H_n(x_0) = 2n H_{n-1}(x_0).$$

Moreover, following Eq. (7) one has that the second derivative of $f_H(x) = \ln\omega_H(x) + \ln(H_n(x))^2$ evaluated at the absolute maximum x_0 has the value

$$f_H''(x_0) = 2x_0^2 - 4n - 2.$$

Then, according to Eq. (5) we obtain that

$$\int_{-\infty}^{+\infty} \left[\omega_H(x) H_n^2(x)\right]^p dx = 2\int_{0}^{+\infty} \left[\omega_H(x) H_n^2(x)\right]^p dx$$
$$= 2\left[\omega_H(x_0) H_n^2(x_0)\right]^p \left[\sqrt{\frac{2\pi}{p(4n-2x_0^2+2)}} + \mathcal{O}(p^{-1})\right]. \tag{8}$$

For the particular cases $n = 0, 1$ and 2 we have that $x_0 = 0, 1$ and $\sqrt{\frac{5}{2}}$, respectively, so that the L_p norm of the corresponding polynomials has the asymptotical values

$$\sqrt{\frac{\pi}{p}},\ 2^{2p+1}e^{-p}\left[\sqrt{\frac{\pi}{2p}}+\mathcal{O}(p^{-1})\right] \quad \text{and} \quad 2^{6p+1}e^{-\frac{5}{2}p}\left[\sqrt{\frac{2\pi}{5p}} + \mathcal{O}(p^{-1})\right]. \tag{9}$$

Remark that the first of these three asymptotical values is the exact value of the functional. To calculate it we take into account that $x_0 = 0$, so that one has to apply the Laplace's method to the whole integration interval $(-\infty, +\infty)$ in (8).

3.2 Laguerre polynomials $L_n^{(\alpha)}(x)$

These polynomials are orthogonal with respect to the weight function $\omega_L(x) = x^\alpha e^{-x}$ on the interval $[0, +\infty)$ and satisfy the differential equation (6) with the coefficients

$$\sigma(x) = x, \quad \tau(x) = 1 + \alpha - x, \quad \lambda_n = n$$

Here, the absolute maximum $x_0 = x_0(n)$ is according to Eq. (4) one solution of the equation

$$\left(\frac{\alpha}{x_0} - 1\right) L_n^{(\alpha)}(x_0) = 2L_{n-1}^{(\alpha+1)}(x_0). \tag{10}$$

Moreover, according to Eq. (7), one has that the second derivative of the function $f_L(x) = \ln \omega_L(x) + \ln \left(L_n^{(\alpha)}(x)\right)^2$ evaluated at x_0 has the value

$$f_L''(x_0) = \frac{\alpha^2}{2x_0^2} - \frac{2n+\alpha+1}{x_0} + \frac{1}{2}.$$

Then, following Eq. (5) we obtain that the pth-power of the weighted L_p norm of Laguerre polynomials $L_n^{(\alpha)}(x)$ has the following asymptotic behavior

$$\int_0^{+\infty} \left[\omega_L(x)\left[L_n^{(\alpha)}(x)\right]^2\right]^p dx = \left[\omega_L(x_0)\left[L_n^{(\alpha)}(x_0)\right]^2\right]^p \times \left[\sqrt{\frac{2\pi}{p\left(-\frac{\alpha^2}{2x_0^2}+\frac{2n+\alpha+1}{x_0}-\frac{1}{2}\right)}} + \mathcal{O}(p^{-1})\right], \tag{11}$$

for $p \to +\infty$ and $\alpha > 0$. For the Laguerre polynomials with $\alpha > 0$ and degrees $n = 0$ and 1, one finds from Eq. (10) the absolute maximum values $x_0 = \alpha$ and $\frac{1}{2}\left(2\alpha + 3 - \sqrt{8\alpha+9}\right)$, respectively. Taking these particular cases into Eq. (11), we obtain that the leading term of the asymptotics ($p \to \infty$) of the weighted L_p norms of the corresponding polynomials $L_0^{(\alpha)}(x) = 1$ and $L_1^{(\alpha)}(x) = \alpha + 1 - x$ is given by

$$\int_0^{+\infty} \left[\omega_L(x)\left[L_0^{(\alpha)}(x)\right]^2\right]^p dx = \alpha^{p\alpha} e^{-p\alpha}\left[\sqrt{\frac{2\pi\alpha}{p}} + \mathcal{O}(p^{-1})\right]$$

and

$$\int_0^{+\infty} \left[\omega_L(x)\left[L_1^{(\alpha)}(x)\right]^2\right]^p dx = \left[x_0^{\alpha} e^{-x_0}(1+\alpha-x_0)^2\right]^p \left[\sqrt{\frac{2\pi}{-pf_L''(x_0)}} + \mathcal{O}(p^{-1})\right],$$

respectively, with

$$f_L''(x_0) = \frac{3\sqrt{8\alpha+9} - 8\alpha - 9}{\left(\sqrt{8\alpha+9} - 2\alpha - 3\right)^2}.$$

Moreover, in the subcase $\alpha = 1$ one finds that $x_0 = \frac{1}{2}\left(5 - \sqrt{17}\right)$ and $f''(x_0) = -\frac{1}{16}\left(51 + 11\sqrt{17}\right)$, so that we obtain the following asymptotics

$$\int_0^{+\infty} \left[\omega_L(x)\left[L_1^{(1)}(x)\right]^2\right]^p dx = \left[\frac{1}{2}\left(31 - 7\sqrt{17}\right) e^{-\frac{1}{2}\left(5-\sqrt{17}\right)}\right]^p \times \left[\sqrt{\frac{32\pi}{p\left(51 + 11\sqrt{17}\right)}} + \mathcal{O}(p^{-1})\right].$$

3.3 Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$

These polynomials are orthogonal with respect to the weight function $\omega_J(x) = (1-x)^\alpha(1+x)^\beta$ on the interval $[-1, +1]$, and satisfy the differential equation (6) with the coefficients

$$\sigma(x) = 1 - x^2, \quad \tau(x) = \beta - \alpha - (\alpha+\beta+2)x, \quad \lambda_n = n(n+\alpha+\beta+1)$$

In this case the absolute maximum x_0 turns out to be, according to Eq. (4), one solution of the equation

$$\frac{P_{n-1}^{(\alpha+1,\beta+1)}(x_0)}{P_n^{(\alpha,\beta)}(x_0)} = -\frac{1}{\alpha+\beta+n+1}\left(\frac{-\alpha}{1-x_0} + \frac{\beta}{1+x_0}\right). \tag{12}$$

Moreover, the use of Eq. (7) allows us to find the following value for the second derivative of the function $f_J(x) = \ln \omega_J(x) + \ln\left(P_n^{(\alpha,\beta)}\right)^2$ evaluated at x_0:

$$\begin{aligned} f_J''(x_0) = &-\left(\alpha + \frac{\alpha^2}{2}\right)\frac{1}{(1-x_0)^2} - \left(\beta + \frac{\beta^2}{2}\right)\frac{1}{(1+x_0)^2} \\ &-\frac{\alpha\beta}{1-x_0^2} - \frac{2n(n+\alpha+\beta+1)}{1-x_0^2} \\ &+\frac{\beta-\alpha-(\alpha+\beta+2)x_0}{1-x_0^2}\left[\frac{\beta}{1+x_0} - \frac{\alpha}{1-x_0}\right]. \end{aligned} \tag{13}$$

Now, from Eq. (5) we find that the pth-power of the weighted L_p norm of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ has the following asymptotic behavior:

$$\begin{aligned} &\int_{-1}^{+1}\left[\omega_J(x)\left[P_n^{(\alpha,\beta)}(x)\right]^2\right]^p dx \\ &\quad = \left[\omega_J(x_0)\left[P_n^{(\alpha,\beta)}(x_0)\right]^2\right]^p\left[\sqrt{\frac{2\pi}{-pf_J''(x_0)}} + \mathcal{O}(p^{-1})\right] \end{aligned} \tag{14}$$

for $p \to \infty$ and $\alpha, \beta > 0$. In the particular case where $n = 0$, $\alpha > 0$ and $\beta > 0$ we can find from Eq. (12) and (13) that

$$x_0 = \frac{\beta-\alpha}{\alpha+\beta} \quad \text{and} \quad f_J''(x_0) = -\frac{(\alpha+\beta)^3}{4\alpha\beta},$$

respectively. Thus, from Eq. (14) with these values of x_0 and $f_J''(x_0)$ we obtain the value

$$\int_{-1}^{+1} \left[\omega_J(x) \left(P_0^{(\alpha,\beta)}(x) \right)^2 \right]^p dx$$
$$= 2^{p(\alpha+\beta)} \left(\frac{\alpha}{\alpha+\beta} \right)^{\alpha p} \left(\frac{\beta}{\alpha+\beta} \right)^{\beta p} \left[\sqrt{\frac{8\pi\alpha\beta}{p(\alpha+\beta)^3}} + \mathcal{O}(p^{-1}) \right]$$

for the leading term of the asymptotics ($p \to \infty$) of $P_0^{(\alpha,\beta)}(x) = 1$. Finally, let us consider another particular case: when $n = 1$ and $\alpha = \beta > 0$. Then, $P_1^{(\alpha,\alpha)}(x) = (1+\alpha)x$ and the associated Rakhmanov density

$$\rho_n^J(x) = \omega_J(x) \left[P_1^{(\alpha,\alpha)} \right]^2 = (1+\alpha)^2 (1-x^2)^\alpha x^2$$

is symmetric with respect to the origin. Then, the corresponding pth-power of the weighted L_p norm can be expressed as

$$\int_{-1}^{+1} \left\{ \omega_J(x) \left[P_1^{(\alpha,\alpha)}(x) \right]^2 \right\}^p dx = 2 \int_{0}^{+1} \left\{ \omega_J(x) \left[P_1^{(\alpha,\alpha)}(x) \right]^2 \right\}^p dx.$$

The application of the Laplace's method to this functional on the interval $(0, +1)$ together with the values

$$x_0 = \sqrt{\frac{1}{1+\alpha}} \quad \text{and} \quad f_J''(x_0) = -\frac{4(1+\alpha)^2}{\alpha}$$

for the absolute maximum and the second derivative of the corresponding function $f_J(x)$ allows us to find from Eq. (5) the expression

$$\int_{-1}^{+1} \left\{ \omega_J(x) \left[P_1^{(\alpha,\alpha)}(x) \right]^2 \right\}^p dx = 2(1+\alpha)^p \left[\frac{\alpha}{1+\alpha} \right]^{\alpha p} \left[\sqrt{\frac{\pi\alpha}{2(1+\alpha)^2 p}} + \mathcal{O}(p^{-1}) \right]$$

for the leading term of the asymptotics ($p \to \infty$) of the weighted L_p norm of the Jacobi polynomial $P_1^{(\alpha,\alpha)}(x)$.

4 Monotonicity of the asymptotic behaviour

In this section we analyse the monotonicity of the asymptotics ($p \to +\infty$) for the Hermite polynomials $H_n(x)$. Then, we describe the difficulties to obtain the same property in the Laguerre and Jacobi cases.

We start from the general expression (5), whose asymptotic behaviour is given by

$$G(p) = \left[\omega(x_0) y_n^2(x_0)\right]^p \sqrt{\frac{2\pi}{-p f''(x_0)}}.$$

This function $G(p)$ is the product of the function $\left[\omega(x_0) y_n^2(x_0)\right]^p$ (which has, as a function of p, an exponential behavior in practice) and the power $p^{-\frac{1}{2}}$. For large values of p, the exponential function gives the increasing or decreasing behaviour of the asymptotics: $G(p)$ increases with p if $\omega(x_0) y_n^2(x_0) > 1$ and $G(p)$ decreases when p increases if $\omega(x_0) y_n^2(x_0) \leq 1$. Thus, notice that the monotonicity of the asymptotic behaviour for large values of p is controlled by the value of the function in the absolute maximum x_0.

Let us first consider the case of the orthogonal ($H_n(x)$) and orthonormal ($\tilde{H}_n(x)$) Hermite polynomials. Notice that $\tilde{H}_n(x) = H_n(x)/\sqrt{d_n^2}$. The orthonormal Hermite polynomials satisfy Eq. 18.14.9 of [53], namely

$$\omega_H(x) \tilde{H}_n^2(x) \leq \frac{1}{\sqrt{\pi}} < 1.$$

Thus, in particular we have that $\omega_H(x_0) \tilde{H}_n^2(x_0) < 1$, so the pth-power of the L_p norm of these polynomials decreases as p increases for large values of p.

On the other hand, the orthogonal Hermite polynomials, with the standard normalization constant d_n^2 given in Table 1, satisfy that [54]

$$\omega_H(x_0) H^2(x_0) > K_n,$$

for $n \geq 6$ with

$$K_n = \begin{cases} \dfrac{27}{61(2n)^{\frac{1}{6}}} \dfrac{2n\sqrt{4n-2}(n!)^2}{\sqrt{8n^2-8n+3}\left(\frac{n}{2}!\right)^2} & \text{if } n \text{ is even,} \\ \dfrac{27}{61(2n)^{\frac{1}{6}}} \dfrac{\sqrt{16n^2-16n+6}n!(n-1)!}{\sqrt{2n-1}\left(\frac{(n-1)}{2}!\right)^2} & \text{if } n \text{ is odd.} \end{cases}$$

Note that K_n reaches its minimum at $n = 6$, with value $K_6 \simeq 15209 > 1$. Then

$$\omega_H(x_0) H_n^2(x_0) > 1, \quad n \geq 6.$$

In fact this condition is also true for $1 \leq n \leq 5$. So finally we have that the pth-power of the L_p norm of these polynomials increases with p for large values of p. Moreover, for $n = 0$, $\omega_H(x_0) H_0^2(x_0) = 1$; so we have a decreasing behaviour in this case, as given by Eq. (9).

Let us now consider the Laguerre case. Then, the standard orthogonal $L_n^{(\alpha)}(x)$ and the orthornormal polynomials are related by $\tilde{L}_n^{(\alpha)}(x) = L_n^{(\alpha)}(x)/\sqrt{d_n^2}$. Regarding upper and lower bounds, we have not found in the literature results for these polynomials so simple and powerful as those for Hermite polynomials. However, notice that

$d_n^2 > 1$ for Laguerre polynomials with $\alpha > 0$. This implies that

$$\omega_L(x_0)\left(L_n^{(\alpha)}(x_0)\right)^2 > \omega_L(x_0)\frac{\left(L_n^{(\alpha)}(x_0)\right)^2}{d_n^2} = \omega_L(x_0)\left(\tilde{L}_n^{(\alpha)}(x_0)\right)^2. \quad (15)$$

Thus, if $\omega_L(x_0)\left(L_n^{(\alpha)}(x_0)\right)^2 < 1 \Rightarrow \omega_L(x_0)\left(\tilde{L}_n^{(\alpha)}(x_0)\right)^2 < 1$. Then, if the pth-power of the L_p norm of the standard orthogonal polynomials decreases as p increases for large values of p, the pth-power of the L_p norm of the orthonormal polynomials has the same behaviour.

For Jacobi polynomials, we do not have results like those for Hermite polynomials, neither their normalization constant is always greater or lower than one. Then, the monotonicity of the asymptotic behaviour remains open for each specific case.

5 Numerical study

In this section we study numerically the behaviour of the asymptotics given in Sect. 3 for the Hermite, Laguerre and Jacobi families of orthogonal polynomials. This is done in each case for the standard orthogonal and orthonormal polynomials. In all the following figures, we represent the numerically calculated exact value of the corresponding pth-power of the L_p norms $\|\rho\|_p^p$ of these polynomials (squared dot), its corresponding asymptotic behaviour γ_p (solid line), as well as the absolute difference (circled dot)

$$\theta_a = |\|\rho\|_p^p - \gamma_p|,$$

and the relative difference (times)

$$\theta_r = \frac{|\|\rho\|_p^p - \gamma_p|}{\|\rho\|_p^p},$$

as a function of p.

Figure 1 shows these values for the orthogonal Hermite polynomial with $n = 1$, $H_1(x)$. Herein we observe the increasing behaviour of the pth-power of the L_p norms and the asymptotic behaviour, as predicted in Sect. 4. The absolute difference increases with p indicating that the asymptotic behaviour can be improved with some increasing terms, while the relative difference goes to zero as expected for a good asymptotic behaviour.

In Fig. 2 we take into account the orthonormal Hermite polynomial $\tilde{H}_1(x)$, whose pth-power of the L_p norm is now decreasing, as expected from the results of Sect. 4. The absolute and relative differences naturally decrease as well.

These behaviours are completely analogous for Hermite polynomials with other values of the degree n.

Now, let us consider the orthogonal Laguerre polynomial with degree $n = 1$ and parameter $\alpha = 1$, $L_1^{(1)}(x)$. Figure 3 shows that the pth-power of the L_p norms

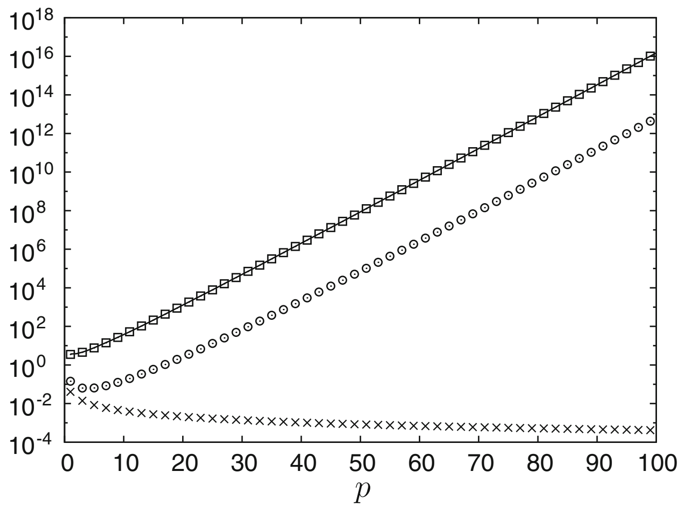


Fig. 1 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the Hermite polynomial $H_1(x)$, as a function of p

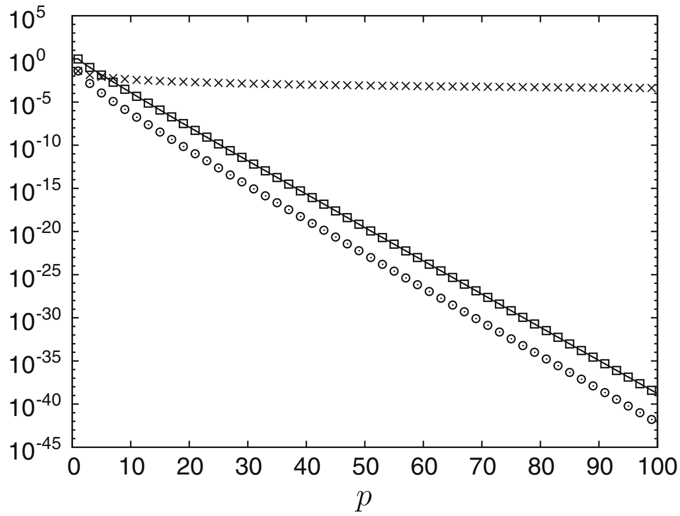


Fig. 2 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the orthonormal Hermite polynomial $\tilde{H}_1(x)$, as a function of p

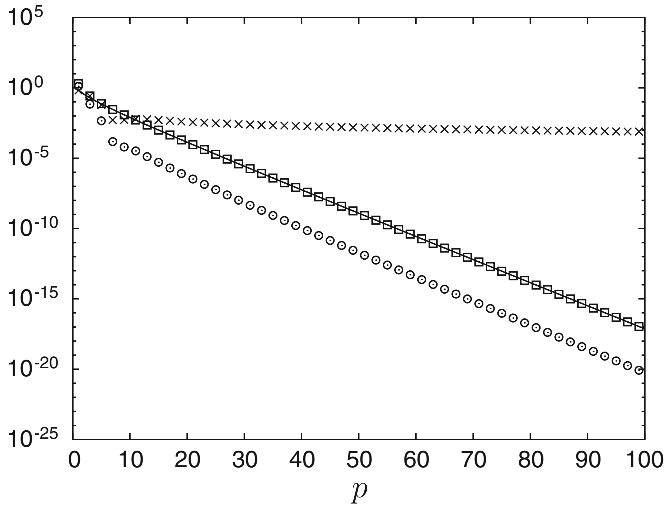


Fig. 3 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the Laguerre polynomial $L_1^{(1)}(x)$, as a function of p

decreases as a function of p. Then, taking into account the result (15) from Sect. 4, we can conclude that the pth-power of the L_p norms of the orthonormal polynomials $\tilde{L}_1^{(1)}(x)$ also decreases as p is increasing. The absolute and relative differences θ_a and θ_r, also decrease as p is increasing.

Fig. 4 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the Laguerre polynomial $L_1^{(2)}(x)$, as a function of p

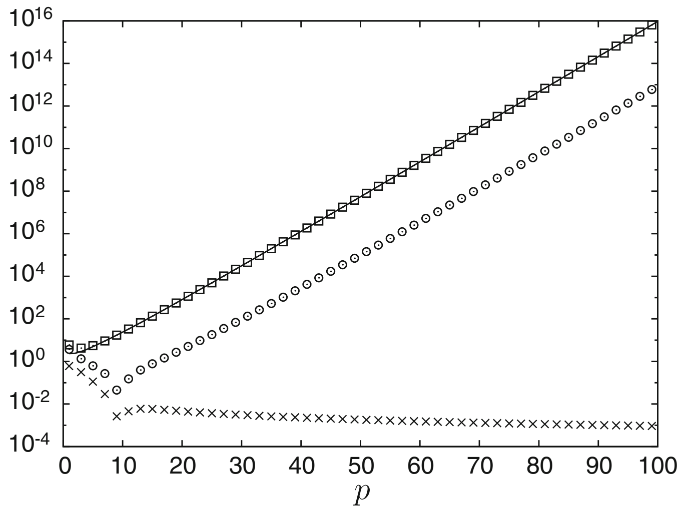
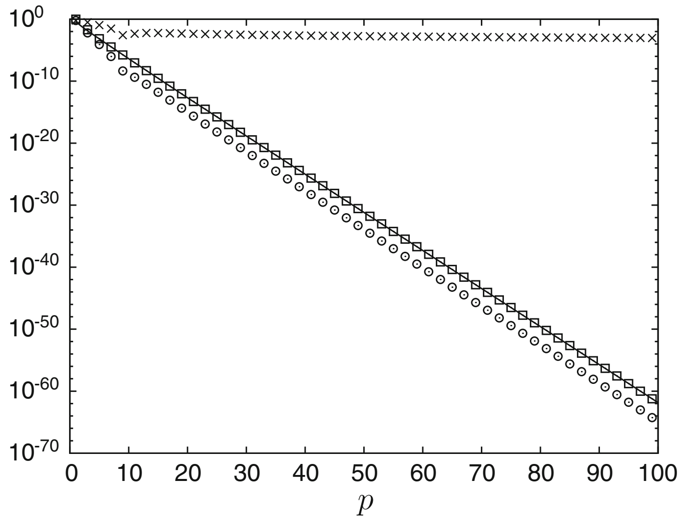


Fig. 5 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the orthonormal Laguerre polynomial $\tilde{L}_1^{(2)}(x)$, as a function of p



In Figs. 4 and 5 we consider the orthogonal $L_1^{(2)}(x)$ and orthonormal $\tilde{L}_1^{(2)}(x)$ Laguerre polynomials, respectively. Now, the pth-power of the L_p norm increases with p in the orthogonal case, but it decreases in the orthonormal case. A brief study of the corresponding functions $x^2e^{-x}\left(L_1^{(2)}(x)\right)^2$ and $x^2e^{-x}\left(\tilde{L}_1^{(2)}(x)\right)^2$ shows that their maximum values are greater and lower than 1, respectively. As in the previous Hermite case, the absolute difference θ_a increases with p for the orthogonal polynomial, indicating that the asymptotic behaviour can be improved with increasing terms.

The Jacobi polynomials, with bounded support, can have maximum values greater or lower than zero, depending on the values of the degree n and the parameters α and β, regardless if we are considering the orthogonal or the orthonormal version of the polynomials. Thus, Figs. 6 and 7 show the behaviour of the pth-power of the L_p norm for the polynomials $P_1^{(\frac{3}{2},\frac{3}{2})}(x)$ and $\tilde{P}_1^{(\frac{3}{2},\frac{3}{2})}(x)$, respectively.We notice that it

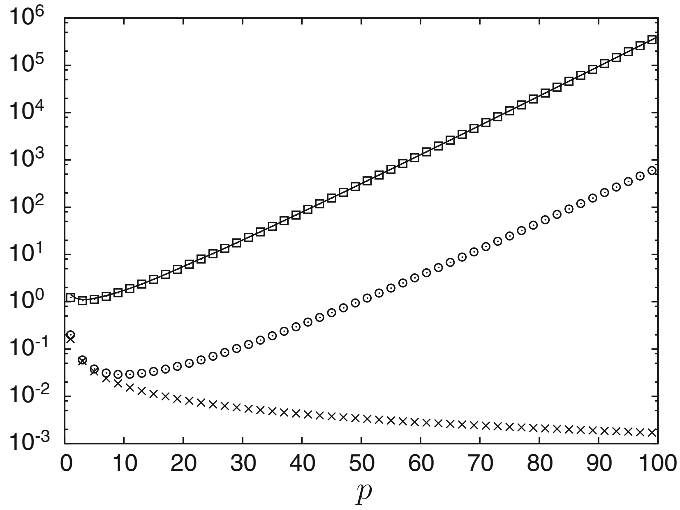


Fig. 6 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the Jacobi polynomial $P_1^{(\frac{3}{2},\frac{3}{2})}(x)$, as a function of p

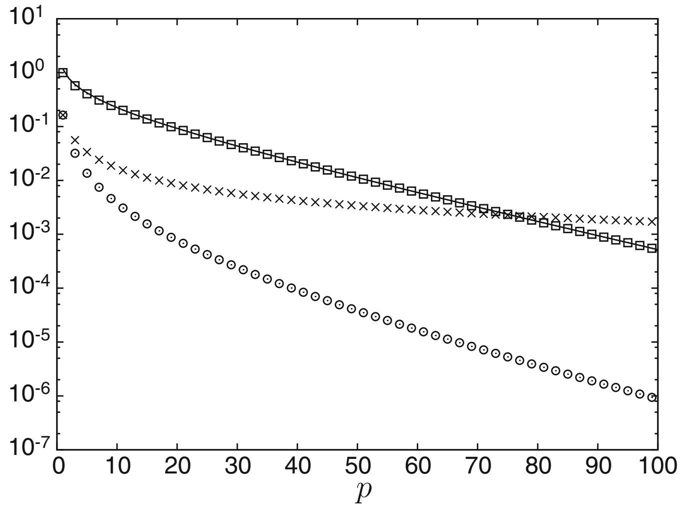


Fig. 7 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the orthonornal Jacobi polynomial $\tilde{P}_1^{(\frac{3}{2},\frac{3}{2})}(x)$, as a function of p

is increasing with p in the orthogonal case, but decreasing in the orthonormal case. According to the reasoning in Sect. 4, this behavior is because

$$\max_{x\in[-1,1]}\left\{(1-x)^{\frac{3}{2}}(1+x)^{\frac{3}{2}}\left(\tilde{P}_1^{(\frac{3}{2},\frac{3}{2})}(x)\right)^2\right\} < 1 < \max_{x\in[-1,1]}\left\{(1-x)^{\frac{3}{2}}(1+x)^{\frac{3}{2}}\left(P_1^{(\frac{3}{2},\frac{3}{2})}(x)\right)^2\right\}.$$

Figures 8 and 9 show the same quantities for polynomials $P_3^{(\frac{1}{2},\frac{1}{2})}(x)$ and $\tilde{P}_3^{(\frac{1}{2},\frac{1}{2})}(x)$, respectively. Now the behaviours are in the opposite direction compared with those of the previous examples in Figs. 6 and 7. The pth-power of the L_p norm is decreasing for the orthogonal polynomial but increasing for the orthonormal one. The reason, again, is that

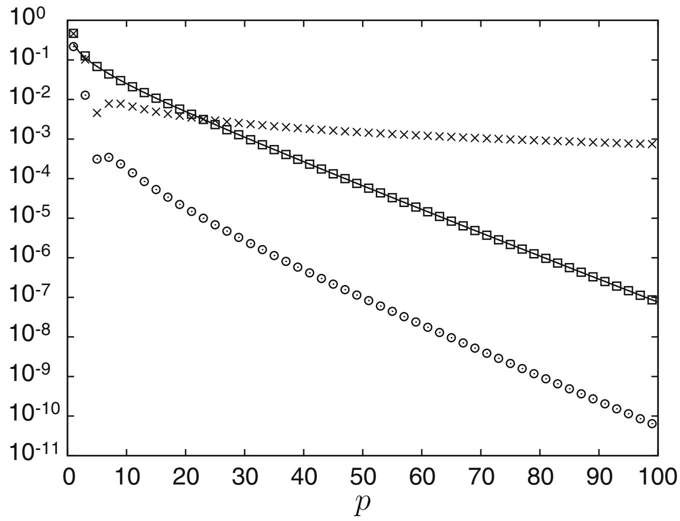


Fig. 8 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the Jacobi polynomial $P_3^{(\frac{1}{2},\frac{1}{2})}(x)$, as a function of p

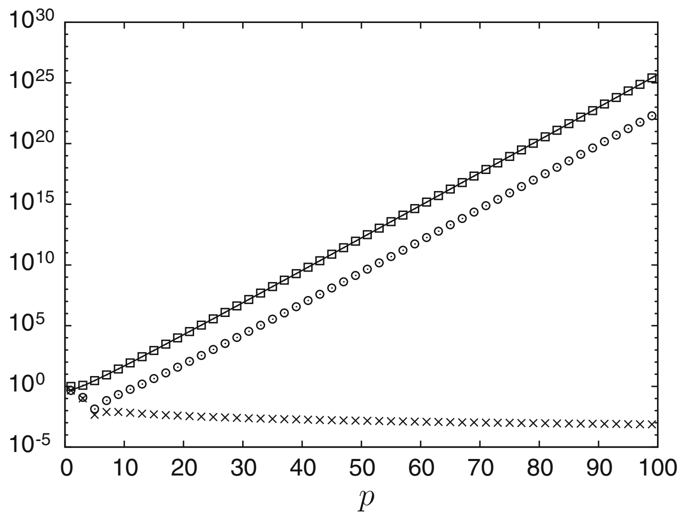


Fig. 9 Exact value of the pth-power of the L_p norms $\|\rho\|_p^p$ (*squared dot*), its corresponding asymptotic behaviour γ_p (*solid line*), absolute difference θ_a (*circled dot*), relative difference θ_r (*times*) for the orthonornal Jacobi polynomial $\tilde{P}_3^{(\frac{1}{2},\frac{1}{2})}(x)$, as a function of p

$$\max_{x\in[-1,1]}\left\{(1-x)^{\frac{1}{2}}(1+x)^{\frac{1}{2}}\left(P_3^{(\frac{1}{2},\frac{1}{2})}(x)\right)^2\right\} < 1 <$$
$$\max_{x\in[-1,1]}\left\{(1-x)^{\frac{1}{2}}(1+x)^{\frac{1}{2}}\left(\tilde{P}_3^{(\frac{1}{2},\frac{1}{2})}(x)\right)^2\right\}.$$

Then, all the numerical examples considered here agree with the analytical monotonicity results of Sect. 4. Furthermore, the relative difference θ_r is always a decreasing function as p increases. Notice also in all the figures the exponential behavior predicted by the Laplace's method for the pth-power of the L_p norms and their asymptotics. Please keep in mind the logarithmic scale in the ordinate axis.

6 Conclusions and open problems

Energetic and entropic quantities of the ground and excited states of exactly and quasi-exactly solvable quantum systems can be often expressed in terms of some weighted L_p norms of the orthogonal polynomials which control the corresponding wavefunctions.

In this work we have determined the asymptotics of the weighted L_p norms of Hermite, Laguerre and Jacobi polynomials of nth degree when $p \to \infty$ by means of the Laplace's method. Moreover we have analyzed its monotonicity, identifying some new open problems. As well, a numerical study of the asymptotics for all classical continuous orthogonal polynomials has been performed.

The extension of these results to other continuous hypergeometric orthogonal polynomials of the Askey tableau [55] (even to those which are orthogonal with respect to a complex contour where the Laplace's method remains valid under certain conditions) and to the classical orthogonal polynomials in a discrete variable are open problems of a great interest in the theory of special functions not only from a fundamental point of view, but also because of their straightforward applications to various fields, from some weighted permutation problems to the quantum-mechanical description of physical systems.

Finally, let us point out that the only results found for the asymptotics of the L_p norms of discrete orthogonal polynomials up until now are the ones for the unweighted norms of Meixner [36] and Charlier [37] polynomials, which were shown to be very useful for some extremal problems in generalised derangements [36]. It is clear that for extensions to other discrete systems we will need the linearisation techniques for the corresponding polynomials [41,56–59].

Acknowledgments This work has been partially funded by the Junta-de-Andalucía Grants FQM-207, FQM-4643 and FQM-7276 as well as the MINECO Grant FIS2011-24540.

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4.3. Medidas de complejidad de los polinomios ortogonales

Esta sección contiene el artículo siguiente que trata el cálculo de medidas de complejidad de polinomios ortogonales:

Complexity analysis of hypergeometric orthogonal polynomials.
J. S. Dehesa, **A. Guerrero** y P. Sánchez-Moreno.
Journal of Computational and Applied Mathematics (2014). Aceptado.

En este artículo se extiende el concepto de complejidad, que tan importante papel juega en Ciencia y Tecnología, a la teoría de funciones especiales y, concretamente, a los polinomios ortogonales hipergeométricos $p_n(x)$. Para ello se hace uso de su densidad de Rakhmanov asociada $\rho_n(x) = \omega(x)p_n^2(x)$, donde $\omega(x)$, $x \in (a, b)$ es la función peso correspondiente, y se calculan las medidas de complejidad de tipo Cramér-Rao, Fisher-Shannon y LMC para las tres familias hipergeométricas canónicas. Entre los resultados obtenidos cabe mencionar la expresión explícita de la complejidad de Cramér-Rao de las tres familias polinómicas, y el término dominante de la asintótica de las complejidades de tipo Fisher-Shannon y LMC para dichas familias.

Por último se lleva a cabo un estudio numérico de estas tres medidas de complejidad, distinguiéndose dos casos. En primer lugar, se fijan los parámetros de los polinomios y se analiza la evolución de las complejidades con respecto al grado n, y en segundo lugar se fija el grado del polinomio y se estudia la evolución de dichas magnitudes con respecto a los parámetros que caracterizan la función peso con respecto a la cual son ortogonales los polinomios considerados.

Complexity analysis of hypergeometric orthogonal polynomials

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Abstract

The complexity measures of the Crámer-Rao, Fisher-Shannon and LMC (López-Ruiz, Mancini and Calvet) types of the Rakhmanov probability density $\rho_n(x) = \omega(x)p_n^2(x)$ of the polynomials $p_n(x)$ orthogonal with respect to the weight function $\omega(x)$, $x \in (a, b)$, are used to quantify various two-fold facets of the spreading of the Hermite, Laguerre and Jacobi systems all over their corresponding orthogonality intervals in both analytical and computational ways. Their explicit (Crámer-Rao) and asymptotical (Fisher-Shannon, LMC) values are given for the three systems of orthogonal polynomials. Then, these complexity-type mathematical quantities are numerically examined in terms of the polynomial's degree n and the parameters which characterize the weight function. Finally, several open problems about the generalised hypergeometric functions of Lauricella and Srivastava-Daoust types, as well as on the asymptotics of weighted L_q-norms of Laguerre and Jacobi polynomials are pointed out.

1. Introduction

The contents of this work are inspired to a great extent by the ideas of Leonhard Euler [1], who long ago ushered in a true revolution in mathematics by combining painstaking observations (which he collected in notebooks) with use of quantities extracted from Physics (e.g., electrostatic properties of the zeros, capacity, mutual energy, logarithmic potential, ...) in order to gain further insights into the structure of mathematical functions, having encountered novel paths, notions and approaches which led to many of the fundamental properties which presently we know about them. These Physics-based notions have contributed in a very important manner to the development of various mathematical fields, such as e.g. the theory of special functions, approximation theory and potential theory. With this spirit in mind, we use concepts and techniques extracted from Information Theory (such as entropy, entropic moments, complexity,...) to define, analyze and discuss new characteristics and structural properties of hypergeometric orthogonal polynomials.

The information-theoretical quantities of the Rakhmanov's probability density associated to these polynomials turn out to describe novel macroscopic facets of them, which possibly cannot be considered otherwise. Moreover, these quantities have not only a relevant mathematical character, but also they have an applied interest. Indeed, for example, they are closely related to physical entropies and measures of complexity of quantum systems which quantify their internal disorder and, consequently, they describe numerous fundamental and/or experimentally accesible quantities of these systems. This is essentially because the hypergeometric orthogonal polynomials often controls the mathematical description of the physical states of the quantum systems whose fundamental wave equations (Schrödinger, Dirac,...) are exactly- or quasi-exactly solvable.

A great challenge in contemporary science is to explore the mixing of simplicity and complexity, regularity and randomness, order and disorder, from particle physics and cosmology up to the adaptive complex systems and ultimately the living beings [2–4]. Many related efforts have been spent in these and other

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disciplines in the last few decades, but still today not so many results have been done in the theory of the mathematical functions which control the classical and quantum phenomena of the involved physical, chemical and biological systems. Not even for the so-called special functions of mathematical physics and applied mathematics and, particularly, the hypergeometric orthogonal polynomials [5, 6], which are very useful because of their numerous simple and elegant algebraic properties (e.g., recursion and ladder relations, Rodrigues formulas, integral representations, second-order differential equations). These "elementary" functions have plenty of applications not only in many mathematical areas but also in applied sciences; in particular, they are used to model and interpret numerous scientific properties and phenomena, as well as to describe the wave functions of classical and quantum-mechanical states of a great deal of physical systems, beginning with the prototypic hydrogenic and oscillator-like systems [5, 7].

The purpose of this paper is to quantify how simple or how complex are the special functions of Applied Mathematics beginning by the classical or hypergeometric-type orthogonal polynomials in a real continuous variable (i.e., Hermite, Laguerre and Jacobi). The issues *How do we understand by simplicity and complexity?* and *In what sense a certain mathematical function is simple and complex another one?* are not at all simple. There does not exist a unique notion of complexity to grasp our intuitive notions in the appropriate manner. Or perhaps various different quantities (possibly not yet known) are required to grasp our intuitive notions of complexity of a mathematical function (e.g., a hypergeometric orthogonal polynomial) in order to capture the great diversity and complexity of its configuration shapes corresponding to the different values of its degree and the parameters which characterize its weight function. Up until now there does not exist such notions, to the best of our knowledge.

We should immediately say that various distinct complexity notions have been published in different contexts (dynamical systems, cellular automata, neuronal networks, social sciences, complex molecules, geophysical and astrophysical processes,...) for several purposes, such as e.g. to study pattern, structure and correlations in systems and processes. In addition, at times, some complexity-type quantities are successfully used to analyze the computational resources (space, time,...) required to solve a problem in computer science and quantum information theory [8, 9], so at the interface of mathematics and computer science; more precisely, they concern the scaling of the resources in terms of the size of the problem. Nevertheless we will not use these complexity measures (heretoforth called by *extrinsic* complexity measures) in the present work because they do depend on the context, such as e.g. the algorithmic and computational complexities; they are closely related to the time required for a computer to solve a given problem; so that it depends on the chosen computer.

Here we will rather use density-dependent complexity measures, such as the Cramér-Rao, Fisher-Shannon and LMC (López-Ruiz-Mancini-Calvet) complexities, recently introduced in a quantum-physical context (see e.g. the reviews [10, 11] and [12–16]), which are of *intrinsic* character in the sense that they do not depend on the context but on the quantum probability density of the system under consideration. Our goal is to quantify how simple or how complex are the classical orthogonal polynomials $p_n(x)$ by means of the complexity measures of its associated Rakhmanov's probability density [17]. Remark that, contrary to other complexity notions (algorithmic, computational,...)[8, 9], the density-dependent complexities are intrinsic properties of the polynomials. Thus, the intrinsic complexity notions are closely related to the main macroscopic features of the associated probability density of the polynomials (irregularities, extent, fluctuations, smoothing,...).

The structure of the paper is the following. In Section 2 we define and describe the meaning of the complexity measures of the classical orthogonal polynomials which we use throughout the paper. Then, in Section 3 we give the values of the Cramér-Rao complexity of the Hermite polynomials and the asymptotics (infinity) of the Fisher-Shannon and LMC complexities of Hermite polynomials. In Sections 4 and 5 we find the Cramér-Rao complexity and the disequilibrium as well as the asymptotics of the Fisher-Shannon and LMC complexities of the Laguerre and Jacobi polynomials, respectively. In Section 6, the previous analytical results are numerically discussed in terms of the polynomial's degree and the parameters which characterize the weight function. Finally, some conclusions and various open problems found throughout the paper are given.

2. Complexity measures of a general probability density

In this Section we give the definitions and mathematical meanings of the complexity measures of a probability distribution.

Let us consider a general one-dimensional random variable X characterized by the continuous probability distribution $\rho(x)$, $x \in \Lambda \subseteq \mathbb{R}$. To quantify the spread of X over the interval Λ we usually employ the statistical root-mean-square or standard deviation Δx, which is the square root of the variance

$$V[\rho] = (\Delta x)^{\frac{1}{2}} = \langle x^2 \rangle - \langle x \rangle^2,$$

where

$$\langle f(x) \rangle = \int_\Lambda f(x)\rho(x)dx.$$

The information theory provides other spreading measures such as the Rényi and Shannon entropies and the Fisher information. The Rényi entropy $R_q[\rho]$ of $\rho(x)$ is defined [18] by

$$R_q[\rho] := \frac{1}{1-q}\ln W_q[\rho] = \frac{1}{1-q}\ln \int_\Lambda [\rho(x)]^q dx,$$

where $W_q[\rho] = \langle \rho^{q-1} \rangle$ denotes the qth-order frequency or entropic moment of $\rho(x)$. The limiting value $q \to 1$, taking into account the normalization condition $W_1[\rho] = 1$, yields the Shannon entropy [19]

$$S[\rho] := \lim_{q\to 1} R_q[\rho] = -\int_\Lambda \rho(x)\ln\rho(x)dx.$$

The Fisher information of $\rho(x)$ is defined [20, 21] as

$$F[\rho] := \int_\Lambda \frac{\left(\frac{d}{dx}\rho(x)\right)^2}{\rho(x)}dx.$$

It is worth remarking that: (a) these three information-theoretic spreading measures do not depend on any particular point of their interval Λ, 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 Rényi 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 [22]

$$N_q[\rho] = \exp\left(R_q[\rho]\right) = \left(W_q[\rho]\right)^{\frac{1}{1-q}}, \quad \text{Rényi length},$$

$$N_1[\rho] = \lim_{q\to 1} N_q[\rho] = \exp\left(S[\rho]\right), \quad \text{Shannon length},$$

$$\delta x = \frac{1}{\sqrt{F[\rho]}}, \qquad \text{Fisher length}.$$

It is straightforward to observe that these three lengths, as well as the standard deviation Δx, have the same units of X.

Let us highlight that the quantities ($V[\rho]$, $R_q[\rho]$, $S[\rho]$, $F[\rho]$), and its related measures (Δx, $N_q[\rho]$, $N_1[\rho]$, δx), are complementary since each of them grasps a single different facet of the probability density $\rho(x)$. So, 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, 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 Λ.

Recently, some composite density-dependent information-theoretic quantities have been introduced; namely, the complexity measures of Crámer-Rao [23–25], Fisher-Shannon [26, 27] and López-Ruiz-Mancini-Calbet (LMC) [28] types. They are given by the product of two of the previous single spreading measures as

$$C_{CR}[\rho] = F[\rho] \times V[\rho], \tag{1}$$

$$C_{FS}[\rho] = F[\rho] \times \frac{1}{2\pi e} e^{2S[\rho]} = \frac{1}{2\pi e} F[\rho] \times N_1^2[\rho], \tag{2}$$

$$C_{LMC}[\rho] = W_2[\rho] \times e^{S[\rho]} = \langle \rho \rangle \times N_1[\rho], \tag{3}$$

for the Crámer-Rao, Fisher-Shannon and LMC complexities, respectively. Each of them grasps the combined balance of two different facets of the probability density. The Crámer-Rao complexity quantifies the wiggliness or 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 second-order entropic moment $W_2[\rho]$, also called disequilibrium $D[\rho]$), and its total extent (as given by the Shannon entropic power $N[\rho] = e^{S[\rho]}$).
Moreover, it may be easily observed that these three complexity measures are (a) dimensionless, (b) bounded from below by unity (when ρ is a continuous density in $\mathbb{R}$ in the Crámer-Rao and Fisher-Shannon cases, and for any ρ in the LMC case), 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 fulfil invariance properties under replication, translation and scaling transformation [29, 30].

3. Complexity measures of Hermite polynomials

In this section we give the values of the Crámer-Rao complexity, as well as the asymptotics ($n \to \infty$) of the Fisher-Shannon and LMC complexities, of the Hermite polynomials $H_n(x)$ characterized by the orthogonality condition (see e.g. [6, 31])

$$\int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} dx = \delta_{m,n}, \quad m, n \in \mathbb{N}.$$

These quantities are defined by the corresponding complexity measures of the Rakhmanov-Hermite probability density

$$\rho_H(x) = H_n^2(x) e^{-x^2}.$$

Let us begin with the Crámer-Rao complexity which, according to Eq.(1), is given by

$$C_{CR}[\rho_H] = F[\rho_H] \times V[\rho_H],$$

where the variance and the Fisher information of the Hermite polynomials are known [24, 32] to be

$$V[\rho_H] = n + \frac{1}{2},$$

and

$$F[\rho_H] = 4n + 2, \tag{4}$$

respectively. Therefore, one easily has the value

$$C_{CR}[\rho_H] = 4n^2 + 4n + 1,$$

for the Crámer-Rao quantity.

Similarly, from Eq. (2) one has that the Fisher-Shannon complexity of Hermite polynomials is given by

$$C_{FS}[\rho_H] = F[\rho_H] \times \frac{1}{2\pi e} N_1^2[\rho_H],$$

where the Shannon length (also called Shannon entropy power) of the Hermite polynomials, $N_1[\rho_H] = \exp(S[\rho_H])$, have not been analytically calculated up until now except in the asymptotical case [33]:

$$N_1[\rho_H] \approx \frac{\pi}{e}\sqrt{2n}; \quad n \gg 1. \tag{5}$$

Then, this expression together with the Fisher value (4) directly lead to the asymptotical value of the Fisher-Shannon of the Hermite polynomials:

$$C_{FS}\left[\rho_H\right] \approx \left(\frac{4\pi}{e^3}\right) n^2, \qquad n \gg 1.$$

Finally, from Eq. (3) one obtains the LMC complexity of Hermite polynomials as

$$C_{LMC}[\rho_H] = W_2[\rho_H] \times N_1[\rho_H],$$

where the second-order entropic moment (also called disequilibrium)

$$W_2[\rho_H] = \langle \rho_H \rangle,$$

can be explicitly calculated both for all n and in the asymptotic case. The latter value is

$$W_2[\rho_H] = 2\pi^{-2}(2n)^{-\frac{1}{2}}\left(\ln(n) + O(1)\right); n \gg 1,$$

as explained in [34]. Then, this expression together with Eq. (5) gives

$$C_{LMC}[\rho_H] \approx \frac{2}{\pi e}\ln n; \qquad n \gg 1,$$

for the asymptotical value of the LMC complexity of the Hermite polynomials $H_n(x)$.

4. Complexity measures of Laguerre polynomials

In this section we give the values of the Crámer-Rao complexity and the asymptotical value of the Fisher-Shannon of the Laguerre polynomials $L_n^{(\alpha)}(x), \alpha > -1$. As well, we point out the issues to calculate the LMC complexity of these mathematical objects both in the general (i.e., for all n) and asymptotical (i.e., at large n) cases. The Rakhmanov probability density associated to the Laguerre polynomials $L_n^{(\alpha)}(x)$ characterized by the orthogonality condition (see e.g. [6, 35])

$$\int_0^{+\infty} L_n^{(\alpha)}(x) L_m^{(\alpha)}(x) x^\alpha e^{-x} dx = \delta_{mn},$$

is defined by

$$\rho_L(x) = \left[L_n^{(\alpha)}(x)\right]^2 x^\alpha e^{-x}.$$

Then, according to Eq.(1), the Crámer-Rao complexity of the Laguerre polynomials is given by

$$C_{CR}[\rho_L] = F[\rho_L] \times V[\rho_L], \tag{6}$$

where the variance and the Fisher information are given [24, 32] by

$$V[\rho_L] = 2n^2 + 2(\alpha+1)n + \alpha + 1, \tag{7}$$

and

$$F[\rho_L] = \begin{cases} 4n+1, & \alpha = 0, \\ \frac{(2n+1)\alpha+1}{\alpha^2-1}, & \alpha > 1, \\ \infty, & \alpha \in [-1,+1], \alpha \neq 0, \end{cases} \tag{8}$$

respectively. The expressions (6)-(8) lead to the following value

$$C_{CR}[\rho_L] = \begin{cases} 8n^3 + [8(\alpha+1)+2]\, n^2 + 6(\alpha+1)n + (\alpha+1), & \alpha = 0, \\ \frac{1}{\alpha^2-1}\left[4\alpha n^3 + (4\alpha^2+6\alpha+2)n^2 + (4\alpha^2+6\alpha+2)n + (\alpha+1)^2\right], & \alpha > 1, \\ \infty, & \text{otherwise}, \end{cases}$$

for the Crámer-Rao complexity of Laguerre polynomials.

Let us now consider the Fisher-Shannon complexity of these polynomials which is defined, according to Eq.(2), by

$$C_{FS}[\rho_L] = F[\rho_L] \times \frac{1}{2\pi e} N_1^2[\rho_L], \tag{9}$$

where the Shannon length or Shannon entropy power $N_1[\rho_L] = \exp(S[\rho_L])$ of the Laguerre polynomial $L_n^{(\alpha)}(x)$ is not yet known for all values of the degree n, mainly because it is a logarithmic functional of the polynomial. However, its asymptotical (large n) value has been found [31] to be

$$N_1[\rho_L] \approx \frac{2\pi n}{e}. \tag{10}$$

Then, from Eqs.(8), (9) and (10) one obtains the following asymptotics for the Fisher-Shannon complexity of the Laguerre polynomial $L_n^{(\alpha)}(x)$:

$$C_{FS}\left[\rho_L\right] \approx \begin{cases} \left(\frac{8\pi}{e^3}\right) n^3, & \alpha = 0, \\ \frac{4\alpha}{\alpha^2-1}\left(\frac{\pi}{e^3}\right) n^3, & \alpha > 1, \\ \infty, & \text{otherwise}. \end{cases}$$

Finally, let us tackle the calculation of the LMC complexity of Laguerre polynomials which is given by

$$C_{LMC}[\rho_L] = W_2[\rho_L] \times N_1[\rho_L].$$

Now, we have two opposite situations when calculating these two factors: while the Shannon length $N_1[\rho_L]$ is only known in the asymptotics case (see Eq.10), the second-order entropic moment $W_2[\rho_L]$ has been recently shown [31] to be expressed in the two following manners for all values of the degree n:

(i) In terms of the four-variate Lauricella function $F_A^{(4)}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ [36]:

$$\begin{aligned} W_2[\rho_L] &= \left(\frac{n!}{\Gamma(\alpha+n+1)}\right)^2 \frac{\Gamma(2\alpha+1)}{2^{2\alpha+1}} \binom{n+\alpha}{n}^4 \\ &\quad \times F_A^{(4)}\left(\begin{matrix} 2\alpha+1; -n,-n,-n,-n \\ \alpha+1,\alpha+1,\alpha+1,\alpha+1 \end{matrix}; \frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right). \end{aligned} \tag{11}$$

(ii) In terms of the multivariate Bell polynomials $B_{m,l}(a_1, a_2 \ldots, a_{m-l+1})$ [37]:

$$W_2[\rho_L] = \left[\sum_{k=0}^{4n} \frac{\Gamma(2\alpha+k+1)}{2^{2\alpha+k+1}} \frac{(4)!}{(k+4)!} B_{k+4,4}\left(c_0^{(n,\alpha)}, 2!c_1^{(n,\alpha)}, ..., (k+1)!c_k^{(n,\alpha)}\right)\right], \tag{12}$$

where the parameters $c_t^{(n,\alpha)}$ are given by

$$c_t^{(n,\alpha)} = \sqrt{\frac{\Gamma(n+\alpha+1)}{n!}} \frac{(-1)^t}{\Gamma(\alpha+t+1)} \begin{pmatrix} n \\ t \end{pmatrix}.$$

Taking into account that $N_1[\rho_L]$ is not known for a generic degree n of the polynomials and the asymptotics of Eqs.(11) and (12) is a formidable task, the evaluation of the LMC complexity of Laguerre polynomials remains to be an open problem in both general and asymptotic situations of n.

5. Complexity measures of Jacobi polynomials

In this section we give the values of the Crámer-Rao complexity of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, with $\alpha, \beta > -1$, as well as the asymptotics (large n) of its Fisher-Shannon complexity. In addition, we discuss the reasons why the evaluation of the LMC complexity cannot yet be done. The Jacobi polynomials are well-known to satisfy the orthogonality condition (see [6, 35])

$$\int_{-1}^{+1} P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x)(1-x)^\alpha (1+x)^\beta dx = \delta_{mn},$$

and its associated Rakhmanov probability density $\rho_J(x)$ is given by

$$\rho_J(x) = \left[P_n^{(\alpha,\beta)}(x)\right]^2 (1-x)^\alpha (1+x)^\beta.$$

The Crámer-Rao complexity of $P_n^{(\alpha,\beta)}(x)$ is defined by the Crámer-Rao of the density $\rho_J(x)$ which, according to Eq.(1), is given by

$$C_{CR}[\rho_J] = F[\rho_J] \times V[\rho_J]. \tag{13}$$

These two factors have been recently calculated [24, 32], having the values

$$\begin{aligned} V[\rho_J] = & \frac{4(n+1)(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2(2n+\alpha+\beta+3)} \\ & + \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)}, \end{aligned} \tag{14}$$

for the variance, and

$$F[\rho_J] = \begin{cases} 2n(n+1)(2n+1), & \alpha, \beta = 0, \\ \frac{2n+\beta+1}{4}\left[\frac{n^2}{\beta+1} + n + (4n+1)(n+\beta+1) + \frac{(n+1)^2}{\beta-1}\right], & \alpha = 0, \beta > 1, \\ \frac{2n+\alpha+\beta+1}{4(n+\alpha+\beta-1)}\left[n(n+\alpha+\beta-1)\left(\frac{n+\alpha}{\beta+1} + 2 + \frac{n+\beta}{\alpha+1}\right)\right. & \\ \left. + (n+1)(n+\alpha+\beta)\left(\frac{n+\alpha}{\beta-1} + 2 + \frac{n+\beta}{\alpha-1}\right)\right], & \alpha, \beta > 1, \\ \infty, & \text{otherwise}, \end{cases} \tag{15}$$

for the Fisher information of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$. Then, from Eqs.(13)-(15) one obtains the value

$$
C_{CR}[\rho_J] = \begin{cases} 2n(n+1)\left[\frac{(n+1)^2}{2n+3} + \frac{n^2}{2n-1}\right], & \alpha=\beta=0, \\ \left[\frac{(n+1)^2(n+\beta+1)^2}{(2n+\beta+2)^2(2n+\beta+3)} + \frac{n^2(n+\beta)^2}{(2n+\beta-1)(2n+\beta)^2}\right] \\ \times\left[\frac{n^2}{\beta+1} + n + (4n+1)(n+\beta+1) + \frac{(n+1)^2}{\beta-1}\right], & \alpha=0, \beta>1, \\ \left[\frac{(n+1)(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+2)^2(2n+\alpha+\beta+3)} + \frac{n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2}\right] \\ \times\frac{1}{n+\alpha+\beta-1}\left[n(n+\alpha+\beta-1)\left(\frac{n+\alpha}{\beta+1}+2+\frac{n+\beta}{\alpha+1}\right)\right. \\ \left.+(n+1)(n+\alpha+\beta)\left(\frac{n+\alpha}{\beta-1}+2+\frac{n+\beta}{\alpha-1}\right)\right], & \alpha>1, \beta>1, \\ \infty, & \text{otherwise.} \end{cases}
$$

The Fisher-Shannon complexity of Jacobi polynomial is, according to Eq.(2), given by

$$
C_{FS}[\rho_J] = F[\rho_J] \times \frac{1}{2\pi e} N_1^2[\rho_J]. \tag{16}
$$

We cannot calculate the exact value of this complexity measure for all values of the polynomial degree n since the Shannon length $N_1[\rho_J]$ has not yet been found for a generic n, because of its logarithmic-functional nature. However, its asymptotic value has been recently shown [37] to be as

$$
N_1[\rho_J] \approx \frac{\pi}{e}, \quad n \to \infty, \tag{17}
$$

so that the asymptotics of the Fisher-Shannon complexity of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ is

$$
C_{FS}[\rho_J] \approx \begin{cases} \left(\frac{2\pi}{e^3}\right) n^3, & \alpha=\beta=0, \\ \frac{1}{4}\left(\frac{\pi}{e^3}\right)\left[\frac{1}{\beta+1} + 4 + \frac{1}{\beta-1}\right] n^3, & \alpha=0, \beta>,1 \\ \frac{1}{2}\left(\frac{\pi}{e^3}\right)\left[\frac{\beta}{\beta^2-1} + \frac{\alpha}{\alpha^2-1}\right] n^3, & \alpha>1, \beta>1, \\ \infty, & \text{otherwise.} \end{cases}
$$

where Eqs.(15), (16) and (17) have been taken into account.

Finally it is worth highlightening that the LMC complexity of Jacobi polynomial defined by

$$
C_{LMC}[\rho_J] = W_2[\rho_J] \times N_1[\rho_J],
$$

cannot yet be evaluated neither for a generic polynomial degree n, nor in the asymptotic case $n \to \infty$. This is so despite we know [37, 38] the asymptotic behavior of the Shannon length $N_1[\rho_J]$ and the two following expressions for the second-order entropic moment $W_2[\rho_J]$ (also called disequilibrium):

(a) In terms of the four-variate Srivastava-Daoust function $F_{1:1;1;1;1}^{1:2;2;2;2}(1,1,1,1)$ [38] [36]:

$$
W_2[\rho_J] = D\left[P_n^{(\alpha,\beta)}\right] = \frac{d_0^{(2\alpha,2\beta)}}{\left(d_n^{(\alpha,\beta)}\right)^2} b_0\left(4, n, \alpha, \beta, 2\alpha, 2\beta\right),
$$

where

$$
d_n^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{n!(\alpha+\beta+2n+1)\Gamma(\alpha+\beta+n+1)},
$$

and

$$b_0(4,n,\alpha,\beta,2\alpha,2\beta) = \begin{pmatrix} n+\alpha \\ n \end{pmatrix}^4$$
$$\times F^{1:2;2;2;2}_{1:1;1;1;1}\left(\begin{matrix} 2\alpha+1 : -n, \alpha+\beta+n+1; \ldots; -n, \alpha+\beta+n+1 \\ 2\alpha+2\beta+2 : \alpha+1; \ldots; \alpha+1 \end{matrix} ; 1,1,1,1 \right).$$

(b) In terms of the Bell polynomials $B_{m,l}(a_1, a_2, \ldots, a_{m-l+1})$ [37]:

$$W_2[\rho_J] = \sum_{k=0}^{4n} \frac{(4)!}{(k+4)!} B_{k+4,4}\left(c_0^{(n,\alpha,\beta)}, 2!c_1^{(n,\alpha,\beta)}, ..., (k+1)!c_k^{(n,\alpha,\beta)}\right) \mathcal{I}(k,2,\alpha,\beta),$$

where the coefficients $c_t^{(n,\alpha,\beta)}$ are given by

$$c_t^{(n,\alpha,\beta)} = \sqrt{\frac{\Gamma(\alpha+n+1)(2n+\alpha+\beta+1)}{n!2^{\alpha+\beta+1}\Gamma(\alpha+\beta+n+1)\Gamma(n+\beta+1)}}$$
$$\times \sum_{i=t}^{n} (-1)^{i-t} \begin{pmatrix} n \\ i \end{pmatrix} \begin{pmatrix} i \\ t \end{pmatrix} \frac{\Gamma(\alpha+\beta+n+i+1)}{2^i \Gamma(\alpha+i+1)},$$

and

$$\mathcal{I}(k,q,\alpha,\beta) = \frac{(-1)^k 2^{1+\alpha q+\beta q}\Gamma(\alpha q+1)\Gamma(\beta q+1)}{\Gamma(\alpha q+\beta q+2)} {}_2F_1\left(\begin{matrix} -k, 1+\beta q \\ 2+(\alpha+\beta)q \end{matrix} ; 2 \right).$$

To find the value of the LMC complexity of $P_n^{(\alpha,\beta)}(x)$ we would further need to know the explicit value of the Shannon length $N_1[\rho]$ and/or the asymptotics of the disequilibrium $D[P_n^{(\alpha,\beta)}(x)]$, what is a formidable task. Therefore the analytical knowledge of the LMC complexity of Jacobi polynomials remains to be an open problem in both general and asymptotic cases.

6. Numerical discussion

In this section the expressions for the Cramer-Rao, Fisher-Shannon and LMC complexities found in the three previous sections are numerically studied for the three classical families of orthogonal polynomials of Hermite, Laguerre and Jacobi. The values of these complexities are computationally discussed in terms of the degree and parameters of the corresponding polynomials.

6.1. Dependence on the polynomial's degree n

Figures 1 and 2 represent the Cramer-Rao and the Fisher-Shannon complexity measures, respectively, for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ (■) and Jacobi $P_n^{(2,2)}(x)$ (•) polynomials as a function of the degree n for $n = 0, 1, \ldots, 40$. In the three cases these complexity measures monotonically grow with the degree n. For different values of the parameters of the Laguerre and Jacobi polynomials, the behaviour of these measures is the same. This behaviour can be explained from an intuitive idea of complexity: The number of maxima of the Rakhmanov density associated to a polynomial of degree n is equal to $n+1$, with one zero between each two consecutive maxima. Therefore, the number of oscillations and, consequently, one form of complexity of the density increases with n. Then, it looks like an intuitive idea of complexity is in agreement with the values of these complexity measures.

Figure 3 shows the LMC complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ (■) and $L_n^{(50)}(x)$ (□), and Jacobi $P_n^{(2,2)}(x)$ (•) and $P_n^{(50,50)}(x)$ (○) polynomials, as a function of the degree n for $n = 0, 1, \ldots, 30$. This complexity measure is a monotonically increasing function of n in the Laguerre and Jacobi cases with small values of the parameters, as can be seen in the figure for the

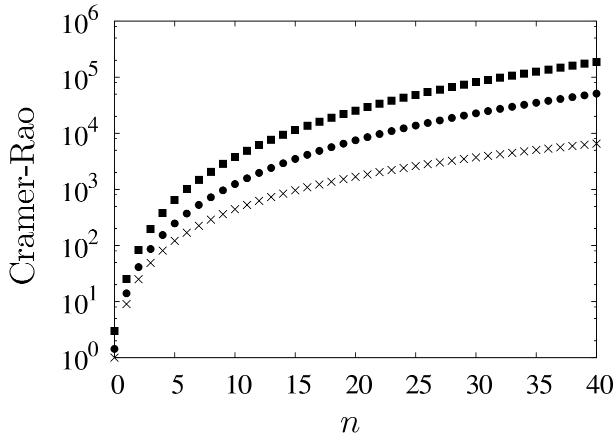

Figure 1: Cramer-Rao complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ ($\blacksquare$) and Jacobi $P_n^{(2,2)}(x)$ ($\bullet$) polynomials as a function of the degree n for $n = 0, 1, \ldots, 40$.

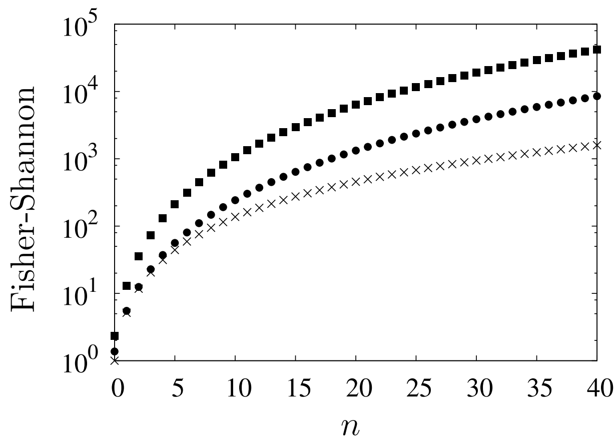

Figure 2: Fisher-Shannon complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ ($\blacksquare$) and Jacobi $P_n^{(2,2)}(x)$ ($\bullet$) polynomials as a function of the degree n for $n = 0, 1, \ldots, 40$.

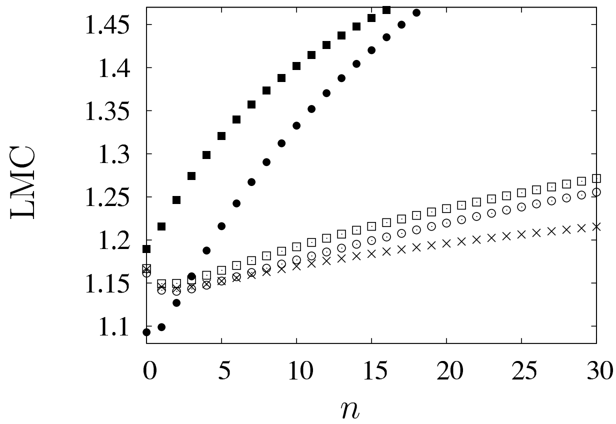

Figure 3: LMC complexity measure for the Rakhmanov densities of the Hermite $H_n(x)$ ($\times$), Laguerre $L_n^{(2)}(x)$ ($\blacksquare$) and $L_n^{(50)}(x)$ ($\square$), and Jacobi $P_n^{(2,2)}(x)$ ($\bullet$) and $P_n^{(50,50)}(x)$ ($\circ$) polynomials, as a function of the degree n for $n = 0, 1, \ldots, 30$.

polynomials $L_n^{(2)}(x)$ and $P_n^{(2,2)}(x)$. However, the LMC complexity measure is a decreasing function of n for small values of n in the Hermite case and also for Laguerre and Jacobi polynomials with large values of the parameters ($\alpha = \beta = 50$ in the figure). This can be explained taking into account that the LMC complexity does not depend on the Fisher information or any other information measure sensitive to the oscillatory character of the density. Then, the increase of the oscillatory content of the density from one maximum ($n = 0$) to two maxima ($n = 1$) is not very relevant to the increment of the complexity, from the point of view of the LMC measure. What provokes the decreasing of the LMC complexity is the decrement experienced by the average height of the density, that is measured by the disequilibrium; while the Shannon entropy remains almost constant. Thus, the LMC complexity is much more sensitive to the smoothness of the density than to its oscillatory character, grasping a different intuitive idea of complexity.

6.2. Dependence on the polynomial's parameters

Figures 4, 5 and 6 represent the Cramer-Rao, Fisher-Shannon and LMC complexity measures, respectively, for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $1 < \alpha < 10$ in the Cramer-Rao and Fisher-Shannon case (as the Fisher information is defined for $\alpha > 1$, apart from the discrete value $\alpha = 0$), and $-\frac{1}{2} < \alpha < 10$ in the LMC case (as the disequilibrium is defined for $\alpha > -\frac{1}{2}$).

For the Laguerre polynomials, the three complexity measures decrease when α increases. Again, this behaviour can be explained from an intuitive idea of complexity: The spreading of these densities increases with α. Since the complexity decreases (and the smoothness increases) as the spreading grows, the complexity of these densities decreases as α increases, as shown by the three studied complexity measures.

In the Jacobi case, the principal characteristic on these figures is the minima that show the three complexity measures as a function of α. This behaviour can also be explained from an intuitive point of view: For a given value of $\beta \in \{0\} \cap (1, +\infty)$, if $\alpha \leq 1$ the density appears more concentrated around positive values of x in the interval $(-1, 1)$. However, as α increases from this value the density moves to negative values of x. Within this transition, the density pass through a configuration of maximal spreading and smoothness, or minimal complexity, that is detected by these complexity measures with the minima that we can see in these figures. Another feature from these figures is the clear separation between points for $n = 0$ and points for $n = 2$ that appear in the Cramer-Rao and Fisher-Shannon representations, contrary to the LMC complexity measure. This behaviour is due to the effect of the Fisher information, very sensitive to the oscillatory character, in the first two complexity measures. However, the LMC complexity measure depend on the disequilibrium, that is not affected directly by the oscillatory content but for the average height of the density. For the three measures, since the density is defined in a bounded interval, the variance

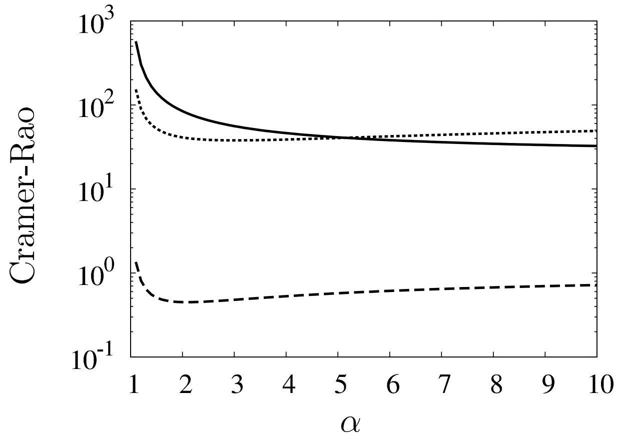

Figure 4: Cramer-Rao complexity measure for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $1 < \alpha < 10$.

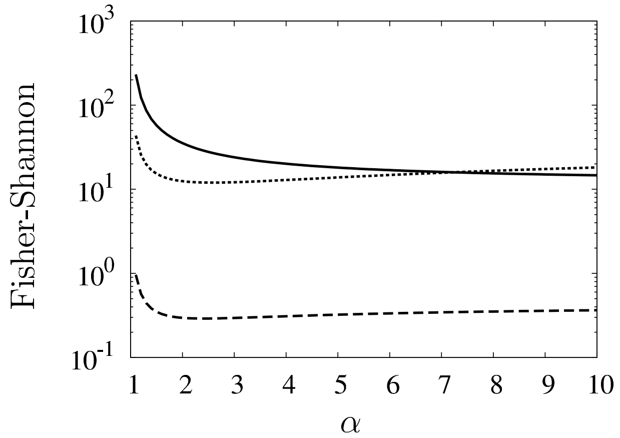

Figure 5: Fisher-Shannon complexity measure for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $1 < \alpha < 10$.

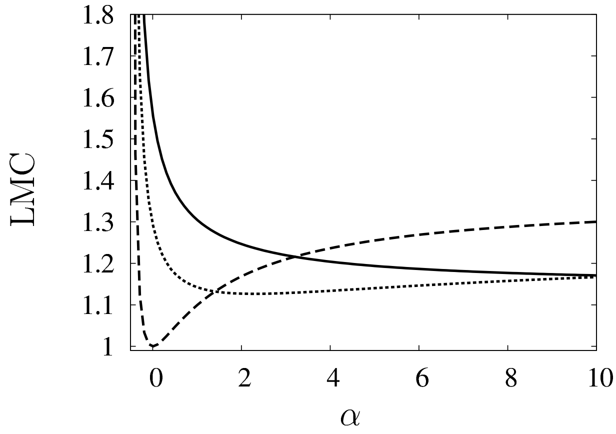

Figure 6: LMC complexity measure for the Rakhmanov densities of the Laguerre $L_2^{(\alpha)}(x)$ (solid line), and the Jacobi $P_0^{(\alpha,0)}(x)$ (dashed line) and $P_2^{(\alpha,2)}(x)$ (dotted line) polynomials, as a function of the parameter α, for $-\frac{1}{2} < \alpha < 10$.

and the Shannon entropy have an upper bound, so the variations of these measures come essentially from the Fisher information and the disequilibrium, respectively.

7. Conclusions and open problems

Nowadays the concept of complexity has become fundamental in Science and Technology because of its usefulness to interpret, explain and predict numerous natural phenomena. However its mathematical realization is manifold, depending not only on the specific discipline where it was created but also on the concrete purpose which generated it. Generally speaking, the different notions of complexity published in the literature can be classified as intrinsic (i.e., the ones which depend on the single-particle probability density of the many-body system under consideration) and extrinsic (i.e., the ones which do not depend on any probability density and take into account the context where the system is related with). The complexities of extrinsic character (e.g., Kolmogorov, computational and algorithmic complexities) were earlier introduced, being mostly used in technological areas [8, 9], while the intrinsic ones (e.g., Cramer-Rao, Fisher-Shannon and LMC complexities) have been recently introduced, being mostly used in scientific disciplines to discuss the internal structure of physical systems as well as to describe the course of chemical and biological processes and reactions [10, 11, 13, 14, 25, 26].

In this work we have introduced various complexities of intrinsic character to study the complexity of the hypergeometric-type orthogonal polynomials in a real continuous variable. We have defined them as the corresponding complexities of the Rakhmanov probability density associated to these polynomials. Then, we have discussed both algebraically and numerically the complexities of Hermite, Laguerre and Jacobi polynomials in terms of both the polynomial degree and the characterizing parameters of their weight functions. Analytically, we have found the explicit expression of the Cramer-Rao complexity in the Hermite case and the asymptotics of the Fisher-Shannon and LMC complexities in the three Hermite, Laguerre and Jacobi cases. Numerically we have shown that, opposite to the single information-theoretic measures (e.g., Shannon entropy, Fisher information, disequilibrium,...), these three composite complexities grasp different aspects of the complex nature that people have about the mathematical functions here considered.

In addition, several open problems have been pointed out throughout the paper. Here we would like to highlight two important issues in the field of generalized hypergeometric functions (namely, the reduction of the Lauricella function $F_A^{(4)}\left(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ and the Srivastava-Daoust function $F^{1:2;2;2;2}_{1:1;1;1;1}(1,1,1,1)$ to much simpler functions) and the following asymptotic problem of classical orthogonal polynomials $y_n(x)$: to find the asymptotical ($n \to \infty$) value of the functional

$$W_q[\rho] = \int_\Lambda [\rho(x)]^q \, dx = \int_\Lambda [\omega(x)]^q \, |y_n(x)|^{2q} \, dx,$$

which is very closely connected to the weighted L_q-norm of these polynomials. Here, $\omega(x)$ ($x \in \Lambda$) is the weight function with respect to which these polynomials are orthogonal, and $\rho(x) = \omega(x)|y_n(x)|^2$ denotes the associated Rakhmanov probability density. This asymptotical issue has been recently solved for the Hermite polynomials [34] but it remains open in the Laguerre and Jacobi cases. The solution of these issues would allow one to calculate not only the disequilibrium but also the LMC complexity of the Laguerre and Jacobi cases and, *in extenso*, the corresponding quantities of numerous physical systems whose quantum-mechanical states are described by wavefunctions controlled by these polynomials. Finally, for the sake of completeness, let us also comment that the asymptotics ($q \to \infty$) of these mathematical objects have been recently considered [39].

Acknowledgements

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4.4. Medidas entrópicas y de complejidad de los armónicos hiperesféricos y aplicaciones cuánticas

Esta sección contiene el artículo siguiente que trata el cálculo de medidas entrópicas y de complejidad de los armónicos hiperesféricos, y los resultados obtenidos se aplican al rotador rígido.

Entropy and complexity analysis of the D-dimensional rigid rotator and hyperspherical harmonics.
J. S. Dehesa, **A. Guerrero** y P. Sánchez-Moreno.
Journal of Mathematical Chemistry (2014). Enviado.

Uno de los prototipos cuánticos más utilizados para caracterizar fenómenos y propiedades moleculares es el rotor o rotador rígido, que es un sistema-modelo constituido por una partícula moviéndose sobre la superficie de una esfera. En este artículo se considera un rotador rígido en D dimensiones, por lo que el movimiento de la partícula tiene lugar sobre una hiperesfera D-dimensional. Las funciones de onda de los estados mecano-cuánticos permitidos para este sistema son los armónicos hiperesféricos. En este trabajo se analiza el movimiento mecano-cuántico de este sistema haciendo uso de las medidas teórico-informacionales. Esto conlleva la determinación de los momentos entrópicos, las medidas entrópicas y las medidas de complejidad de los armónicos hiperesféricos. Finalmente se hace un análisis numérico exhaustivo de estas magnitudes.

Entropy and complexity analysis of the D-dimensional rigid rotator and hyperspherical harmonics

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Abstract

In this paper we carry out an information-theoretic analysis of the D-dimensional rigid rotator by studying the entropy and complexity measures of its wavefunctions, which are controlled by the hyperspherical harmonics. These measures quantify single and two-fold facets of the rich intrinsic structure of the system which are manifest by the intricate and complex variety of D-dimensional geometries of the hyperspherical harmonics. We calculate the explicit expressions of the entropic moments and the Rényi entropies as well as the Fisher-Rényi, Fisher-Shannon and LMC complexities of the system. The explicit expression for the last two complexity measures is not yet possible, mainly because the logarithmic functional of the Shannon entropy has not yet been obtained up until now in a closed form.

Keywords: Hyperspherical harmonics, rigid rotor, complexity measures, Shannon entropy, Rényi entropy, Fisher information

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I. INTRODUCTION

The manifestations of quantum mechanics in D-dimensional physical systems are generally analytically inaccessible, basically because the associated Schrödinger equations cannot be explicitly solved except for a very few cases which correspond to a quantum potential with some known symmetry. The particle-in-a-box, the harmonic oscillator, the hydrogen atom, the particle moving in a Dirac-delta-like potential, and the rigid rotator are possibly the five major prototypical systems which are used to model the quantum-mechanical behavior of most 3- and D-dimensional physical systems (see e.g. [1, 2]).

The information-theoretic properties of these physical prototypes have been recently investigated for the first four cases in references [3–7]; see also the review papers [8, 9]. However, the corresponding properties for the rigid rotator have not yet been found, although many other properties of this system are well known, such as the specific heat [10], potential energy surfaces [11], spectral quantities in external fields [12], among others. This is a serious lack because of the numerous applications of this model; in particular, it has been extensively used to characterize the rotation of diatomic molecules (and is easily extended to linear polyatomic molecules). In this work we investigate the entropy and complexity properties of the wavefunctions of the rigid rotator; i.e., the hyperspherical harmonics.

The D-dimensional ($D \geq 3$) spherical harmonics (or simply, hyperspherical harmonics) do not only play a central role in harmonic analysis and approximation theory [13–15] but also in quantum theory [16, 17]. As well, they have been shown to be the solutions of a very broad class of equations of a form into which numerous equations of D-dimensional physics can be transformed, ranging from the Schrödinger equation of the rigid rotator till the Bethe-Salpeter equation of some quark systems [2, 14, 16–22]. Indeed, e.g. they are the eigenfunctions of the D-dimensional rigid rotator (i.e., a point mass μ rotating around a fixed center in the hyperspace at a given distance r_0) corresponding to the eigenvalues $l(l+D-2)/(2I)$, for $l = 0, 1, 2, \ldots$, where the moment of inertia $I = \mu r_0^2$. Moreover, they are the functions that give the anisotropic character of the eigenfunctions of D-dimensional central potentials, since the remaining radial part is spherically symmetric. The hyperspherical harmonics are functions defined on the $(D-1)$-dimensional unit sphere $S_{D-1} \subset \mathbb{R}_D$ which arise as eigenfunctions of the Laplace-Beltrami operator corresponding to the eigenvalues $l(l+D-2)$. They are basis vectors in certain irreducible representation spaces of $SO(D, 2)$

[13–15], and in fact constitute a basis for integrable functions defined on the unit sphere.

The hyperspherical harmonics are known [4, 16, 21] to have the form

$$Y_{l,\{\mu\}}(\Omega_D) = \frac{1}{\sqrt{2\pi}} e^{i\mu_{D-1}\theta_{D-1}} \prod_{j=1}^{D-2} \hat{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j)(\sin\theta_j)^{\mu_{j+1}}, \tag{1}$$

where $\Omega_D \equiv (\theta_1, \theta_2, \cdots, \theta_{D-1})$ represents the $D-1$ angular coordinates of the sphere S_{D-1} so that $0 \leq \theta_j \leq \pi$ for $j = 1, \cdots, D-2$ and $0 \leq \theta_{D-1} \leq 2\pi$. The $D-1$ integer numbers $l \equiv \mu_1$ and $\{\mu_2, \cdots, \mu_{D-1} \equiv m\} \equiv \{\mu\}$ have the values $l = 0, 1, 2, \cdots$ and $\mu_1 \geq \mu_2 \geq \ldots \geq |\mu_{D-1}| \geq 0$. The parameter $\alpha_j = (D-j-1)/2$. And the symbol $\hat{C}^{\lambda}_n(x)$, $\lambda > -\frac{1}{2}$, denotes the orthonormal Gegenbauer polynomial of degree n and parameter λ which satisfies the orthogonality condition

$$\int_{-1}^{+1} \hat{C}^{\lambda}_n(x)\hat{C}^{\lambda}_m(x)\omega_\lambda(x)dx = \delta_{mn}, \tag{2}$$

where the weight function is defined as

$$\omega_\lambda(x) = (1-x^2)^{\lambda-\frac{1}{2}}. \tag{3}$$

The algebraic properties of these functions are widely known in mathematical physics [2, 16, 17, 20–24]; in particular, they satisfy the orthogonality relation

$$\int_{S_{D-1}} Y^*_{l,\{\mu\}}(\Omega_D)Y_{l',\{\mu'\}}(\Omega_D)d\Omega_D = \delta_{ll'}\delta_{\{\mu\},\{\mu'\}},$$

where the generalized solid angle element is

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

The spread of the hyperspherical harmonics all over the hyperspace is, however, not so well known. This is a serious lack since these functions control the angular distribution of the charge and momentum distributions of numerous quantum mechanical systems with a central potential, by means of the density function

$$\rho_{l,\{\mu\}}(\Omega_D) = \left|Y_{l,\{\mu\}}\left(\Omega_D\right)\right|^2, \tag{4}$$

which is called as Rakhmanov probability density of the hyperspherical harmonics in the theory of special functions, and gives the distribution of the particle all over the hyperspace.

The information-theoretic measures of this density function allows us to quantify single and composite facets of the rich variety of D-dimensional geometries of the system in the hyperspace.

The goal of this paper is three-fold. First, we calculate the analytical expressions of various single information-theoretic measures of spreading (entropic moments and Rényi entropies) beyond the recently found Fisher information [25], and the following two-component complexity measures: Fisher-Shannon, Fisher-Rényi and LMC complexities. Second, we apply these results to eigenfunctions of the standard (i.e., three-dimensional) rigid rotator; that is to the hyperspherical harmonics. Third, we carry out a numerical study of these entropy and complexity quantities for various orders and dimensionalities of the harmonics.

The structure of the paper is the following. In Section II we give the definitions of the entropies and complexities to be used throughout the paper. Then, in Section III we give the expression of the Fisher information and calculate the entropic moments and Rényi entropies of the wavefunctions of the quantum-mechanical D-dimensional rigid rotator, which are controlled by the hyperspherical harmonics. In Section IV the expressions of the two-component complexity measures of the type Fisher-Shannon, Fisher-Rényi and LMC types are given, and a numerical study is performed. Finally, some conclusions are given and various open problems are pointed out.

II. ENTROPY AND COMPLEXITY MEASURES: BASICS

In this Section we describe briefly the information-theoretic spreading measures of a general probability density $\rho(\vec{\mathbf{r}})$ which will be used throughout the paper; namely, the entropic moments, the Rényi, Tsallis and Shannon entropies, the Fisher information and the associated two-component complexity measures: Fisher-Shannon, Fisher-Rényi, and LMC.

The qth-frequency or entropic moment of the density $\rho(\vec{\mathbf{r}})$, $\vec{\mathbf{r}} \in \mathbb{R}^D$, is defined by

$$W_q[\rho] := \langle \rho^{q-1} \rangle = \int_{\mathbb{R}^D} [\rho(\vec{\mathbf{r}})]^q \, d\vec{\mathbf{r}}, \quad q \in \mathbb{R}^+ \tag{5}$$

where the expectation value of a function $f(\vec{\mathbf{r}})$, $\langle f(\vec{\mathbf{r}}) \rangle$, is given by

$$\langle f(\vec{\mathbf{r}}) \rangle = \int_{\mathbb{R}^D} f(\vec{\mathbf{r}}) \rho(\vec{\mathbf{r}}) d\vec{\mathbf{r}}.$$

Mathematically, these moments are often more useful than the ordinary moments $\langle r^k \rangle$ because the later ones give too much weight to the tail of the distribution and, at times, they are undefined [26]. From a physical point of view the entropic moments describe numerous functionals of the electron density which characterize fundamental and/or experimentally-measurable quantities of atomic and molecular systems according to the Hohenberg-Kohn density-functional theory [27–30]; e.g. the Thomas-Fermi and Dirac exchange energies. See also [31] for their connection with other atomic density functionals, [32, 33] for the existence conditions, [34] for further mathematical properties, [8] for various applications in D-dimensional quantum systems, and [35] for potential applications in statistics and imaging.

The Rényi and Tsallis entropies of $\rho(\vec{\mathbf{r}})$ are defined in terms of the entropic moments as [36]

$$R_q[\rho] = \frac{1}{1-q} \log W_q[\rho] = \frac{1}{1-q} \log \int_{\mathbb{R}^D} [\rho(\vec{\mathbf{r}})]^q \, d\vec{\mathbf{r}}, \quad q > 0, \; q \neq 1, \tag{6}$$

and [37]

$$T_q[\rho] = \frac{1}{q-1} \left(1 - W_q[\rho]\right) = \frac{1}{q-1} \left(1 - \int_{\mathbb{R}^D} [\rho(\vec{\mathbf{r}})]^q \, d\vec{\mathbf{r}}\right), \quad q > 0, \; q \neq 1, \tag{7}$$

respectively, which when $q \to 1$ reduce to the well-known Shannon entropy

$$S[\rho] = -\int_{\mathbb{R}^D} \rho(\vec{\mathbf{r}}) \log \rho(\vec{\mathbf{r}}) d\vec{\mathbf{r}}. \tag{8}$$

It is interesting to remark that these quantities are global measures of spreading of the density $\rho(\vec{\mathbf{r}})$ because they are power (Rényi) or logarithmic (Shannon) functionals of $\rho(\vec{\mathbf{r}})$. They provide various complementary ways to quantify the extent of $\rho(\vec{\mathbf{r}})$ all over the hyperspace.

The (translationally invariant) Fisher information of $\rho(\vec{\mathbf{r}})$ is defined [38, 39] by

$$F[\rho] = \int_{\mathbb{R}^{\mathbb{D}}} \rho(\vec{\mathbf{r}}) \left|\nabla_D \log \rho(\vec{\mathbf{r}})\right|^2 d\vec{\mathbf{r}} = 4 \int_{\mathbb{R}^{\mathbb{D}}} \left|\nabla_D \sqrt{\rho(\vec{\mathbf{r}})}\right|^2 d\vec{\mathbf{r}}, \tag{9}$$

where ∇_D denotes the D-dimensional gradient. This notion was first introduced in the one-dimensional case for statistical estimation [38], but nowadays it is used in a wide variety of scientific fields [39] mainly because of its close resemblance with kinetic and Weiszäcker energies [40]. Contrary to the Rényi and Shannon entropies, the Fisher information is a local measure of spreading of the density because it is a gradient functional of $\rho(\vec{\mathbf{r}})$. 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.

Recently, some composite density-dependent information-theoretic quantities have been introduced. They are called complexity measures because they grasp more than a single facet (macroscopic property) of the density. We refer to the Fisher-Shannon, and the more general Fisher-Rényi, and the LMC shape complexities. They have a number of very interesting mathematical properties. Here we would like to highlight some common characteristics. They are dimensionless, opposite to the previously defined single-component entropies (entropic moments, Shannon and Rényi entropies, Fisher information), what allows them to be mutually compared. They are defined essentially by the product of two single entropies, what allows them to quantify two-fold facets of the density. Moreover, they are intrinsic quantities of the density what differenciate them from other complexity notions already used (computational complexity, algorithmic complexity, ...), which depend on the context. Finally, they are close to the intuitive notion of complexity because they are minimum for the extreme or least complex distribution which correspond to maximum disorder (i.e. the highly flat distribution).

The Fisher-Rényi complexity of $\rho(\vec{\mathbf{r}})$ is defined [41] by

$$C_{FR}^{(q)}\left[\rho\right] := F\left[\rho\right] \times J_q\left[\rho\right] \tag{10}$$

where $F\left[\rho\right]$ is the Fisher information (9) and $J_q\left[\rho\right]$ denotes the qth-order Rényi power entropy of $\rho(\vec{\mathbf{r}})$ given by

$$J_q\left[\rho\right] = \frac{1}{2\pi e} e^{\frac{2}{D} R_q[\rho]} \tag{11}$$

where $R_q\left[\rho\right]$ is the Rényi entropy (6). This complexity measure quantifies wiggliness or gradient content of the density jointly with its total extent all over the hyperspace, the parameter q weighting different regions of $\rho(\vec{\mathbf{r}})$. The special case $q \to 1$ of (10) leads to the Fisher-Shannon complexity as

$$C_{FS}\left[\rho\right] = F\left[\rho\right] \times \frac{1}{2\pi e} e^{\frac{2}{D} S[\rho]}, \tag{12}$$

where $S\left[\rho\right]$ is the Shannon entropy (8). All the relevant invariance properties (replication, translation, scaling) of $C_{FS}\left[\rho\right]$ are also fulfilled by the Fisher-Rényi complexities $C_{FR}^{(q)}\left[\rho\right]$ for any $q > 0$, $q \neq 1$.

The LMC complexity of $\rho(\vec{\mathbf{r}})$ is given [42, 43] by

$$C_{LMC}\left[\rho\right] = D\left[\rho\right] \times e^{S[\rho]}, \tag{13}$$

where

$$D[\rho] = W_2[\rho] = \langle \rho \rangle \tag{14}$$

is the second-order entropic moment of ρ, also called disequilibrium in some contexts. This complexity measure quantifies the combined balance of the average height of $\rho(\vec{\mathbf{r}})$ and the total extent of the spread of the density over the whole hyperspace.

III. ENTROPY MEASURES OF HYPERSPHERICAL HARMONICS

In this Section we give the algebraic expression of the Fisher information and obtain those of the entropic moments and Rényi and Tsallis entropies of the hyperspherical harmonics $Y_{l,\{\mu\}}(\Omega_D)$, which are given by the corresponding quantities, $F[\rho]$, $W_q[\rho]$ and $R_q[\rho]$ respectively, of the associated Rakhmanov probability density $\rho = \rho_{l,\{\mu\}}(\Omega_D)$. They will be expressed in terms of the hyperquantum numbers $(\mu_1 \equiv l, \mu_2, \ldots, \mu_{D-1}) \equiv (l, \{\mu\})$ and the dimensionality D.

First we realize from Eqs. (1) and (4) that the Rakhmanov density of the hyperspherical harmonics is

$$\rho_{l,\{\mu\}}(\Omega_D) = \frac{1}{2\pi}\prod_{j=1}^{D-2}\left[\hat{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j)\right]^2(\sin\theta_j)^{2\mu_{j+1}}. \tag{15}$$

Then, according to Eq. (9), the Fisher information of this density is [25, 44]

$$F[\rho_{l,\{\mu\}}] = 4L(L+1) - 2|\mu_{D-1}|(2L+1) - (D-1)(D-3), \tag{16}$$

where $L = l + \frac{D-3}{2}$. In the three-dimensional case ($D = 3$) this yields

$$F_{l,m}[\rho] = 4l(l+1) - 2|m|(2l+1). \tag{17}$$

The entropic moments of this density are, according to Eq. (5),

$$\begin{aligned} W_q[\rho_{l,\{\mu\}}] &= \int_{\mathbb{S}_{D-1}}\left[\rho_{l,\{\mu\}}(\Omega_D)\right]^q d\Omega_D \qquad (18)\\ &= \frac{1}{(2\pi)^{q-1}}\prod_{j=1}^{D-2}\int_0^{\pi}\left|\hat{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j)\right|^{2q}(\sin\theta_j)^{2(q\mu_{j+1}+\alpha_j)}d\theta_j \end{aligned}$$

The change of variable $\theta_j \to x_j = \cos\theta_j$ allows us to write these quantities as follows

$$\begin{aligned} W_q[\rho_{l,\{\mu\}}] &= \frac{1}{(2\pi)^{q-1}}\prod_{j=1}^{D-2}\int_{-1}^{+1}\left|\hat{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(x_j)\right|^{2q}\left(1-x_j^2\right)^{q\mu_{j+1}+\alpha_j-\frac{1}{2}}dx_j \qquad (19)\\ &= \frac{1}{(2\pi)^{q-1}}\prod_{j=1}^{D-2}\int_{-1}^{+1}\left|\hat{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(x_j)\right|^{2q}\omega_{q\mu_{j+1}+\alpha_j}(x_j)\,dx_j \qquad (20) \end{aligned}$$

where $\omega_\lambda(x)$ is defined in (3).

For $q \in \mathbb{N}$ we can apply the linearization method for Jacobi polynomials by Srivastava [45], particularized for Gegenbauer polynomials. This method yields the following linearization formula:

$$\left[\hat{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(x_j)\right]^{2q} = \sum_{i=0}^{2q(\mu_j-\mu_{j+1})} \beta^{(i)}_{j,q,D} \frac{d_i^{\left(q\mu_{j+1}+\alpha_j-\frac{1}{2},q\mu_{j+1}+\alpha_j-\frac{1}{2}\right)}}{\left[d_{\mu_j-\mu_{j+1}}^{\left(\mu_{j+1}+\alpha_j-\frac{1}{2},\mu_{j+1}+\alpha_j-\frac{1}{2}\right)}\right]^{2q}} \hat{C}_i^{\alpha_j+q\mu_{j+1}}(x_j)$$

which, together with the orthogonality relation of the Gegenbauer polynomials, allows us to obtain the following expression for the entropic moments:

$$W_q[\rho_{l,\{\mu\}}] = \frac{1}{(2\pi)^{q-1}} \prod_{j=1}^{D-2} \beta^{(0)}_{j,q,D} \frac{\left[d_0^{\left(q\mu_{j+1}+\alpha_j-\frac{1}{2},q\mu_{j+1}+\alpha_j-\frac{1}{2}\right)}\right]^2}{\left[d_{\mu_j-\mu_{j+1}}^{\left(\mu_{j+1}+\alpha_j-\frac{1}{2},\mu_{j+1}+\alpha_j-\frac{1}{2}\right)}\right]^{2q}}, \tag{21}$$

where

$$d_n^{(\alpha,\beta)} = \sqrt{\frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)}} \tag{22}$$

is the normalization constant of the Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ and

$$\beta^{(0)}_{j,q,D} = c\left(2q, \mu_j-\mu_{j+1}, \alpha_j+\mu_{j+1}-\frac{1}{2}, \alpha_j+\mu_{j+1}-\frac{1}{2}, \alpha_j+q\mu_{j+1}-\frac{1}{2}, \alpha_j+q\mu_{j+1}-\frac{1}{2}\right)$$

with

$$\begin{aligned} &c(r,n,\alpha,\beta,\gamma,\delta) \\ &\quad= \binom{n+\alpha}{n}^r F^{1:2;\ldots;2}_{1:1;\ldots;1}\left(\begin{array}{c} \gamma+1 : -n, \alpha+\beta+n+1; \ldots ; -n, \alpha+\beta+n+1 \\ \gamma+\delta+2 : \alpha+1; \ldots ; \alpha+1 \end{array} ; 1, \ldots, 1\right) \\ &= \binom{n+\alpha}{n}^r \sum_{j_1,\ldots,j_r=0}^{n} \frac{(\gamma+1)_{j_1+\cdots+j_r}}{(\gamma+\delta+2)_{j_1+\cdots+j_r}} \frac{(-n)_{j_1}(\alpha+\beta+n+1)_{j_1}\cdots(-n)_{j_r}(\alpha+\beta+n+1)_{j_r}}{(\alpha+1)_{j_1}\cdots(\alpha+1)_{j_r} j_1!\cdots j_r!}, \end{aligned} \tag{23}$$

where $F^{1:2;\ldots;2}_{1:1;\ldots;1}$ is a Srivastava-Daoust function [45]. This expression generalizes to any q the expression of the entropic moment with $q=4$ already obtained in [25].

Let us now consider some examples: In the case $D=3$ we obtain the expressions

$$W_q[\rho_{0,0}] = 2^{2-2q}\pi^{1-q}$$

for $l = m = 0$,

$$W_q[\rho_{1,0}] = \frac{2^{2-2q}3^q\pi^{1-q}}{2q+1}$$

for $l = 1$, $m = 0$,

$$W_q[\rho_{l,l}] = (2\pi)^{1-q}\frac{2^{2ql+1}\left(\Gamma(ql+1)\right)^2}{(2ql+1)\Gamma(2ql+1)}\left(\frac{(2l+1)\Gamma(2l+1)}{2^{2l+1}\left(\Gamma(l+1)\right)^2}\right)^q$$

for $m = l$, and

$$W_q[\rho_{l,l-1}] = (2\pi)^{1-q}l^{2q}\frac{\Gamma\left(q+\frac{1}{2}\right)\Gamma\left(q(l-1)+\frac{3}{2}\right)}{\sqrt{\pi}\Gamma\left(ql+\frac{3}{2}\right)}\frac{\left(d_0^{(q(l-1),q(l-1))}\right)^2}{\left(d_1^{(l-1,l-1)}\right)^{2q}}$$

for $m = l-1$.

For $D = 2$ the spherical harmonic reduces to $Y_m(\theta) = \frac{1}{\sqrt{2\pi}}e^{im\theta}$, $m \in \mathbb{Z}$, so the entropic moment of order q have the constant value

$$W_q[\rho_m] = (2\pi)^{1-q}.$$

For $D = 4$ we can obtain the values of the entropic moments

$$W_q[\rho_{0,0,0}] = 2^{1-q}\pi^{2-2q}$$

for $\mu_1 = \mu_2 = \mu_3 = 0$,

$$W_q[\rho_{1,0,0}] = \frac{2^{1+q}\pi^{\frac{3}{2}-2q}\Gamma\left(\frac{1}{2}+q\right)}{\Gamma(2+q)}$$

for $\mu_1 = 1$ and $\mu_2 = \mu_3 = 0$,

$$W_q[\rho_{l,l,l}] = (2\pi^2)^{1-q}\frac{(l+1)^q}{lq+1}$$

for $\mu_1 = \mu_2 = \mu_3 = l$,

$$W_q[\rho_{l,l-1,l-1}] = 2\pi^{\frac{3}{2}-2q}(l(l+1))^q\frac{\Gamma\left(q+\frac{1}{2}\right)\Gamma\left(q(l-1)+1\right)}{\Gamma(lq+2)}$$

for μ_l and $\mu_2 = \mu_3 = l-1$,

$$W_q[\rho_{l-1,l-1,l-2}] = 2^{1+q}\pi^{1-2q}(l(l^2+1))^q\frac{\left(\Gamma\left(q+\frac{1}{2}\right)\right)^2\Gamma\left(q(l-2)+1\right)}{\Gamma(lq+2)}$$

for μ_l, $\mu_2 = l-1$ and $\mu_3 = l-2$.

For any value of the dimensionality D we can obtain the following results:

$$W_q[\rho_{0,0,\dots,0}] = (2\pi)^{1-q} 2^{(D-1)(D-2)(1-q)/2} ((D-2)!)^{q-1} \prod_{j=1}^{D-2} \frac{\left(\Gamma\left(\frac{D-j}{2}\right)\right)^{2-2q}}{\left(\Gamma\left(D-j-1\right)\right)^{1-q}}$$

for $\mu_1 = \mu_2 = \cdots = \mu_{D-1} = 0$,

$$W_q[\rho_{l,l,\dots,l}] = (2\pi)^{1-q} 2^{(D-1)(D-2)(1-q)/2} \frac{((2l+1)_{D-2})^q}{(2ql+1)_{D-2}} \times \prod_{j=1}^{D-2} \frac{\left(\Gamma\left(ql + \frac{D-j}{2}\right)\right)^2}{\Gamma(2ql+D-j-1)} \left(\frac{\Gamma(2l+D-j-1)}{\left(\Gamma\left(l+\frac{D-j}{2}\right)\right)^2} \right)^q$$

for $\mu_1 = \mu_2 = \cdots = \mu_{D-1} = l$.

These expressions together with Eqs. (6) and (14) allow us to obtain the Rényi and Tsallis entropies of the quantum-mechanical states of the D-dimensional rigid rotator, respectively, in a straightforward manner in terms of the hyperquantum numbers characterizing the states and the dimensionality D.

IV. COMPLEXITY MEASURES OF HYPERSPHERICAL HARMONICS

In this Section we consider the complexity measures of Fisher-Shannon, Fisher-Rényi and LMC of the eigenfunctions of the D-dimensional rigid rotator (i.e., the hyperspherical harmonics) which are described by the corresponding quantities of the associated probability density given by Eq. (4) or (15). We should immediately say that these quantities cannot be obtained in analytical form, mainly because of the highbrow expression of the Rényi entropy (as seen in the previous section) and the logarithmic character of the Shannon functional. Therefore, our study has to be necessarily numerical. We will fix the dimensionality $D = 3$, so that we will investigate the behavior of the abovementioned complexity measures for the eigenfunctions of the three-dimensional rigid rotator (i.e., the standard spherical harmonics $Y_{l,m}(\theta,\phi)$) in terms of the quantum numbers l and m. We will numerically perform a complexity analysis of the three-dimensional rigid rotator (i.e. a point-mass particle freely moving on the two-dimensional sphere) whose ground and excited states (l,m) have the associated probability density

$$\rho_{l,m}(\theta,\phi) = \frac{1}{2\pi} \left[\hat{C}_{l-m}^{\frac{1}{2}+m}(\cos\theta) \right]^2 (\sin\theta)^{2m}. \tag{24}$$

It is well known that this system models a great number of physical systems, such as e.g. the rotating diatomic molecules. Indeed, a diatomic molecule is an extremely complicated many body problem (e.g., the HCl molecule is a 20-body problem), but at very low energies no excitations associated with the electron degrees of freedom come into play since the electron cloud binds the two atomic nuclei into a nearly rigid structure. For further details and applications of the three-dimensional rigid rotator, see e.g. [14, 19, 21].

A. Fisher-Shannon complexity

According Eq. (12), the Fisher-Shannon complexity of the three-dimensional rotator state (l, m) is given by the Fisher-Shannon complexity of the density $\rho_{l,m}(\theta, \phi)$; that is,

$$C_{FS}[\rho_{l,m}] = F[\rho_{l,m}] \times \frac{1}{2\pi e} e^{\frac{2}{3}S[\rho_{l,m}]} = (4l(l+1) - 2|m|(2l+1)) \times \frac{1}{2\pi e} e^{\frac{2}{3}S[\rho_{l,m}]},$$

where the Shannon entropy $S[\rho_{l,m}]$ is given by Eq. (8). The variation of this complexity measure in terms of l and m is investigated in Figures 1, 2 and 3. Figure 1 shows the values of the Fisher-Shannon complexity for fixed values of the angular quantum number $l = 10, 20, 50, 80$, for m from 0 to l. Notice that this complexity measure depends on the absolute value of m, so we have that $C_{FS}[\rho_{l,-m}] = C_{FS}[\rho_{l,m}]$. In this case we observe that the function $C_{FS}[\rho_{l,m}]$ decreases monotonically as m increases. We can also remark that the values of the complexity measure grow when l increases.

Figure 2 shows specifically how the complexity measure grows with l ($l \geq m$) for fixed values of m.

Finally, Figure 3 represents the values of $C_{FS}[\rho_{l,m}]$ as a function of l when $m = l - a$ with $a = 0, 1, 2$, for l from m to 80. The complexity measure increases monotonically with l in all the cases, and we see that the larger the difference between l and m, the higher the growth rate.

B. Fisher-Rényi complexity

Following Eqs. (6), (10), (11), (17) and (18) we can express the Fisher-Rényi complexity $C^{(q)}_{FR}[\rho_{l,m}]$ of the three-dimensional rigid rotator in terms of the quantum numbers l and m via the entropic moments $W_q[\rho_{l,m}]$ already calculated in Section III for any dimension; that

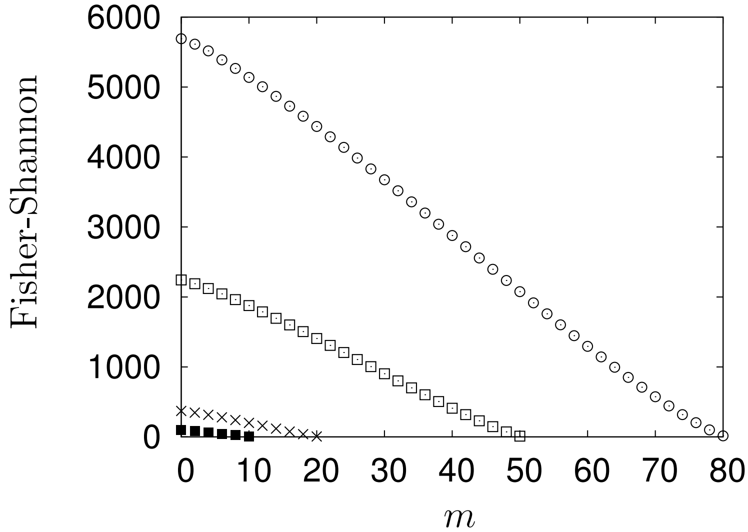

FIG. 1: Dependence of the Fisher-Shannon complexity on the magnetic quantum number $m = 0, \ldots, l$, for various spherical harmonics $Y_{l,m}(\theta, \phi)$ with a fixed orbital quantum number $l = 10$ (■), 20 ($\times$), 50 (⊡) and 80 (⊙).

is,

$$C_{FR}^{(q)}[\rho_{l,m}] = \frac{1}{2\pi e} F[\rho_{l,m}] \times W_q[\rho_{l,m}]^{\frac{2}{3(1-q)}}$$
$$= \frac{1}{2\pi e} \left(4l(l+1) - 2|m|(2l+1)\right) \times W_q[\rho_{l,m}]^{\frac{2}{3(1-q)}}, \quad \text{with } q > 0. \qquad (25)$$

Let us now explore the dependence of this complexity for a given q (say e.g., $q = 2$) on the quantum parameters l and m by means of Figures 4, 5 and 6. Figure 4 represents the Fisher-Rényi complexity measure $C_{FR}^{(q)}[\rho_{l,m}]$ for $q = 2$ as a function of m for fixed values of $l = 10, 20, 50$. The most notable feature of this figure is the maximum value achieved by this complexity measure for a given value $m_0 \geq 0$ that depends on l and q. This contrasts with Figure 1, where the maximum value of the Fisher-Shannon complexity measure is achieved for $m_0 = 0$ in all the cases.

Figure 5 shows the complexity $C_{FR}^{(q)}[\rho_{l,m}]$ for $q = 2$ as a function of l for $m = 0, 1, 2, 5$. We observe the same monotonically increasing behaviour shown by the Fisher-Shannon complexity in Figure 2.

Figure 6 represents the complexity $C_{FR}^{(q)}[\rho_{l,m}]$ for $q = 2$ as a function of l for $m = l - a$, with $a = 0, 1, 2$. This figure is completely analogous to the corresponding Figure 3 for the Fisher-Shannon complexity, where the complexity measure increases monotonically as l

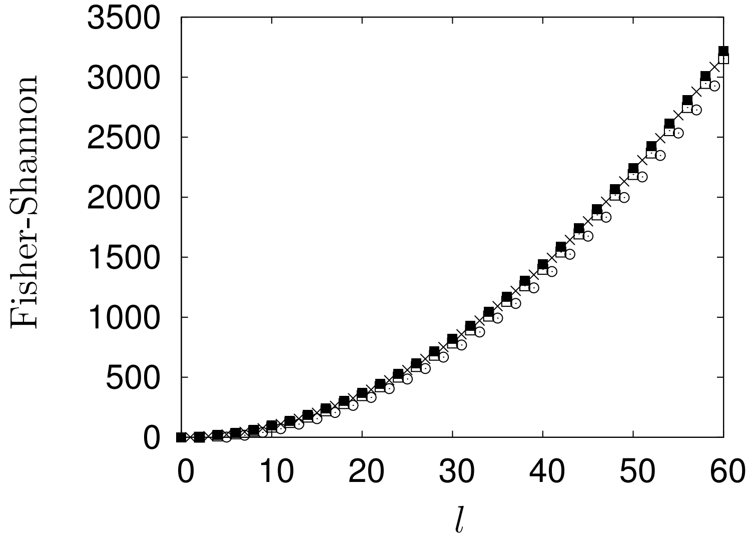

FIG. 2: Growth of the Fisher-Shannon complexity with l for various spherical harmonics $Y_{l,m}(\theta, \phi)$ for fixed $m = 0$ (■), 1 ($\times$), 2 (⊡) and 5 ($\odot$).

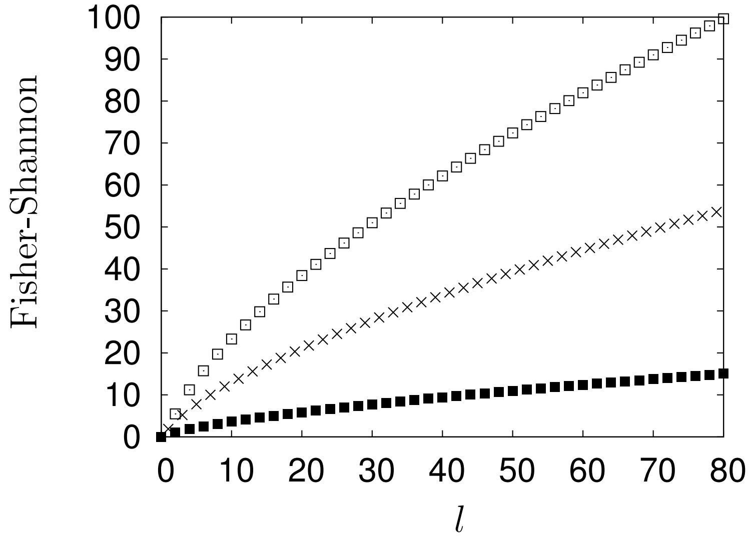

FIG. 3: Behaviour of the Fisher-Shannon complexity of the spherical harmonics $Y_{l,m}(\theta, \phi)$ with $m = l - a$, where $a = 0$ (■), 1 ($\times$) and 2 (⊡), as a function of l when l goes from a to 80.

grows.

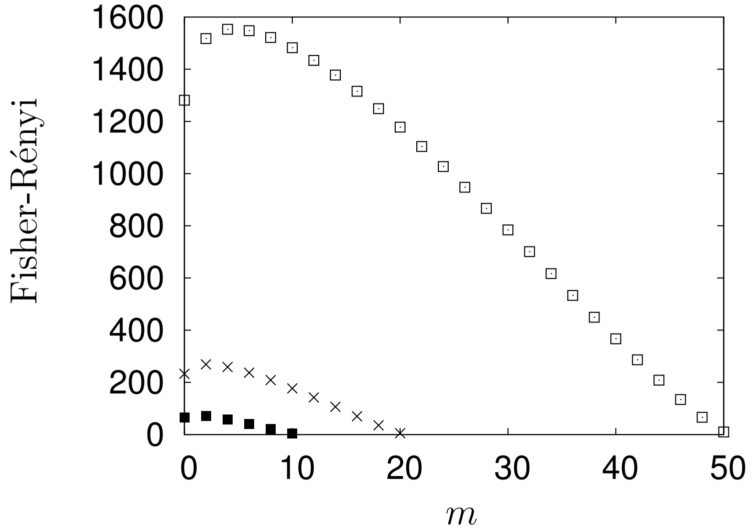

FIG. 4: Study of the Fisher-Rényi complexity measure $C_{FR}^{(2)}$ in terms of m for various spherical harmonics $Y_{l,m}(\theta,\phi)$ with fixed values of $l = 10$ (■), 20 (×) and 50 (⊡).

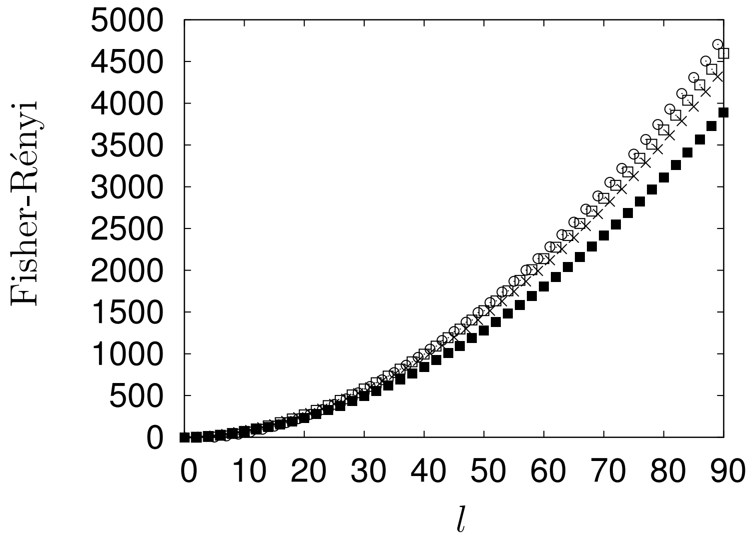

FIG. 5: Study of the Fisher-Rényi complexity measure $C_{FR}^{(2)}$ in terms of l for various spherical harmonics $Y_{l,m}(\theta,\phi)$ with fixed values of $m = 0$ (■), 1 (×), 2 (⊡) and 5 (⊙).

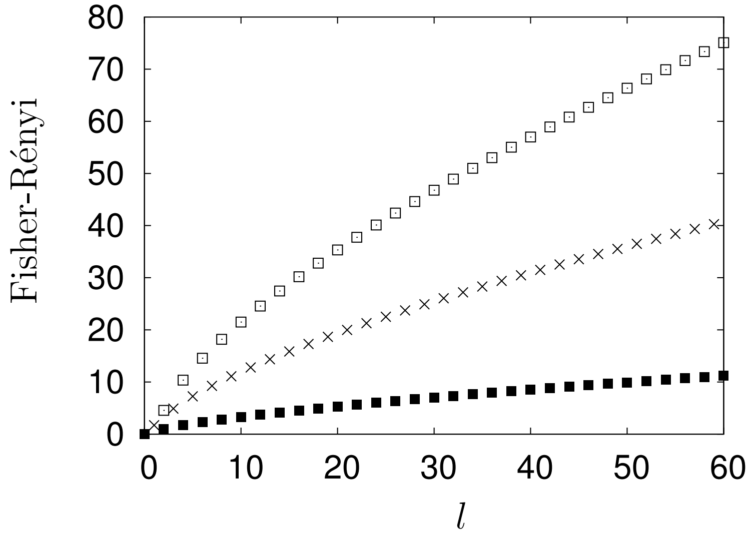

FIG. 6: Study of the Fisher-Rényi complexity measure $C_{FR}^{(2)}$ for various spherical harmonics $Y_{l,m}(\theta,\phi)$ with $m = l - a$, where $a = 0$ (■), 1 (×), and 2 (⊙), as a function of l when l goes from a to 60.

C. LMC complexity

According to Eqs. (8), (13) and (14) we have that the LMC complexity of the rotator states (l, m) is given by the expression

$$C_{LMC}[\rho_{l,m}] = W_2[\rho_{l,m}] \times e^{S[\rho_{l,m}]} \tag{26}$$

where $W_2[\rho_{l,m}]$ have been already calculated in Section III. Figure 7 shows the LMC complexity measure as a function of m and fixed values $l = 10, 20, 50, 80$. This complexity measure has a decreasing behaviour as m increases up to the position $m \sim l$ where a minimum is found and the complexity measure starts increasing.

Figure 8 shows the LMC complexity $C_{LMC}[\rho_{l,m}]$ as a function of l for fixed values $m = 0, 1, 2, 5$. For $l \gg m$ this complexity have a clear increasing behaviour. But for some cases it has a minimum when $l \sim m$. These minima correspond to those found on Figure 7. They appear when the values of l and m have similar values.

This behaviour is better explained in Figure 9, where $C_{LMC}[\rho_{l,m}]$ is represented as a function of l for $m = l - a$, with $a = 0, 1, 2$. Thus, $l \sim m$ in all the cases. We observe that for large and moderate values of l ($l \gtrsim 5$) the complexity measure is larger when $m = l$ than in the other two cases.

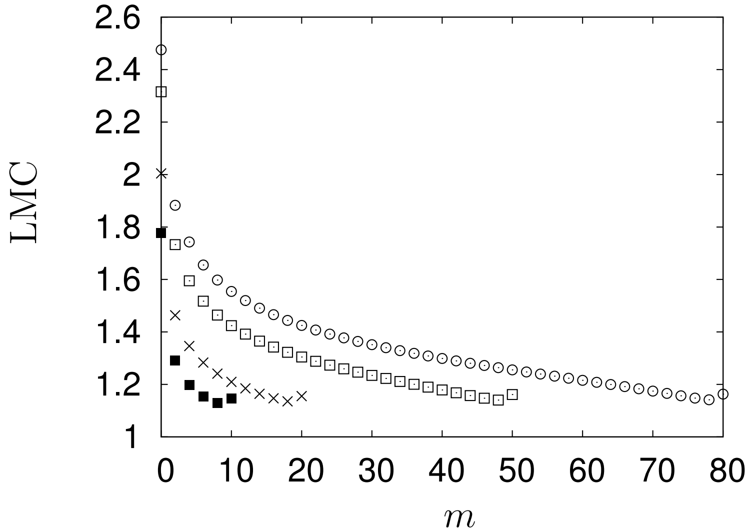

FIG. 7: Dependence of the LMC complexity measure on m for various spherical harmonics $Y_{l,m}(\theta,\phi)$ with fixed orbital quantum number $l = 10$ (■), 20 ($\times$), 50 (⊡), and 80 ($\odot$).

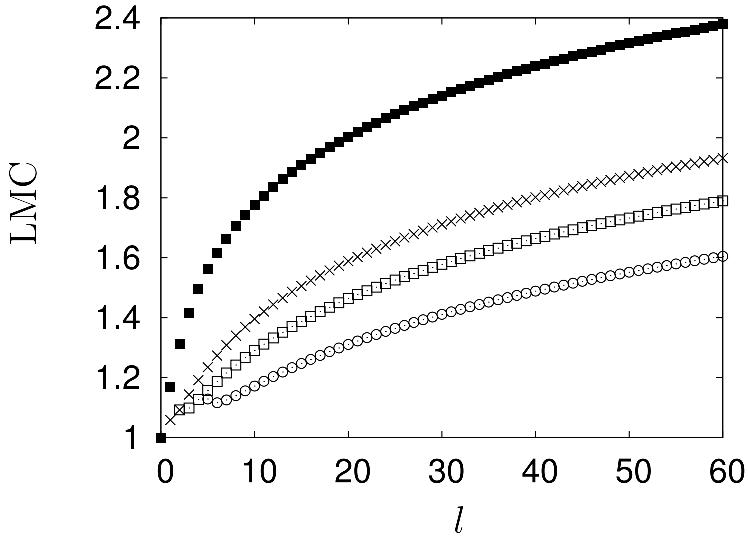

FIG. 8: Study of the LMC complexity measure as a function of l for various spherical harmonics $Y_{l,m}(\theta,\phi)$ with fixed values of $m = 0$ (■), 1 ($\times$), 2 (⊡), and 5 ($\odot$).

V. CONCLUSIONS

The rigid rotator model has been used in numerous mathematical and physical directions [13–16]; in particular it has been used to characterize the rotation of diatomic molecules

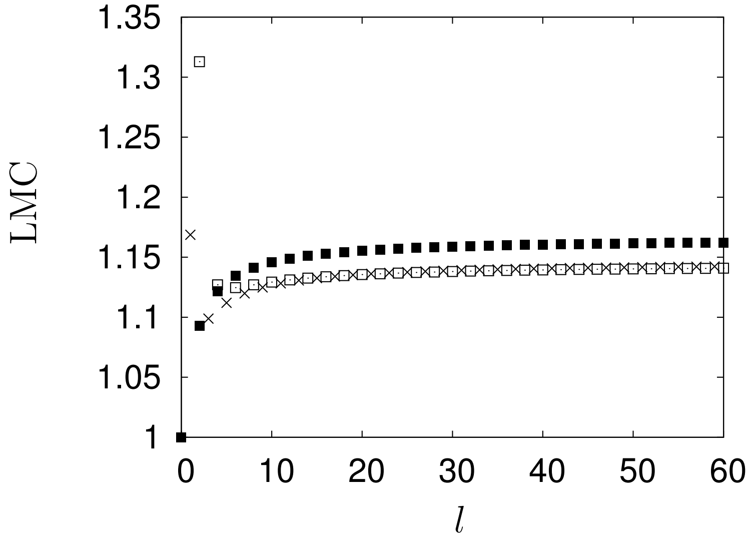

FIG. 9: Behavior of the LMC complexity measure for various spherical harmonics $Y_{l,m}(\theta, \phi)$ with $m = l - a$, where $a = 0$ (■), 1 (×), and 2 (⊡), as a function of l when l goes from a to 60.

(and is easily extended to linear polyatomic molecules), so that the entropy and complexity properties of these molecules can be referenced with respect to the corresponding rotator quantitites [46]. In this work we have investigated the entropy and complexity measures of the eigenfunctions of the D-dimensional rigid rotator model (namely, the hyperspherical functions) in terms of the dimensionality and the hyperquantum numbers which characterize them.

Since the hyperspherical harmonics describe the angular part of the stationary states of any central potential with arbitrary dimensionality, these information-theoretic quantities provide estimations for the angular anisotropy of the eigenfunctions of a central potential in the hyperspace. In other terms, they quantify the rich variety of D-dimensional geometries of the lobe-structure of the quantum states of the corresponding system (e.g., hydrogenic orbitals for the hydrogen atom), which are described by means of D integer hypernumbers (e.g., the principal, orbital and azimuthal quantum numbers n, l and m, in the three dimensional case).

Specifically, besides the explicit expression for the Fisher information, first we have found the entropic or frequency moments of the hyperspherical harmonics, which allows one to find the Rényi and Tsallis entropies of the rigid rotator in a straightforward manner. Then, we numerically study the dependence on the quantum numbers (l, m) for the complexity measures of Fisher-Shannon, Fisher-Rényi and LMC types of the spherical harmonics $Y_{l,m}(\theta, \phi)$, which are the eigenfunctions of the three-dimensional rigid rotator.

Let us highlight that the spatial complexity of the associated probability densities (24) to the spherical harmonics is clearly related to the number of lobes of their three-dimensional representations. In fact the degree of the involved Gegenbauer polynomial is connected to its number of maxima, and hence to the number of lobes, that is equal to $l - |m| + 1$; so the complexity is expected to grow as the difference $l - |m|$ increases. This behaviour is only grasped by the Fisher-Shannon complexity. Indeed the Fisher-Rényi and the LMC complexities, although follow this behaviour in most cases, show pointwise differences with respect to the Fisher-Shannon complexity. This can be seen e.g. in Figure 1, where the Fisher-Rényi measure increases with $|m|$ at low values of $|m|$. Similarly, this counterintuitive behaviour can also be seen for the LMC complexity in Figures 7 and 8 for the cases where $l \simeq |m|$. As well, this phenomena is also apparent in Figure 9 in a transparent manner, where $|m| \simeq l$ in all the cases and a clear monotonic behaviour in the plotted data is not observed. In turn, it is remarkable that the Fisher-Shannon complexity grasps the visual, intuitive complexity of the density associated to the spherical harmonics. From this point of view we can endorse this quantity as the most appropriate complexity measure in this system.

Finally, let us also point out that the entropy and complexity quantities used in this work do not only quantify the anisotropic character of the stationary states of the central potentials in any dimensionality, but they can potentially be used to visualize D-dimensional models that are becoming integral components of data processing in many fields, including medicine, chemistry, architecture, agriculture and biology over last few years. Moreover, they could be employed to carry out volumetric shape analyses which permit an evaluation of the actual structures that are implicitly represented in D-dimensional image data.

Acknowledgements

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4.5. Acotación de productos de incertidumbre y medidas de complejidad de sistemas cuánticos

Esta sección contiene el artículo siguiente:

Upper bounds on quantum uncertainty products and complexity measures.
A. Guerrero, P. Sánchez-Moreno y J. S. Dehesa
Physical Review A 84 (2011), 042105.

En este artículo se presentan cotas superiores a las medidas de información y a las medidas de complejidad. En la introducción se hacen presentes cotas inferiores para las principales medidas de complejidad (Cramér-Rao, Fisher-Shannon y LMC).

Posteriormente se hayan diversas cotas superiores tanto a los productos de incertidumbre de Shannon y Rényi como a las medidas de complejidad, en términos del producto de Heisenberg generalizado, que involucra valores esperados de los espacios de posiciones y momentos de un sistema cuántico. Se hayan cotas tanto para sistemas generales como para sistemas centrales (i.e., aquellos cuyo potencial depende únicamente de la distancia al origen).

Upper bounds on quantum uncertainty products and complexity measures

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The position-momentum Shannon and Rényi uncertainty products of general quantum systems are shown to be bounded not only from below (through the known uncertainty relations), but also from above in terms of the Heisenberg-Kennard product $\langle r^2\rangle\langle p^2\rangle$. Moreover, the Cramér-Rao, Fisher-Shannon, and López-Ruiz, Mancini, and Calbet shape measures of complexity (whose lower bounds have been recently found) are also bounded from above. The improvement of these bounds for systems subject to spherically symmetric potentials is also explicitly given. Finally, applications to hydrogenic and oscillator-like systems are done.

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I. INTRODUCTION

The uncertainty principle is a basic physico-mathematical aporia. It is not only a relevant issue in harmonic analysis [1], but also a statement of the human and technical limitations to perform measurements on a system without disturbing it [2]. Moreover, the position-momentum uncertainty principle describes a characteristic feature of quantum mechanics whose first mathematical realization is the Heisenberg-Kennard relation [2,3] based on the second-order power moment of the position and momentum probability densities $(\rho(\vec{r}),\gamma(\vec{p}))$ which characterize the quantum state of a physical system. This relation is given in atomic units $\hbar = 1$ by

$$\langle r^2\rangle\langle p^2\rangle \geqslant \tfrac{9}{4}, \tag{1}$$

valid for all quantum-mechanical states of any three-dimensional physical system. Here the symbol $\langle f(r)\rangle$ denotes the expectation value

$$\langle f(r)\rangle := \int_{\mathbb{R}^3} f(r)\rho(\vec{r})d^3r, \quad \text{with} \quad r = |\vec{r}|$$

in position space, and similarly in momentum space. Then the relation (1) was generalized for any power moments $(\langle r^a\rangle,\langle p^b\rangle)$ in the sense [4,5]

$$\langle r^a\rangle^{\frac{1}{a}}\langle p^b\rangle^{\frac{1}{b}} \geqslant \left[\frac{\pi ab}{16\Gamma\left(\frac{3}{a}\right)\Gamma\left(\frac{3}{b}\right)}\right]^{\frac{1}{3}}\left(\frac{3}{a}\right)^{\frac{1}{a}}\left(\frac{3}{b}\right)^{\frac{1}{b}}e^{1-\frac{1}{a}-\frac{1}{b}}, \tag{2}$$

valid for $a,b > 0$. See also [6] for further inequalities with moments of negative orders. For the case $a = b$ we have

$$\langle r^a\rangle\langle p^a\rangle \geqslant \left[\frac{\pi a^2}{16\Gamma^2\left(\frac{3}{a}\right)}\right]^{\frac{a}{3}}\left(\frac{3}{a}\right)^2 e^{a-2}; \quad a > 0, \tag{3}$$

which reduces to (1) when $a = 2$. However, the Heisenberg-Kennard relation is much too weak to express the uncertainty principle (see, e.g., [7,8]).

Presently it is well known that quantities based not on the position and momentum power moments $(\langle r^\alpha\rangle, \langle p^\beta\rangle)$, but instead on the frequency or entropic moments,

$$W_\alpha[\rho] := \int_{\mathbb{R}^3}[\rho(\vec{r})]^\alpha d^3r, \quad W_\beta[\gamma] := \int_{\mathbb{R}^3}[\gamma(\vec{p})]^\beta d^3p,$$

are much more appropriate and stringent uncertainty measures for quantum systems. These quantities are called information-generating functionals in other contexts [9]. The position Rényi entropy [10–12], defined as

$$R_\alpha[\rho] := \frac{1}{1-\alpha}\ln W_\alpha[\rho]; \quad 0 < \alpha < \infty; \quad \alpha \neq 1,$$

and the corresponding momentum quantity $R_\beta[\gamma]$ provide the most relevant canonical class of position and momentum uncertainty measures [13]. These quantities have been widely used in a large variety of quantum systems, phenomena, and processes, as briefly summarized in Refs. [14] and [15]. It is worth noting that the (Boltzmann-Gibbs)-Shannon entropy $S[\rho] = -\int\rho(\vec{r})\ln\rho(\vec{r})d^3r$ is the limiting case $\alpha \to 1$ of $R_\alpha[\rho]$ (see, e.g., [16]), and the Tsallis entropy [17] is a linear approximation of $R_\alpha[\rho]$ with respect to $W_\alpha[\rho]$. Moreover, uncertainty-type inequalities associated with the Shannon and Tsallis entropies have been obtained by Beckner [18] and Bialynicki-Birula–Mycielski [19], and Maassen-Uffink [20] and Rajagopal [21], respectively.

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Bialynicki-Birula [14] has shown in 2006 that the Renyi entropies satisfy the uncertainty relation

$$R_\alpha[\rho] + R_\beta[\gamma] \geqslant -\frac{\ln\left(\frac{\alpha}{\pi}\right)}{2(1-\alpha)} - \frac{\ln\left(\frac{\beta}{\pi}\right)}{2(1-\beta)}; \quad \text{with } \frac{1}{\alpha} + \frac{1}{\beta} = 2,$$

which has been extended and rewritten in 2009 by Zozor *et al.* [22] in the form

$$N_\alpha[\rho] N_\beta[\gamma] \geqslant C(\alpha,\beta), \tag{4}$$

where $N_\alpha[\rho]$ denotes the position Renyi α-entropy power [22,23]

$$N_\alpha[\rho] := \exp\left(\frac{1}{3} R_\alpha[\rho]\right) = \{W_\alpha[\rho]\}^{\frac{1}{3(1-\alpha)}} \tag{5}$$

in position space, and $N_\beta[\gamma]$ the corresponding momentum quantity. The constant $C(\alpha,\beta)$ has the value

$$C(\alpha,\beta) = 2\pi\,(2\alpha)^{\frac{1}{2(\alpha-1)}}\,(2\beta)^{\frac{1}{2(\beta-1)}}. \tag{6}$$

On the other hand, the translationally invariant Fisher information [24], defined by

$$F[\rho] := \int_{\mathbb{R}^3} \frac{[\vec{\nabla}\rho(\vec{r})]^2}{\rho(\vec{r})}\, d^3\vec{r},$$

has been shown to be a particularly useful uncertainty measure. This is because, contrary to the previous measures, it has a locality property: it is very sensitive to the fluctuations or irregularities of the position probability density of the stationary states of the quantum systems. Moreover, it has the bounds

$$\frac{81}{\langle r^2\rangle\langle p^2\rangle} \leqslant F[\rho]F[\gamma] \leqslant 16\langle r^2\rangle\langle p^2\rangle,$$

where we have used the Cramér-Rao inequalities [23]

$$F[\rho] \geqslant \frac{9}{\langle r^2\rangle}, \quad F[\gamma] \geqslant \frac{9}{\langle p^2\rangle},$$

and the Stam relation [25]

$$F[\rho] \leqslant 4\langle p^2\rangle, \quad F[\gamma] \leqslant 4\langle r^2\rangle.$$

Let us also mention, for the sake of completeness, that the Fisher information also satisfies the uncertainty relation

$$F[\rho]F[\gamma] \geqslant 36$$

for quantum systems when either the position wave function or the momentum wave function is real [26].

Furthermore, there exist some products of two single information-theoretic measures which have been shown to be most appropriate to grasp various facets of the internal disorder of quantum systems and to disentangle among their rich three-dimensional geometries: the Cramér-Rao [16,27,28], Fisher-Shannon [29–31], and López-Ruiz, Mancini, and Calbet (LMC) [32,33] complexities. These composite quantities are defined as

$$C_{CR}[\rho] = F[\rho]V[\rho] \tag{7}$$

for the Cramér-Rao complexity; as

$$C_{FS}[\rho] = F[\rho]J[\rho] = \frac{1}{2\pi e} F[\rho]N_1^2[\rho] \tag{8}$$

for the Fisher-Shannon complexity; and as

$$C_{\rm LMC}[\rho] = D[\rho]\exp(S[\rho]) = D[\rho]N_1^3[\rho] = \left[\frac{N_1[\rho]}{N_2[\rho]}\right]^3 \tag{9}$$

for the LMC shape complexity. The symbols $V[\rho]$ and $J[\rho]$ denote the variance $V[\rho] = \langle r^2\rangle - |\langle\vec{r}\rangle|^2$ and the Shannon quantity $J[\rho] = (2\pi e)^{-1}\exp(\frac{2}{3}S[\rho]) = (2\pi e)^{-1} N_1^2[\rho]$, where $N_1[\rho] = \exp(\frac{1}{3}S[\rho])$ gives the Shannon entropy power, and the disequilibrium $D[\rho] = \langle\rho\rangle = W_2[\rho] = N_2^{-3}[\rho]$ of the system. These three dimensionless two-ingredient measures of complexity, which quantify how easily a quantum system may be modeled, differ from the remaining complexities in the following properties: (i) mathematical simplicity, (ii) invariance under replication, translation, and scaling transformations, and (iii) minimal values in the two extreme cases: perfect order (i.e., for completely ordered systems, that is, when the density denotes a Dirac δ function) and perfect disorder (i.e., for completely disordered systems which have a uniform or highly spread density and an ideal gas in one and three dimensions, respectively). Moreover, they are bounded from below as

$$C_{CR}[\rho] \geqslant 9, \quad C_{FS}[\rho] \geqslant 3, \quad \text{and} \quad C_{\rm LMC}[\rho] \geqslant 1 \tag{10}$$

for general three-dimensional systems.

In this work we first highlight (see Sec. II) the connection between the Rényi- and Shannon-entropy-based uncertainty products of general quantum systems, as well as the two-ingredient measures of complexity mentioned above, with the Heisenberg-like uncertainty products $\langle r^a\rangle\langle p^b\rangle$. Then in Sec. III we show that the resulting upper bounds can be improved for systems subject to central potentials of arbitrary analytical form. Finally, these quantities are explicitly given and numerically discussed for the hydrogen atom and harmonic oscillator quantum systems in Sec. IV. Some conclusions and open problems are also given.

II. UNCERTAINTY PRODUCTS AND COMPLEXITY MEASURES FOR GENERAL SYSTEMS: UPPER BOUNDS

In this section we first study the relation of the Rényi- and Shannon-entropy-based uncertainty products with the Heisenberg-like products in general quantum systems. Then, we derive upper bounds on the Cramér-Rao, Fisher-Shannon, and LMC shape complexities in terms of Heisenberg-like products.

A. Uncertainty products

We will first show the uncertainty character of the product $N_\alpha[\rho]N_\beta[\gamma]$ of the Rényi entropy powers in position and momentum spaces via its connection with the Heisenberg-like products (1), (2), and (3). To do this we use the variational optimization procedure described in Ref. [34], subject to the constraint $\langle r^a\rangle$, $a = 1,2,\ldots$, to obtain the following lower bound to the position entropic moment $W_\alpha[\rho]$:

$$W_\alpha[\rho] \geqslant A_1(\alpha,a)\langle r^a\rangle^{-[3(\alpha-1)/a]}; \quad \alpha > 1,$$

with the constant

$$A_1(\alpha,a) = \frac{a\alpha}{(a+3)\alpha - 3} \times \left\{ \frac{a}{4\pi B\left(\frac{\alpha}{\alpha-1},\frac{3}{a}\right)} \left[\frac{3\alpha-3}{(a+3)\alpha-3}\right]^{\frac{3}{a}} \right\}^{\alpha-1},$$

where $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ denotes the β function. Similarly, we find the lower bound

$$W_\beta[\gamma] \geqslant A_1(\beta,b)\langle p^b\rangle^{-[3(\beta-1)/b]}; \quad b = 1,2,\ldots; \quad \beta > 1,$$

for the entropic moment $W_\beta[\gamma]$ of the momentum density $\gamma(\vec{p})$ in terms of the momentum expectation value $\langle p^b\rangle$.

For $\alpha < 1$ we have the following upper bound [35]:

$$W_\alpha[\rho] \leqslant \tilde{A}_1(\alpha,a)\langle r^a\rangle^{[3(1-\alpha)/a]}; \quad \alpha < 1, \quad a > 3\frac{1-\alpha}{\alpha},$$

with the constant

$$\tilde{A}_1(\alpha,a) = \frac{\alpha a}{[(a+3)\alpha-3]^\alpha} \times \left\{ \frac{\alpha a^2}{4\pi B\left(\frac{\alpha}{1-\alpha} - \frac{3}{a},\frac{3}{a}\right)} \left[\frac{3-3\alpha)}{(a+3)\alpha-3}\right]^{\frac{3}{a}} \right\}^{\alpha-1}.$$

Then, taking into account Eq. (5) we have the following upper bounds:

$$N_\alpha[\rho] \leqslant A_2(\alpha,a)\langle r^a\rangle^{1/a} \tag{11}$$

and

$$N_\beta[\gamma] \leqslant A_2(\beta,b)\langle p^b\rangle^{1/b}, \tag{12}$$

for the position and momentum Rényi entropy power, where the constant A_2 is given by

$$A_2(\alpha,a) = \begin{cases} [A_1(\alpha,a)]^{1/3(1-\alpha)}, & \alpha > 1, \\ [\tilde{A}_1(\alpha,a)]^{1/3(1-\alpha)}, & \alpha < 1. \end{cases}$$

The expression (11) extends and generalizes various inequalities of similar type obtained differently by various authors [36,37]. Then, from (11) and (12) we obtain the inequality

$$N_\alpha[\rho]N_\beta[\gamma] \leqslant A_2(\alpha,a)A_2(\beta,b)\langle r^a\rangle^{\frac{1}{a}}\langle p^b\rangle^{\frac{1}{b}}, \tag{13}$$

for $\alpha > 1, \beta > 1$, for the position-momentum Rényi products. Remark that a and $b = 1,2,3,\ldots$ In case that $a = b$, one has

$$N_\alpha[\rho]N_\beta[\gamma] \leqslant A_2(\alpha,a)A_2(\beta,a)[\langle r^a\rangle\langle p^a\rangle]^{1/a}, \tag{14}$$

for $a = 1,2,\ldots;\alpha > 1,\beta > 1$, which connects the Rényi products with the Heisenberg-like uncertainty products $\langle r^a\rangle\langle p^a\rangle$. Moreover, from Eqs. (4)–(6) and Eq. (14) with $a = 2$ one finds

$$N_\alpha[\rho]N_\beta[\gamma] \leqslant A_2(\alpha,2)A_2(\beta,2)(\langle r^2\rangle\langle p^2\rangle)^{1/2}. \tag{15}$$

To obtain the corresponding Shannon-entropy-based uncertainty products, either we carefully take the limits $\alpha \to 1$ and $\beta \to 1$ in the expressions (11), (12), (13), (14), and (15), or we start from the variational bound [38,39] on the Shannon entropy $S[\rho]$ given by

$$S[\rho] \leqslant A_3(a) + \frac{3}{a}\ln\langle r^a\rangle, \quad \forall a > 0,$$

with

$$A_3(a) = \ln\left[\frac{4\pi}{a}\Gamma\left(\frac{3}{a}\right)\left(\frac{ae}{3}\right)^{3/a}\right].$$

Then one easily obtains the following lower bound on the Shannon entropy power $N_1[\rho] = \exp(\frac{1}{3}S[\rho])$ in position space:

$$N_1[\rho] \leqslant A_4(a)\langle r^a\rangle^{1/a}, \tag{16}$$

with

$$A_4(a) = \left[\frac{4\pi}{|a|}\Gamma\left(\frac{3}{a}\right)\right]^{\frac{1}{3}}\left(\frac{ae}{3}\right)^{1/a}.$$

A similar result can be obtained for the upper bound on the momentum Shannon entropy power $N_1[\gamma]$ in terms of an arbitrary expectation value $\langle p^b\rangle$, $b > 0$. So the uncertainty product $N_1[\rho]N_1[\gamma]$ is bounded from above as

$$N_1[\rho]N_1[\gamma] \leqslant A_4(a)\,A_4(b)\,\langle r^a\rangle^{\frac{1}{a}}\,\langle p^b\rangle^{1/b}.$$

In case that $a = b$, one has that

$$N_1[\rho]N_1[\gamma] \leqslant [A_4(a)]^2\,(\langle r^a\rangle\langle p^a\rangle)^{1/a} \tag{17}$$

for $a = 1,2,\ldots$, which connects the Shannon-entropy-power-based products with the Heisenberg-like uncertainty products $\langle r^a\rangle\langle p^a\rangle$. Moreover, from Eq. (15) with ($\alpha \to 1$, $\beta \to 1$) or from Eqs. (4)–(6) with $\alpha \to 1$ and (17) with $a = 2$ we have the Shannon product

$$N_1[\rho]N_1[\gamma] \leqslant \frac{2\pi e}{3}(\langle r^2\rangle\langle p^2\rangle)^{1/2} \tag{18}$$

in terms of the Heisenberg-Kennard uncertainty relation $\langle r^2\rangle\langle p^2\rangle$.

B. Complexity measures

In Eq. (10) of Sec. I we have pointed out the lower bounds of the Cramer-Rao, Fisher-Shannon, and LMC measures of complexity. Let us now explore the upper bounds on these three measures.

1. Cramér-Rao complexity $C_{CR}[\rho]$

Taking into account its definition (7) and the Cramér-Rao inequality [i.e., the first expression in (10)], the Stam relation $F[\rho] \leqslant 4\langle p^2\rangle$, and that $V[\rho] \leqslant \langle r^2\rangle$, one obtains that the Cramér-Rao complexity is bounded from both sides as

$$9 \leqslant C_{CR}[\rho] \leqslant 4\langle r^2\rangle\langle p^2\rangle. \tag{19}$$

2. Fisher-Shannon complexity $C_{FS}[\rho]$

Let us start with its definition (8). Taking into account the Stam relation $F[\rho] \leqslant 4\langle p^2\rangle$ and the upper bound $N_1[\rho] \leqslant (\frac{2\pi e}{3}\langle r^2\rangle)^{1/2}$ on the Shannon power entropy previously mentioned, we obtain the upper bound $C_{FS}[\rho] \leqslant \frac{4}{3}\langle r^2\rangle\langle p^2\rangle$ on the Fisher-Shannon complexity. This result together with the lower bound (10) allows us to write the following chain of inequalities:

$$3 \leqslant C_{FS}[\rho] \leqslant \tfrac{4}{3}\langle r^2\rangle\langle p^2\rangle. \tag{20}$$

3. LMC shape complexity $C_{\rm LMC}[\rho]$

From its definition (9) one has that

$$C_{\rm LMC}[\rho] = D[\rho]N_1^3[\rho].$$

Now, taking into account that $N_1^3[\rho] \leqslant (\frac{2\pi e}{3}\langle r^2\rangle)^{3/2}$ because of Eq. (16), and the Gadre-Chakraborty inequality for the disequilibrium [40]

$$D[\rho] \leqslant \frac{4}{3\sqrt{3}\pi^2}\langle p^2\rangle^{3/2}, \tag{21}$$

one obtains the upper bound

$$1 \leqslant C_{\rm LMC}[\rho] \leqslant \frac{2^{7/2}}{3^3\sqrt{\pi}}\, e^{3/2}(\langle r^2\rangle\langle p^2\rangle)^{3/2}. \tag{22}$$

We know from the very beginning that the upper bound (21) on the disequilibrium is not so accurate because it is the result of two concatenated general inequalities (namely, Cauchy-Schwarz and Sobolev) [40,41]. Consequently, the upper bound in Eq. (22) is poor; nevertheless, it is the only existing one to the best of our knowledge.

III. UNCERTAINTY PRODUCTS AND COMPLEXITY MEASURES FOR CENTRAL POTENTIALS: UPPER BOUNDS

In this section we study the improvement of the upper bounds on the uncertainty products and complexity measures found in the previous section, when the potential of the quantum system is spherically symmetric.

A. Uncertainty products

Let us first improve the inequality (15) between the Rényi-entropy-based product $N_\alpha[\rho]N_\beta[\gamma]$ and the Heisenberg product $\langle r^2\rangle\langle p^2\rangle$ for central potentials.

The stationary states of a single-particle system in a spherically symmetric potential $V(r)$ are known to be described by the wave functions

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

which are characterized through the quantum numbers (n,l,m), where the principal quantum number $n = 0,1,\ldots$, the orbital quantum number $l = 0,1,\ldots$, and the magnetic quantum number $m = -l,-l+1,\ldots,l-1,l$. The angular part is given by the well-known spherical harmonics $Y_{lm}(\theta,\phi)$, and the radial part $R_{nl}(r)$ depends on the analytical form of the potential.

Recently, Sánchez-Moreno *et al.* [42] have used a variational method to bound the Rényi entropy $N_\alpha[\rho]$ with the covariance matrix as a constraint. They found that

$$N_\alpha[\rho] \leqslant B(l,m)\, A_2(\alpha,2)\,\langle r^2\rangle^{1/2} \tag{23}$$

with

$$B(l,m) = \sqrt{3}\left(\frac{2l(l+1)-2m^2-1}{4l(l+1)-3}\right)^{1/6} \times \left(\frac{l(l+1)+m^2-1}{4l(l+1)-3}\right)^{1/3}.$$

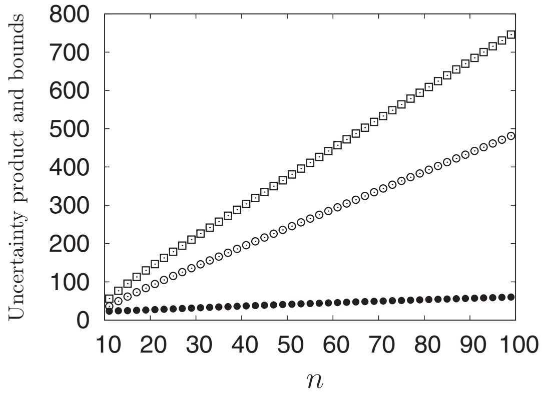

FIG. 1. Uncertainty product $N_2[\rho]N_2[\gamma]$ (•), central upper bound (⊙), and general upper bound (⊡), with $\alpha = \beta = 2$, for the states of the hydrogen atom with quantum numbers $l = m = 10$, as a function of the principal quantum number n, for $n = 11$–100.

It is worth noting that $B(0,0) = 1$. Moreover, $B(l,m) \leqslant 1$ so that the bound (23) is lower (so, better) than the bound given by Eq. (11) with $a = 2$.

By working in momentum space we can obtain a similar bound for the momentum Rényi entropy $N_\beta[\gamma]$ in terms of the expectation value $\langle p^2\rangle$. Then, we can obtain in a straightforward manner the following inequality between the Rényi-entropy-based and Heisenberg uncertainty products:

$$N_\alpha[\rho]N_\beta[\gamma] \leqslant [B(l,m)]^2\, A_2(\alpha,2)\, A_2(\beta,2)\,(\langle r^2\rangle\langle p^2\rangle)^{1/2}. \tag{24}$$

Now, let us show the improvement of the upper bound (18) on the Shannon-entropy-based uncertainty product $N_1[\rho]N_1[\gamma]$ for the central potentials. This is obtained either by taking the limit $\alpha \to 1$ in expressions (23) and (24) or by using the corresponding variational result [42]. The former one yields the value

$$N_1[\rho] \leqslant \left(\frac{2\pi e}{3}\right)^{1/2} B(l,m)\,\langle r^2\rangle^{1/2} \tag{25}$$

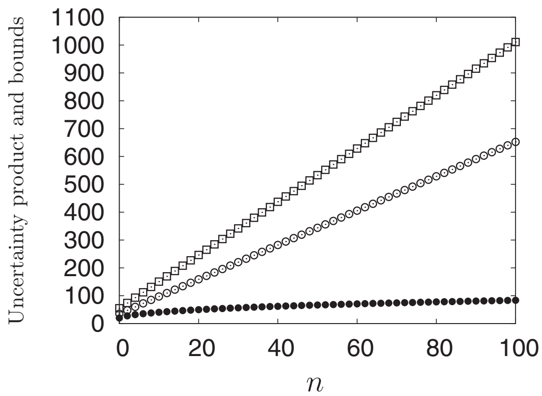

FIG. 2. Uncertainty product $N_2[\rho]N_2[\gamma]$ (•), central upper bound (⊙), and general upper bound (⊡), with $\alpha = \beta = 2$, for the states of the harmonic oscillator with quantum numbers $l = m = 10$, as a function of the principal quantum number n, for $n = 0$ to 100.

for the upper bound on the Shannon entropy power $N_1[\rho]$. And from Eq. (24) one obtains the inequality

$$N_1[\rho]N_1[\gamma] \leqslant \frac{2\pi e}{3}[B(l,m)]^2(\langle r^2\rangle\langle p^2\rangle)^{1/2},$$

which improves the general upper bound (18) because $B(l,m) \leqslant 1$.

B. Complexity measures

Here we improve for central potentials the upper bounds on the Cramer-Rao, Fisher-Shannon, and LMC measures of complexity given in Eqs. (19), (20), and (22), respectively.

1. Cramer-Rao complexity $C_{CR}[\rho]$

Since, for central potentials, the variance is $V[\rho] = \langle r^2\rangle$ and the Fisher information is given [43] as

$$F[\rho] = 4\langle p^2\rangle - 2(2l+1)|m|\langle r^{-2}\rangle, \tag{26}$$

one has the following exact value,

$$C_{CR}[\rho] = 4\langle p^2\rangle\langle r^2\rangle - 2(2l+1)|m|\langle r^{-2}\rangle\langle r^2\rangle, \tag{27}$$

for the Cramer-Rao complexity of physical systems with central potentials, as a function of the expectation values $\langle p^2\rangle$, $\langle r^2\rangle$, and $\langle r^{-2}\rangle$. Notice that for $m = 0$, this expression reduces to $C_{CR}[\rho] = 4\langle p^2\rangle\langle r^2\rangle$. Thus these states saturate the previous general upper bound (19).

2. Fisher-Shannon complexity $C_{FS}[\rho]$

The combination of its definition (8) with the inequality (25) for the Shannon entropy power and the exact expression (26) of the Fisher information for central potentials, yields the upper bound

$$C_{FS} \leqslant \tfrac{1}{3}[4\langle p^2\rangle\langle r^2\rangle - 2(2l+1)|m|\langle r^{-2}\rangle\langle r^2\rangle]\,[B(l,m)]^2 \tag{28}$$

on the Fisher-Shannon complexity of the central potentials, which clearly improves the general upper bound $\frac{4}{3}\langle r^2\rangle\langle p^2\rangle$ of Eq. (20).

3. LMC shape complexity $C_{\mathrm{LMC}}[\rho]$

From the definition (9) and the inequality (25) for the Shannon entropy power $N_1[\rho]$ of central potentials one has that

$$C_{\mathrm{LMC}}[\rho] = D[\rho]N_1^3[\rho] \leqslant \left(\frac{2\pi e}{3}\right)^{3/2}[B(l,m)]^3\, D[\rho]\,\langle r^2\rangle^{3/2}.$$

On the other hand, we have the general inequality (21) that allows us to find the upper bound

$$C_{\mathrm{LMC}}[\rho] \leqslant \frac{1}{3^3}\left(\frac{2^7e^3}{\pi}\right)^{1/2}[B(l,m)]^3\,(\langle r^2\rangle\langle p^2\rangle)^{3/2} \tag{29}$$

on the LMC complexity of central potentials. It is worth emphasizing that this inequality, which certainly improves the generalized upper bound, can be more refined, provided that we improve for central potentials the inequality (21) of the disequilibrium $D[\rho]$.

IV. APPLICATION TO HYDROGENIC AND OSCILLATOR-LIKE SYSTEMS

In this section we examine the improvement of the general upper bounds on the uncertainty Rényi product and the complexity measures studied in Sec. II by the inclusion of the spherical symmetry (see Sec. III). This is done by comparing the bounds on the uncertainty product and on the complexity measures found in Sec. III for central systems, with respect to the corresponding ones described in Sec. II for general systems. We study these bounds in the two main prototype systems in quantum physics [44]: the hydrogen atom, characterized by the Coulomb potential $V(r) = -\frac{1}{r}$, and the harmonic oscillator, characterized by the potential $V(r) = \frac{1}{2}r^2$. Specifically, we consider the bounds described by the inequalities (15), (19), (20), and (22) for general systems, and (24), (27), (28), and (29) for central systems. Notice that all these bounds are expressed in terms of the expectation values $\langle r^2\rangle$, $\langle p^2\rangle$, and $\langle r^{-2}\rangle$. These expectation values have the expressions

$$\langle r^2\rangle = \frac{n^2}{2}[5n^2 - 3l(l+1)+1],$$
$$\langle p^2\rangle = \frac{1}{n^2}, \quad \langle r^{-2}\rangle = \frac{2}{n^3}\frac{1}{2l+1},$$

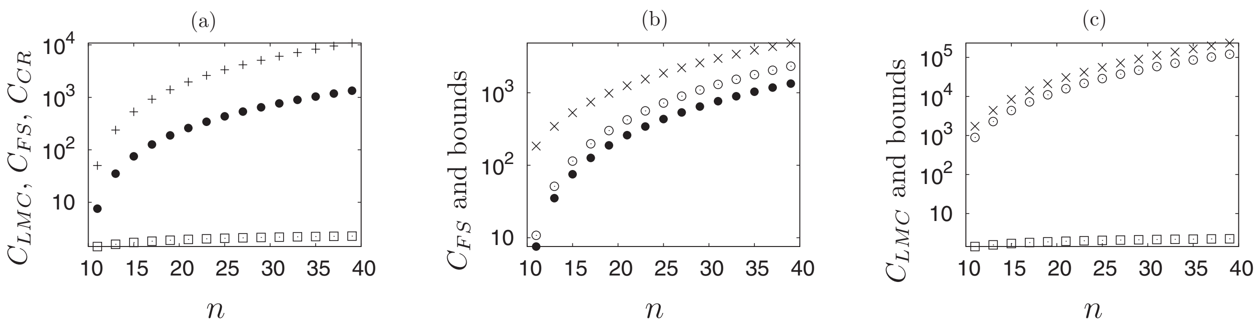

FIG. 3. (a) Cramer-Rao (+), Fisher-Shannon (•), and LMC (⊡) complexity measures. (b) Fisher-Shannon complexity measure (•), central upper bound (⊙), and general upper bound (×). (c) LMC complexity measure (⊡), central upper bound (⊙), and general upper bound (×). All the quantities are plotted for the states of the hydrogen atom with $l = m = 10$ from $n = 11$ to 40.

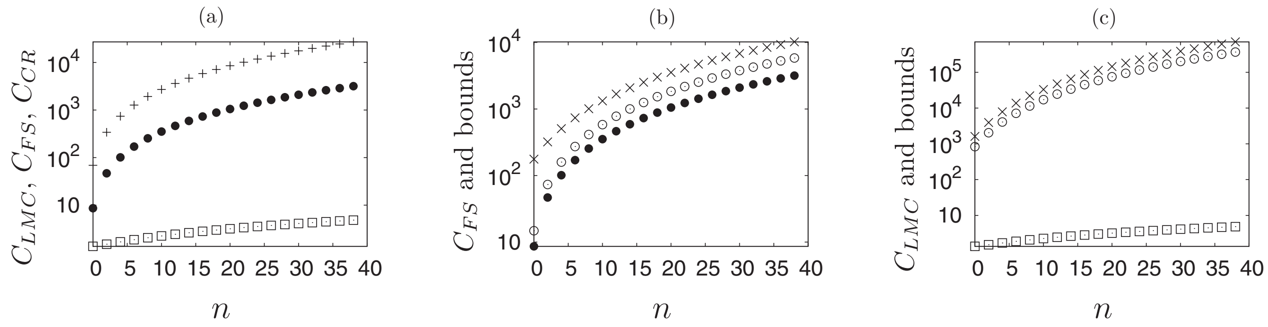

FIG. 4. (a) Cramer-Rao (+), Fisher-Shannon (•), and LMC (⊡) complexity measures. (b) Fisher-Shannon complexity measure (•), central upper bound (⊙), and general upper bound (×). (c) LMC complexity measure (⊡), upper bound for central systems (⊙), and general upper bound (×). All the quantities are plotted for the states of the harmonic oscillator with $l = m = 10$ from $n = 0$ to 40.

for the hydrogen atom, and

$$\langle r^2\rangle = \langle p^2\rangle = 2n + l + \frac{3}{2}, \quad \langle r^{-2}\rangle = \frac{2}{2l+1},$$

for the harmonic oscillator. With these expressions we can calculate the upper bounds of the hydrogen and the oscillator systems on the uncertainty Rényi product and the Cramer-Rao, Fisher-Shannon, and LMC complexities, valid for general and central systems.

First, we study the dependence on n with (l,m) fixed. Figure 1 shows the exact value of the uncertainty product $N_2[\rho]N_2[\gamma]$ (•), the upper bound for central systems given by (24) (⊙), and the general upper bound described in (15) (⊡), with $\alpha = \beta = 2$ for the states of the hydrogen atom, and with quantum numbers $l = m = 10$ as a function of the principal quantum number n for $n = 11 - 100$. Figure 2 shows the same quantities for the harmonic oscillator states with quantum numbers $l = m = 10$ as a function of n for $n = 0 - 100$. In both figures we can see how the upper bound for central systems represents a significant improvement with respect to the general upper bound. Nevertheless, notice that there is still room for much sharper bounds.

Figure 3(a) shows the exact value of the hydrogenic Cramer-Rao (+), Fisher-Shannon (•), and LMC (⊡) complexity measures as a function of the principal quantum number n when $l = m = 10$. Figures 3(b) and 3(c) show the exact values of the hydrogenic Fisher-Shannon (•) and LMC (⊡) complexity measures, respectively, together with their upper bounds for central systems (⊙), and their general upper bounds (×) as a function of the principal quantum number n when $l = m = 10$. Figures 4(a)–4(c) represent the same quantities for the harmonic oscillator states with $l = m = 10$.

The three complexity measures increase with n, since the spreading and the oscillatory behavior of these densities grows with n, both for the hydrogen atom and the harmonic oscillator. Furthermore, in Figs. 3(b) and 4(b) we see that for the Fisher-Shannon complexity, the central upper bound is much sharper than the general bound. This is not the case for the LMC complexity measure, whose bounds, as seen in Figs. 3(c) and 4(c), are relatively far from the exact value, mainly because the upper bound of one of its ingredients (the disequilibrium) has not yet been improved for central potentials.

Second, we study the dependence on l with (n,m) fixed. Figures 5 and 6 represent the same quantities as in Figs. 3 and 4 for the hydrogen atom and the harmonic oscillator, respectively. In Fig. 5 the quantities are given for the hydrogen atom states with $n = 20$ and $m = 0$ as a function of l. Figure 6 shows these quantities for the harmonic oscillator states with $n = m = 0$ as a function of l. In the hydrogen atom case, as shown in Fig. 5(a), the Cramer-Rao and the Fisher-Shannon complexities have a decreasing behavior as l increases. This indicates that the complexity of the density is lower for the states with higher values of l, from the point of view of these measures. However, the LMC complexity

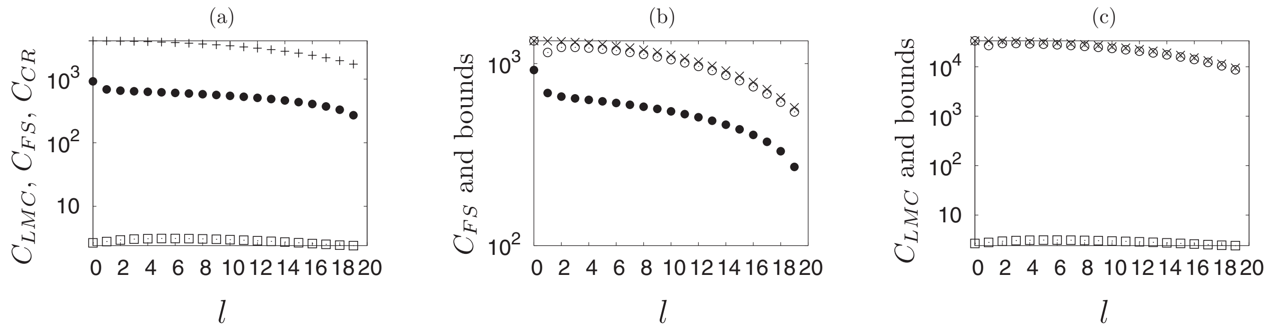

FIG. 5. (a) Cramer-Rao (+), Fisher-Shannon (•), and LMC (⊡) complexity measures. (b) Fisher-Shannon complexity measure (•), central upper bound (⊙), and general upper bound (×). (c) LMC complexity measure (⊡), upper bound for central systems (⊙), and general upper bound (×). All the quantities are plotted for the states of the hydrogen atom with $n = 20$ and $m = 0$ from $l = 0$ to 19.

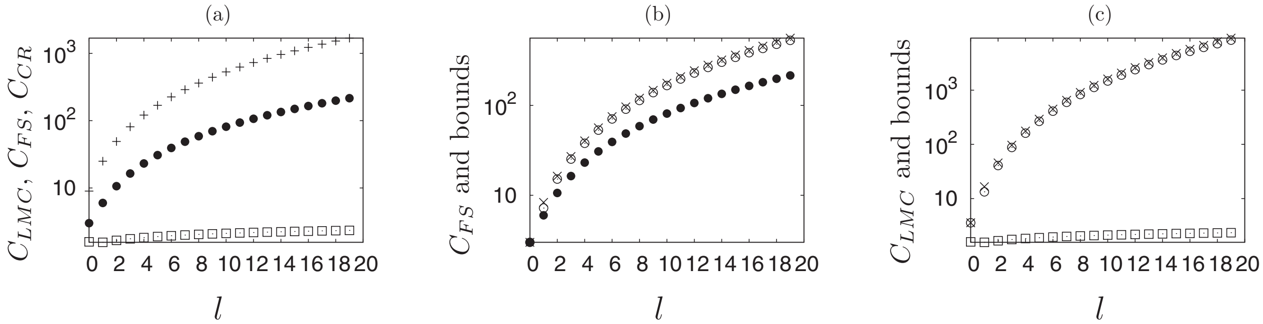

FIG. 6. (a) Cramer-Rao (+), Fisher-Shannon (•), and LMC (⊡) complexity measures. (b) Fisher-Shannon complexity measure (•), central upper bound (⊙), and general upper bound (×). (c) LMC complexity measure (⊡), upper bound for central systems (⊙), and general upper bound (×). All the quantities are plotted for the states of the harmonic oscillator with $n = 0$ and $m = 0$ from $l = 0$ to 19.

shows an increasing behavior for low values of l, which indicates a lower complexity for values of l near 0 for this complexity measure. For the harmonic oscillator, all the complexity measures have an increasing behaviour with l. The reason is that the oscillatory behavior of the density, and hence its complexity, increases with l, as well as with n, for this system. Figures 5(b) and 5(c), and 4(b) and 4(c), show the Fisher-Shannon and LMC complexity measures for the hydrogen atom and harmonic oscillator, respectively, together with the central and general upper bounds. We can clearly see in these figures the improvement of the bound for central potentials. However, this improvement is very small, especially for the LMC complexity for the aforementioned reason.

V. CONCLUSIONS

In this paper we first highlight the uncertainty character of the product of the Rényi entropy powers of position and momentum spaces by showing its inequality-based relationship with the Heisenberg-like uncertainty products. Then the Cramer-Rao, Fisher-Shannon, and LMC complexity measures are shown to be upper-bounded by the Heisenberg-Kennard product. Later on, the resulting bounds are improved for arbitrary spherically symmetric (i.e., central) potentials. Finally, the accuracy of all these bounds is studied in various states of the hydrogenic and oscillator-like systems. In summary, we observe that the inclusion of spherical symmetry considerably improves the general upper bounds found on the Shannon and Rényi uncertainty product as well as on the three complexity measures.

ACKNOWLEDGMENTS

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Conclusiones y problemas abiertos

En esta tesis se estudian las propiedades teórico-informacionales de los polinomios ortogonales hipergeométricos y de los armónicos hiperesféricos. Estas propiedades corresponden a las medidas entrópicas y a las medidas de complejidad intrínseca de la densidad de Rakhmanov de (o densidad de probabilidad asociada a) tales funciones especiales de la matemática aplicada. Estas magnitudes cuantifican el esparcimiento o distribución de dichas funciones en su dominio soporte desde la perspectiva de la Teoría de la Información; o sea, mas allá de la desviación estándar y de sus generalizaciones basadas en los momentos ordinarios de orden arbitrario. Las magnitudes teórico-informacionales de los polinomios ortogonales se expresan en términos de los momentos de frecuencia o momentos entrópicos de su densidad de Rakhmanov, que son funcionales integrales de tipo potencia de dicha densidad (y, por tanto, estrechamente relacionados con las normas L_p de tales funciones).

Los contenidos de esta tesis están en gran medida inspirados por las ideas y el enfoque empleado por Leonhard Euler [22] en sus trabajos para profundizar en el conocimiento de las funciones matemáticas. Euler introdujo, analizó y aplicó en distintas direcciones muchos conceptos extraídos de la Física (e.g., energía mutua, potencial logarítmico, electrostática de ceros,...) que han contribuido poderosamente al desarrollo de lo que ahora se entiende en matemática aplicada por teoría de funciones especiales, teoría de aproximación y teoría de potencial. En este trabajo se introducen, analizan y aplican conceptos y técnicas extraídos de la Teoría de la Información para aumentar el (ya de por sí, enorme) caudal de conocimientos de que se dispone actualmente sobre los polinomios ortogonales hipergeométricos [2, 7, 21, 47, 57–59, 78] y los armónicos esféricos [8–11, 26, 55]. Su interés y relevancia no son solo de carácter fundamental en matemática aplicada (dado que las nuevas medidas consideradas en esta tesis describen aspectos de las funciones especiales no contemplados hasta ahora), sino también de carácter aplicado: las magnitudes teórico-informacionales de estas funciones especiales están estrechamente relacionados con las entropías físicas y las medidas de complejidad que describen y cuantifican el desorden interno (y por ende, las propiedades macroscópicas) de los sistemas cuánticos. Esto se debe a que los polinomios ortogonales hipergeométricos y los armónicos esféricos controlan las funciones de onda que caracterizan los estados mecano-cuánticamente permitidos de la mayoría de los sistemas físicos cuyas ecuaciones de movimiento fundamentales (ecuaciones de Schrödinger y Dirac) son exacta o cuasi-exactamente resolubles.

A continuación se describen brevemente las conclusiones principales de este trabajo y algunos problemas abiertos encontrados.

1. Se han estudiado tanto analítica como numéricamente las longitudes entrópicas de Fisher, Rényi y Shannon de las tres familias canónicas de los polinomios ortogonales hipergeométricos (Hermite, Laguerre y Jacobi) en términos del grado n y de los parámetros que caracterizan su función peso. Estas magnitudes permiten cuantificar diferentes as-

pectos del esparcimiento de tales polinomios a lo largo de su intervalo de ortogonalidad, más allá de los que proporcionan la simple desviación estándar y los momentos ordinarios (que dependen de un punto específico del intervalo, bien sea el centroide o el origen). Se han encontrado expresiones cerradas y simples para, no solo la desviación estándar y los momentos ordinarios, sino también para la longitud entrópica de Fisher. Para la longitud entrópica de Rényi hemos encontrado dos algoritmos diferentes de cálculo: uno basado en los polinomios de Bell, de uso frecuente en Combinatoria, y otro basado en las funciones hipergeométricas generalizadas de Lauricela y Srivastava-Daoust. La longitud entrópica de Shannon no se deja calcular analíticamente debido a su carácter de funcional logarítmico de los polinomios, por lo que nos hemos limitado a su acotación por medios variacionales y teórico-informacionales, analizándose la precisión numérica de las cotas resultantes.
Una continuación natural de gran interés sería la determinación de las longitudes entrópicas de todos los polinomios ortogonales de la tabla de Askey, incluyendo el sistema más general que engloba a los polinomios de Askey-Wilson [49].

2. Se han obtenido las expresiones de las normas L_q (así como los momentos entrópicos y las entropías de Rényi) de los polinomios ortogonales hipergeométricos, incluyendo los polinomios de Hermite generalizados, por medio de ciertas funciones especiales de tipo Lauricella y Srivastava-Daoust de $2q$ variables evaluadas en algunos valores específicos de dichas variables.
Estas expresiones abren la posibilidad de generar una técnica alternativa a los métodos más sofisticados de Riemann-Hilbert y Tulyakov, para la determinación de la asintótica de estas tres magnitudes matemáticas teórico-informacionales cuando el grado n de los polinomios se hace grande o muy grande, por medio de la obtención de la asintótica concomitante de las funciones hipergeométricas multivariadas antes mencionadas para grandes valores de sus parámetros. El cálculo de las normas L_q y las entropías de Rényi R_q, $q > 0$ para grandes valores de n no solo tiene un interés matemático *per se* sino que también presenta aplicaciones físicas interesantes, dado que su resolución permitiría determinar los valores exactos de varias propiedades fundamentales y/o experimentalmente accesibles de los estados Rydberg o estados altamente excitados de los sistemas atómicos o moleculares.

3. Se ha determinado la asintótica de las normas L_q de los polinomios de Hermite, Laguerre y Jacobi de grado n cuando $q \to \infty$, mediante el método de Laplace. Y se han analizado las propiedades de monotonía de estas normas. Asimismo se ha llevado a cabo un estudio numérico exhaustivo de la asintótica de todos los polinomios ortogonales clásicos. La extensión de estos resultados a otros polinomios ortogonales de tipo hipergeométrico en variable continua [49] y a los polinomios ortogonales clásicos en variable discreta son problemas abiertos cuya resolución sería de gran interés no solo desde un punto de vista matemático sino también en otros campos científicos, particularmente en mecánica cuántica. Ha de mencionarse inmediatamente que los únicos resultados de este tipo publicados hasta ahora son los correspondientes a los polinomios de Charlier y Meixner [48, 50].

4. Se han calculado y discutido varias nociones de complejidad de los polinomios ortogonales hipergeométricos, que fueron inicialmente introducidas en la descripción mecano-cuántica de los sistemas atómicos y moleculares y de varios procesos físico-químicos. Se han estudiado analítica y numéricamente las medidas de complejidad de Cramér-Rao, Fisher-Shannon y LMC de la densidad de probabilidad de Rakhmanov de los polinomios de Hermite, Laguerre y Jacobi en términos del grado n y de los parámetros que caracterizan la función peso de tales polinomios. Se ha obtenido, en particular, la expresión explícita de la complejidad de Cramér-Rao y las expresiones asintóticas para las medidas de Fisher-Shannon y LMC. Y se pone de manifiesto la necesidad de avanzar en el problema de la reducción a

funciones mas simples de las funciones hipergeométricas generalizadas de tipo Lauricella y Srivastava-Daoust para poder profundizar en el conocimiento de las medidas de complejidad polinómicas antes mencionadas.

5. Se ha estudiado tanto analítica como numéricamente una batería de medidas teórico-informacionales de los armónicos hiperesféricos constituida por los momentos entrópicos, las medidas entrópicas y las medidas de complejidad. Para ello ha sido de gran ayuda la estrecha relación existente entre los armónicos hiperesféricos y los polinomios ortogonales hipergeométricos de tipo Gegenbauer. Esto ha permitido la determinación de las correspondientes magnitudes de uno de los prototipos físicos más utilizados en la descripción e interpretación de múltiples propiedades de los sistemas moleculares; a saber, el rotador rígido. En esta tesis se han investigado los valores de entropía y complejidad de las funciones de onda (que están controladas por los armónicos hiperesféricos) en D dimensiones en términos de la dimensión y los números hipercuánticos del estado del sistema. Se ha obtenido, en particular, la expresión explícita tanto para la información de Fisher como para los momentos entrópicos y las entropías de tipo Rényi. Dado que los armónicos hiperesféricos describen la parte angular de los estados estacionarios de cualquier potencial central en dimensión arbitraria D, las medidas teórico-informacionales aquí consideradas permiten cuantificar la anisotropía angular de las funciones de onda no solo del rotador rígido sino de cualquier otro sistema multidimensional sujeto a un potencial central. Es decir, estas medidas cuantifican de diversas formas la estructura geométrica de los estados cuánticos del correspondiente sistema.

6. Finalmente, se han analizado y comparado relativamente entre sí las medidas de complejidad y algunos productos de incertidumbre de sistemas cuánticos arbitrarios. En particular, se han encontrado cotas superiores a las medidas de complejidad de Cramér-Rao, Fisher-Shannon y LMC en términos del producto de incertidumbre de Heisenberg. Y se ha mostrado numéricamente la precisión de estas cotas en varios potenciales centrales específicos de tipo coulombiano y de tipo armónico. Se ha mostrado, por último, que la consideración de la simetría esférica en el potencial del sistema mejora sustancialmente las cotas en todos los casos.

Apéndice A

Polinomios ortogonales hipergeométricos: propiedades básicas

Los polinomios ortogonales hipergeométricos $y_n(x)$ son las soluciones polinómicas de la ecuación diferencial de tipo hipergeométrico [58]

$$\sigma(x)\, y''(x) + \tau(x)\, y'(x) + \lambda\, y(x) = 0, \tag{A.1}$$

donde $\sigma(x)$ es un polinomio de grado menor o igual a 2, $\tau(x)$ es un polinomio de grado menor o igual a 1 y λ es una constante que satisface la condición

$$\lambda = \lambda_n = -n\, \tau'(x) - \frac{n(n-1)}{2}\, \sigma''(x), \tag{A.2}$$

donde $n = 0, 1, 2, \ldots$ es un número natural. Estas funciones polinómicas $y_n(x)$ pueden escribirse à la Rodrigues [58]

$$y_n(x) = \frac{B_n}{\omega(x)} \frac{d^n}{dx^n} \left[\sigma^n(x)\, \omega(x)\right], \tag{A.3}$$

donde B_n es una constante y $\omega(x)$ es la función peso que verifica la ecuación de Pearson

$$\left[\sigma(x)\, \omega(x)\right]' = \tau(x)\, \omega(x). \tag{A.4}$$

Existen tres familias canónicas de polinomios ortogonales hipergeométricos reales (a saber, los polinomios de Hermite, Laguerre y Jacobi) que satisfacen las ecuaciones (A.1)-(A.4) con los parámetros que recoge la Tabla A.1. Estas funciones $y_n(x)$ verifican una serie de propiedades algebraicas que, aunque conocidas en la literatura, señalamos aquí por completitud: ecuación diferencial de segundo orden, fórmula de Rodrigues, ortogonalidad, relación de recurrencia a tres términos, desarrollo en serie de potencias, relaciones de inversión y momentos ordinarios.

- Ecuación diferencial de segundo orden y fórmula de Rodrigues

  - Hermite $H_n(x)$:
    $\omega(x) = e^{-x^2}$, $\sigma(x) = 1$, $\tau(x) = -2x$, $\lambda_n = 2n$.
    La ecuación diferencial resultante es

$$H_n''(x) - 2x\, H_n'(x) + 2n\, H_n(x) = 0, \tag{A.5}$$

	Hermite $H_n(x)$	Laguerre $L_n^{(\alpha)}(x)$	Jacobi $P_n^{(\alpha,\beta)}(x)$
$\sigma(x)$	1	x	$1-x^2$
$\tau(x)$	$-2x$	$1+\alpha-x$	$-(\alpha+\beta+2)x+\beta-\alpha$
λ_n	$2n$	n	$n(n+\alpha+\beta+1)$
B_n	$(-1)^n$	$1/n!$	$(-1)^n/(2^n\, n!)$
$\omega(x)$	e^{-x^2}	$x^\alpha e^{-x}$	$(1-x)^\alpha(1+x)^\beta$

Tabla A.1: Parámetros de los polinomios ortogonales hipergeométricos.

y la correspondiente fórmula de Rodrigues con $B_n = (-1)^n$ es

$$H_n(x) = (-1)^n \frac{d^n}{dx^n}\left[e^{-x^2}\right]. \tag{A.6}$$

- Laguerre $L_n^{(\alpha)}(x)$:
$\omega(x) = x^\alpha\, e^{-x}$, $\sigma(x) = x$, $\tau(x) = -x+\alpha+1$, $\lambda_n = n$.
La ecuación diferencial resultante es

$$x\left[L_n^{(\alpha)}(x)\right]'' + (\alpha+1-x)\left[L_n^{(\alpha)}(x)\right]' + n\left[L_n^{(\alpha)}(x)\right] = 0, \tag{A.7}$$

y la fórmula de Rodrigues con $B_n = \frac{1}{n!}$ correspondiente es

$$L_n^{(\alpha)}(x) = \frac{1}{n!}\, e^x\, x^{-\alpha} \frac{d^n}{dx^n}\left[x^{\alpha+n}\, e^{-x}\right]. \tag{A.8}$$

- Jacobi $P_n^{(\alpha,\beta)}(x)$:
$\omega(x) = (1-x)^\alpha(1+x)^\beta$, $\sigma(x) = 1-x^2$, $\tau(x) = -(\alpha+\beta+2)x+\beta-\alpha$, $\lambda_n = n(n+\alpha+\beta+1)$.
La fórmula de Rodrigues con $B_n = \frac{1}{2^n\, n!}$ es

$$P_n^{(\alpha,\beta)}(x) = \frac{1}{2^n\, n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left[(1-x)^{n+\alpha}(1+x)^{n+\beta}\right]. \tag{A.9}$$

- Ortogonalidad. Los polinomios ortogonales hipergeométricos $y_n(x)$ cumplen la condición de ortogonalidad siguiente:

$$\int_a^b y_n(x)\, y_m(x)\, \omega(x)\, dx = d_n^2\, \delta_{nm}, \tag{A.10}$$

donde $\omega(x)$ es la función peso, d_n es la constante de normalización, δ_{nm} es la delta de Kronecker y $[a,b]$ es el intervalo de ortogonalidad. Para cada uno de los P.O.C., con sus respectivos pesos tendremos distintos valores de la constante d_n^2 (también presentamos su valor para los polinomios mónicos, o sea aquellos que tienen como coeficiente principal 1) y del intervalo de ortogonalidad. Todos estos datos se resumen a continuación de forma esquemática.

- Hermite $H_n(x)$:
$(a,b) = (-\infty,+\infty)$,
$d_n^2 = 2^n\, n!\,\sqrt{\pi}$, y para mónicos $d_n^2 = \frac{n!\sqrt{\pi}}{2^n}$.

	Hermite $H_n(x)$	Laguerre $L_n^{(\alpha)}(x)$	Jacobi $P_n^{(\alpha,\beta)}(x)$
α_n	$1/2$	$-(n+1)$	$\frac{2(n+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}$
β_n	0	$2n+\alpha+1$	$\frac{\beta^2-\alpha^2}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)}$
γ_n	n	$-(n+\alpha)$	$\frac{2(n+\alpha)(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}$

Tabla A.2: Valores de α_n, β_n y γ_n en la relación de recurrencia a tres términos para polinomios estándar.

	Hermite $H_n(x)$	Laguerre $L_n^{(\alpha)}(x)$	Jacobi $P_n^{(\alpha,\beta)}(x)$
α_n	1	1	1
β_n	0	$2n+\alpha+1$	$\frac{\beta^2-\alpha^2}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)}$
γ_n	$n/2$	$n(n+\alpha)$	$\frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)(n+\alpha+\beta+1)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)}$

Tabla A.3: Valores de α_n, β_n y γ_n en la relación de recurrencia a tres términos para polinomios mónicos.

- Laguerre $L_n^{(\alpha)}(x)$
  $(a,b)=(0,+\infty)$,
  $d_n^2=\frac{\Gamma(n+\alpha+1)}{n!}$, y para mónicos $d_n^2=n!\,\Gamma(n+\alpha+1)$.
- Jacobi $P_n^{(\alpha,\beta)}(x)$
  $(a,b)=(-1,+1)$,
  $d_n^2=\frac{2^{\alpha+\beta+1}\,\Gamma(n+\alpha+1)\,\Gamma(n+\beta+1)}{n!(2n+\alpha+\beta+1)\,\Gamma(n+\alpha+\beta+1)}$,
  y para mónicos $d_n^2=\frac{2^{\alpha+\beta+2n+1}\,n!\,\Gamma(n+\alpha+1)\,\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\,\Gamma(n+\alpha+\beta+1)\,(n+\alpha+\beta+1)_n^2}$.

▪ Relación de recurrencia a tres términos

Una de las principales características de los polinomios ortogonales clásicos es que satisfacen una relación de recurrencia a tres términos que conecta tres polinomios de grados consecutivos $y_{n-1}(x)$, $y_n(x)$, $y_{n+1}(x)$; a saber,

$$x\,y_n(x)=\alpha_n\,y_{n+1}(x)+\beta_n\,y_n(x)+\gamma_n\,y_{n-1}(x), \tag{A.11}$$

(se suele tomar $y_{-1}(x)=0$ y $y_0(x)=1$) donde α_n, β_n y γ_n son constantes cuyos valores se recogen en las Tablas A.2 Y A.3 para polinomios con normalización estándar y mónicos, respectivamente.

▪ Desarrollo en serie de potencias

A continuación presentaremos los distintos desarrollos para los P.O.C. que estudiamos en este trabajo. Para los polinomios de Hermite y de Laguerre estas expresiones se encuentran fácilmente en la literatura [1]. Los polinomios de Jacobi requieren un poco de trabajo adicional.

- Hermite $H_n(x)$

$$H_n(x)=\sum_{m=0}^{\left[\frac{n}{2}\right]} b_{n,m}\,x^{n-2m}, \tag{A.12}$$

donde $\left[\frac{n}{2}\right]$ indica la parte entera de $\frac{n}{2}$, y los coeficientes $b_{n,m}$ tienen la forma

$$b_{n,m} = (-1)^m \frac{2^{n-2m}\, n!}{m!(n-2m)!}. \tag{A.13}$$

- Laguerre $L_n^{(\alpha)}(x)$

$$L_n^{(\alpha)}(x) = \sum_{m=0}^{n} a_{n,m}^{\alpha}\, x^m. \tag{A.14}$$

donde los coeficientes del desarrollo son

$$a_{n,m}^{\alpha} = (-1)^m \binom{n+\alpha}{n-m} \frac{1}{m!}. \tag{A.15}$$

- Jacobi $P_n^{(\alpha,\beta)}(x)$
La expresión explícita de estos polinomios que más aparece en la literatura [1] es

$$P_n^{(\alpha,\beta)}(x) = \sum_{m=0}^{n} a_{n,m}^{\alpha,\beta}\, (x-1)^m. \tag{A.16}$$

donde los coeficientes del desarrollo tienen la forma

$$a_{n,m}^{\alpha,\beta} = \binom{n}{m} \frac{\Gamma(\alpha+n+1)\,\Gamma(\alpha+\beta+n+m+1)}{n!\, 2^m\, \Gamma(\alpha+\beta+n+1)\,\Gamma(\alpha+m+1)}, \tag{A.17}$$

Ahora bien, teniendo en cuenta la serie de potencias del binomio

$$(x-1)^m = \sum_{l=0}^{m} \binom{m}{l} (-1)^{m-l}\, x^l. \tag{A.18}$$

se obtiene la siguiente expresión explícita de los polinomios de Jacobi

$$P_n^{(\alpha,\beta)}(x) = \sum_{k=0}^{n} c_k\, x^k, \tag{A.19}$$

donde los coeficiente c_k tienen la forma

$$c_k = \sum_{i=k}^{n} \binom{n}{i} \frac{\Gamma(\alpha+n+1)\,\Gamma(\alpha+\beta+n+i+1)}{n!\, 2^i\, \Gamma(\alpha+\beta+n+1)\,\Gamma(\alpha+i+1)} \binom{i}{k} (-1)^{i-k}, \tag{A.20}$$

que es mucho más adecuada para los propósitos de nuestro trabajo.

- Relaciones de inversión

En este apartado se recogen las relaciones de inversión de los polinomios ortogonales hipergeométricos $y_n(x)$, esto es los desarrollos del tipo

$$x^m = \sum_{n=0}^{m} c_{m,n}\, y_n(x), \tag{A.21}$$

donde los coeficientes c_{mn} tienen la forma general [65, 71]

$$c_{m,n} = \frac{1}{d_n^2} \int_a^b x^m\, y_n(x)\, \omega(x)\, dx, \tag{A.22}$$

donde $\omega(x)$ denota la función peso con respecto a la cual son ortogonales los polinomios en el intervalo (a, b). A continuación se detallan los coeficientes de las fórmulas de inversión de los polinomios de Hermite, Laguerre y Jacobi:

- Hermite $H_n(x)$

$$c_{m,n} = \begin{cases} \frac{m!}{2^m\, n!\,((m-n)/2)!} \quad \text{para} \quad m-n \quad \text{par} \\ \\ 0 \quad \text{para} \quad m-n \quad \text{impar} \end{cases} \tag{A.23}$$

- Laguerre $L_n^{(\alpha)}(x)$

$$c_{m,n} = \frac{(-1)^n\, m!\,\Gamma(m+\alpha+1)}{(m-n)!\,\Gamma(n+\alpha+1)}. \tag{A.24}$$

- Jacobi $P_n^{(\alpha,\beta)}(x)$

$$c_{m,n} = \frac{m!\,(-1)^{m-n}\,2^n\,\Gamma(n+2\alpha+1)}{(m-n)!\,\Gamma(2n+2\alpha+1)}\,{}_2F_1(n-m, n+\beta+1; 2n+\alpha+\beta+2; 2). \tag{A.25}$$

  donde ${}_2F_1(a,b;c;2)$ es la función hipergeométrica de Gauss.

- Momentos ordinarios de la densidad de Rakhmanov En esta sección se recogen los momentos ordinarios de la densidad de Rakhmanov $\rho_n(x)$ (2.1) de los polinomios ortogonales hipergeométricos $y_n(x)$. Estas medidas de esparcimiento de los polinomios a lo largo del intervalo de ortogonalidad (a,b), que juegan un papel relevante en algunas cuestiones de este trabajo, se definen por

$$\langle x^k \rangle = \int_a^b x^k\,\rho_n(x)\,dx = \frac{1}{d_n^2}\int_a^b x^k y_n^2(x)\,\omega(x)\,dx, \tag{A.26}$$

Estos momentos pueden obtenerse a partir de la relación de ortogonalidad y de la relación de recurrencia a tres términos que genéricamente satisfacen tales polinomios; a saber,

$$x\,y_n(x) = \alpha_n\,y_{n+1}(x) + \beta_n\,y_n(x) + \gamma_n\,y_{n-1}(x), \tag{A.27}$$

obteniéndose por ejemplo que

$$\langle x \rangle = \frac{1}{d_n^2}\,\beta_n \int_a^b \omega(x)\,y_n^2(x)\,dx = \beta_n, \tag{A.28}$$

$$\langle x^2 \rangle = \frac{d_{n+1}^2}{d_n^2} + \beta_n^2 + \gamma_n^2\,\frac{d_{n-1}^2}{d_n^2}, \tag{A.29}$$

y así sucesivamente. En particular, para los sistemas canónicos de Hermite, Laguerre y Jacobi se obtiene que:

- Hermite $H_n(x)$

$$\langle x^0 \rangle = 1, \qquad \langle x \rangle = 0, \qquad \langle x^2 \rangle = n + \frac{1}{2},$$

$$\langle x^3 \rangle = 0, \qquad \langle x^4 \rangle = \frac{3}{2}\left[n^2 + n + \frac{1}{2}\right].$$

- Laguerre $L_n^{(\alpha)}(x)$

$$\langle x^0\rangle = 1, \qquad \langle x\rangle = 2n+\alpha+1,$$
$$\langle x^2\rangle = 6n^2+6(\alpha+1)n+(\alpha+1)(\alpha+2),$$
$$\langle x^3\rangle = 4n^4+(2\alpha+7)n^3+(10\alpha+13)n^2+(4\alpha^2+12\alpha+14)n+(\alpha+1)(3\alpha+4).$$

- Jacobi $P_n^{(\alpha,\beta)}(x)$

$$\langle x^0\rangle = 1, \qquad \langle x\rangle = \frac{\beta^2-\alpha^2}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)},$$

$$\begin{aligned}\langle x^2\rangle &= \frac{4(n+1)(n+\alpha+1)(n+\beta+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)^2(2n+\alpha+\beta+3)} + \langle x\rangle^2 \\ &+ \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)}.\end{aligned}$$

Y, en general, para los momentos ordinarios de orden arbitrario k se obtienen los valores [71]:

- Hermite $H_n(x)$

$$\langle x^k\rangle = \begin{cases} \sum_{m=0}^{\frac{k}{2}}(-1)^m \frac{(k+n-2m)!}{2^k\, m!\,(n-2m)!\,[(k-2m)/2]!} & \text{para} \quad k \quad \text{par} \\ \\ 0 \qquad \text{para} \quad k \quad \text{impar} \end{cases} \tag{A.30}$$

- Laguerre $L_n^{(\alpha)}(x)$

$$\langle x^k\rangle = \frac{1}{\Gamma(n+\alpha+1)} \sum_{p=n-k}^{n} (-1)^{p+n} \binom{n+\alpha}{n-p} \frac{(k+p)!\,\Gamma(k+p+\alpha+1)}{(k+p-n)!\,p!}. \tag{A.31}$$

- Jacobi $P_n^{(\alpha,\beta)}(x)$

$$\begin{aligned}\langle x^k\rangle &= \sum_{i=n-k}^{n}\left(\sum_{t=i}^{n}(-1)^{t-i}\binom{n}{t}\frac{\Gamma(\alpha+n+1)\,\Gamma(\alpha+\beta+n+t+1)}{n!\,2^t\,\Gamma(\alpha+\beta+n+1)\,\Gamma(\alpha+t+1)}\binom{t}{i}\right) \\ &\times \frac{(-1)^{k+i-n}\,2^n\,(k+i)!\,\Gamma(n+\alpha+\beta+1)}{(k+i-n)!\,\Gamma(2n+\alpha+\beta+1)} \\ &\times {}_2F_1\left(\begin{matrix} n-k-i, n+\beta+1 \\ 2n+\alpha+\beta+2\end{matrix}\,\middle|\, 2\right).\end{aligned} \tag{A.32}$$

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