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Position and momentum information entropies of the D-dimensional harmonic oscillator and hydrogen atom

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The position- and momentum-space entropies of the isotropic harmonic oscillator and the hydrogen atom in D dimensions are shown to be related to some entropy integrals which involve classical orthogonal polynomials. These integrals are exactly calculated for Chebyshev polynomials and only in an approximate way for Gegenbauer polynomials. The physical entropies are explicitly obtained in the ground state and in a few low-lying excited states. Finally, the dimensionality dependence of the ground-state entropies of the two above-mentioned quantum-mechanical systems is analyzed (numerically) and the values of the entropies in a large class of excited states of the D-dimensional ($D = 1, 2, 3$) harmonic oscillator and hydrogen atom are tabulated and discussed.

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I. INTRODUCTION

A D-dimensional n-particle system is completely characterized in quantum mechanics by means of its wave function $\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n)$, where $\vec{r} \equiv (x_1, x_2, \ldots, x_D)$. The basic variable in the modern density-functional approaches [1–3] to study the physical and chemical properties of these systems is the single-particle density $\rho(\vec{r})$, i.e.,

$$\rho(\vec{r}) = \sum_{\sigma_i=-1/2}^{+1/2} \int |\Psi(\vec{r}, \vec{r}_2, \ldots, \vec{r}_n, \sigma_1, \sigma_2, \ldots, \sigma_n)|^2 \times d\vec{r}_2 d\vec{r}_3 \cdots d\vec{r}_n, \tag{1}$$

where $(\vec{r}_i, \sigma_i)$ denotes the position-spin coordinates of the ith particle and the wave function Ψ is assumed to be normalized and antisymmetrized in the pairs $(\vec{r}_i, \sigma_i)$. The density $\rho(\vec{r})$ is then normalized to unity.

An information measure closely related to the concept of entropy and disorder in thermodynamics is the so-called Boltzmann-Shannon entropy [4,5], which is defined as

$$S_\rho = -\int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r} \tag{2}$$

in the position space and

$$S_\gamma = -\int \gamma(\vec{p}) \ln \gamma(\vec{p}) d\vec{p} \tag{3}$$

in the momentum space. The momentum single-particle density $\gamma(\vec{p})$ is given as in (1) for the momentum wave function $\hat{\Psi}(\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_n, \sigma_1, \sigma_2, \ldots, \sigma_n)$, which is the Fourier transform of the position wave function Ψ.

These two entropies have shown to play an important role in the quantum-mechanical description of physical systems [6–11]. They have allowed Bialynicki-Birula and Mycielski (BBM) [6] to find a new and stronger version of the Heisenberg uncertainty relation; the corresponding BBM inequality for $n = 1$ is given by

$$S_\rho + S_\gamma \geq D(1 + \ln \pi), \tag{4}$$

which emphasizes the reciprocity between the position and momentum spaces. Indeed, in particular, high values of S_γ are associated with low values of S_ρ, which indicates that a diffuse $\gamma(\vec{p})$ is associated with a highly localized $\rho(\vec{r})$.

In addition, they show a close relationship [7–11] with fundamental and/or experimentally measurable quantities, such as, e.g., the kinetic energy and the magnetic susceptibility. Both characteristics have been used in the study of the dynamics of atomic and molecular systems [1].

Here we will initiate a detailed physico-mathematical study of both position and momentum information entropies. To begin with, we consider the simplest quantum-mechanical system, namely, a spinless particle in a central potential $V(r)$. The D-dimensional motion of this system is governed by the associated Schrödinger equation which, in atomic units, is

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$$\left[-\frac{1}{2}\vec{\nabla}^2 + V(r)\right]\Psi(\vec{r}) = \Psi(\vec{r}), \tag{5}$$

where

$$r^2 = \sum_{j=1}^{D} x_j^2.$$

Then the position and momentum single-particle densities are simply given by

$$\rho(\vec{r}) = |\Psi(\vec{r})|^2, \quad \gamma(\vec{p}) = |\hat{\Psi}(\vec{p})|^2, \tag{6}$$

respectively, where $\hat{\Psi}(\vec{p})$ is the Fourier transform of $\Psi(\vec{r})$. The corresponding information entropies S_ρ and S_γ, given by Eqs. (2) and (3), give a measure of the "spread" of the single-particle density in position and momentum space, respectively. Thus, S_ρ measures the uncertainty in the localization of the particle in the position space and S_γ measures the uncertainty in predicting the momentum of the particle. Atomic units ($m = e = \hbar = 1$) will be used throughout the paper.

Our attention will be centered around two specific systems: the isotropic harmonic oscillator whose potential is

$$V_{\mathrm{HO}}(r) = \frac{1}{2}\lambda^2 r^2 \tag{7}$$

and the hydrogen atom for which we use the Coulomb potential

$$V_{\mathrm{HA}}(r) = -\frac{1}{r}. \tag{8}$$

First, in Sec. II the energies and wave functions of these two D-dimensional systems are collected in both position and momentum spaces and the corresponding single-particle densities are explicitly shown. Then, in Sec. III we face the calculation of the position and momentum information entropies of the harmonic oscillator. The same problem is attacked in Sec. IV for the hydrogen atom. Briefly, as main results in these two sections, one has the following.

(i) The position and momentum information entropies of the aforementioned systems in the ground state and a few low-lying excited states are explicitly given. One finds, in particular, that the BBM inequality gets exhausted in the ground state of the harmonic oscillator.

(ii) For a general wave function of these systems, the entropies are shown to be expressed in terms of the entropy integrals

$$\int p_n^2(x)\ln p_n^2(x)d\mu(x) \tag{9}$$

and other closely related ones, where $p_n(x)$ are orthonormal polynomials with respect to a measure μ. The sign-reversed integrals (9) are to be called "entropies of the orthonormal polynomials $p_n(x)$." Specifically, the polynomials that appear in the two physical problems considered in the present work are the classical orthogonal polynomials corresponding to the names of Gegenbauer, Laguerre, and Hermite.

The analytical evaluation of the entropy integrals (9) has never been undertaken to the best of our information. In this paper we initiate this project by calculating the values of the entropy of Chebyshev polynomials $T_n(x) = \frac{n}{2}\lim_{\alpha\to 0} C_n^\alpha(x)$ in an exact form (Sec. V) and the values of the entropy of Gegenbauer polynomials $C_n^\alpha(x)$ in an approximate way (Sec. VI).

Finally, to have an idea of the spread or extent of the wave functions which describe the physical states of the systems under consideration, we have numerically computed the position and momentum information entropies of the one-, two-, and three-dimensional harmonic oscillator and hydrogen atom in the ground state and a few excited states (Sec. VII). The resulting values are discussed and the fulfillment of the BBM inequality is checked in all cases. Then some concluding remarks are given and a few open problems are pointed out.

II. THEORETICAL BACKGROUND

A. The D-dimensional harmonic oscillator

The Schrödinger equation of this system, given by Eqs. (5) and (7), can be transformed into

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr} - \frac{\Lambda^2}{r^2}\right) + \frac{1}{2}\lambda^2 r^2\right]\Psi_{n,l,\{\mu\}}(\vec{r}) = E\Psi_{n,l,\{\mu\}}(\vec{r}), \tag{10}$$

where the kinetic-energy operator has been written down by means of the spherical polar coordinates (r, Ω_D). The principal quantum number n, the orbital quantum number l, and the magnetic quantum numbers $\{\mu\}$ are integers satisfying

$$l = \mu_1 \geq \mu_2 \geq \cdots \geq |\mu_{D-1}|,$$

with $\mu_{D-1} = m$. The nonradial part Λ^2 of the Hamiltonian operator is known [12] to fulfill

$$\Lambda^2 Y_{l,\{\mu\}}(\Omega_D) = l(l+D-2)Y_{l,\{\mu\}}(\Omega_D), \tag{11}$$

where $Y_{l,\{\mu\}}(\Omega_D)$ are the hyperspherical harmonics defined by

$$Y_{l,\{\mu\}}(\Omega_D) = N_{l,\{\mu\}}e^{im\varphi}\prod_{j=1}^{D-2} C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j) \times(\sin\theta_j)^{\mu_{j+1}}, \tag{11a}$$

with the normalization constant

$$N_{l,\{\mu\}}^2 = \frac{1}{2\pi}\prod_{j=1}^{D-2}\frac{(\alpha_j+\mu_j)(\mu_j-\mu_{j+1})!\,[\Gamma(\alpha_j+\mu_{j+1})]^2}{\pi 2^{1-2\alpha_j-2\mu_{j+1}}\Gamma(2\alpha_j+\mu_j+\mu_{j+1})}. \tag{11b}$$

Here $2\alpha_j = D - j - 1$, $C_n^{\lambda}(t)$ is the Gegenbauer polynomial of degree n and parameter λ, and the angles $\theta_1, \theta_2, \ldots, \theta_{D-2}, \phi$ are given by

$$\begin{aligned} x_1 &= r \sin\theta_1 \sin\theta_2 \cdots \sin\theta_{D-2} \cos\varphi, \\ x_2 &= r \sin\theta_1 \sin\theta_2 \cdots \sin\theta_{D-2} \sin\varphi, \\ x_3 &= r \sin\theta_1 \sin\theta_2 \cdots \cos\theta_{D-2}, \\ &\vdots \\ x_{D-1} &= r \sin\theta_1 \cos\theta_2, \\ x_D &= r \cos\theta_1, \end{aligned}$$

with $0 \le \theta_j \le \pi$, $j = 1, \ldots, D-2$, and $0 \le \varphi < 2\pi$.

Since the hyperspherical harmonics are eigenfunctions of the operator Λ^2, we can look for solutions of the Schrödinger equation (10) having the separable form

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = R_{n,l}(r) Y_{l,\{\mu\}}(\Omega_D), \tag{12}$$

where $R_{n,l}(r)$ is a radial function which remains to be found. Inserting (12) into the Schrödinger equation (10) and taking into account (11), we obtain, for the radial function, the differential equation

$$\left[-\frac{1}{2}\left(\frac{d^2}{dr^2} + \frac{D-1}{r}\frac{d}{dr} - \frac{l(l+D-2)}{r^2}\right) + \frac{1}{2}\lambda^2 r^2\right] \times R_{n,l}(r) = E R_{n,l}(r). \tag{13}$$

Note that the magnetic quantum numbers do not appear in this equation; therefore, the radial function is independent of this quantum number.

Equation (13) can be solved in the conventional manner. One obtains the following normalized solutions:

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = \left[\frac{2n!\lambda^{l+\frac{D}{2}}}{\Gamma\left(n+l+\frac{D}{2}\right)}\right]^{\frac{1}{2}} r^l e^{-\frac{\lambda r^2}{2}} L_n^{l+\frac{D}{2}-1} \times \left(\lambda r^2\right) Y_{l,\{\mu\}}(\Omega_D),$$

where $n = 0, 1, 2, \ldots$ and $l = 0, 1, 2, \ldots$, which corresponds to the energy

$$E_{n,l} = \lambda\left(2n + l + \frac{D}{2}\right). \tag{14}$$

On the other hand, the Fourier transform of the eigenfunction $\Psi_{n,l,\{\mu\}}(\vec{r})$ gives the wave function in the momentum space

$$\hat{\Psi}_{n,l,\{\mu\}}(\vec{p}) = \left[\frac{2n!\lambda^{-l-\frac{D}{2}}}{\Gamma\left(n+l+\frac{D}{2}\right)}\right]^{\frac{1}{2}} p^l e^{-\frac{p^2}{2\lambda}} L_n^{l+\frac{D}{2}-1}\left(\frac{p^2}{\lambda}\right) \times Y_{l,\{\mu\}}(\hat{\Omega}_D),$$

where $\hat{\Omega}_D$ is the solid angle in momentum space. The symbol $L_n^{\alpha}(t)$ used in the description of the eigenfunctions in both position and momentum spaces denotes the well-known Laguerre polynomial.

As pointed out by Eq. (6), the modulus squared of these two eigenfunctions describes the position and momentum densities of the D-dimensional harmonic oscillator. These quantities are

$$\rho(\vec{r}) = \frac{2n!\lambda^{l+\frac{D}{2}}}{\Gamma\left(n+l+\frac{D}{2}\right)} r^{2l} e^{-\lambda r^2} \left[L_n^{l+\frac{D}{2}-1}\left(\lambda r^2\right)\right]^2 \times \left|Y_{l,\{\mu\}}(\Omega_D)\right|^2, \tag{15a}$$

$$\gamma(\vec{p}) = \frac{2n!\lambda^{-l-\frac{D}{2}}}{\Gamma\left(n+l+\frac{D}{2}\right)} p^{2l} e^{-p^2/\lambda} \left[L_n^{l+\frac{D}{2}-1}\left(p^2/\lambda\right)\right]^2 \times \left|Y_{l,\{\mu\}}(\hat{\Omega}_D)\right|^2 = \frac{1}{\lambda^D}\rho\left(\frac{\vec{p}}{\lambda}\right), \tag{15b}$$

respectively.

Finally, let us consider the special case $D = 1$. For the one-dimensional harmonic oscillator we only have one quantum number n and no angular part in the Schrödinger equation. The energy of this system is given by

$$E_n = \lambda(n + \tfrac{1}{2}) \tag{16}$$

and the eigenfunctions can be expressed by means of the Hermite polynomials [13]. The corresponding position and momentum densities are

$$\rho(x) = \sqrt{\frac{\lambda}{\pi}} \frac{1}{2^n n!} e^{-\lambda x^2} \left[H_n\left(\sqrt{\lambda} x\right)\right]^2, \tag{17a}$$

$$\gamma(p) = \frac{1}{\sqrt{\lambda\pi} 2^n n!} e^{-p^2/\lambda} \left[H_n\left(p/\sqrt{\lambda}\right)\right]^2. \tag{17b}$$

B. The D-dimensional hydrogen atom

The Schrödinger equation (5) for the D-dimensional radially symmetric Coulomb potential (8) can be solved in a similar way to the oscillator case. The eigenfunctions in the position space are given in atomic units by [14]

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = N_{n,l} e^{-\frac{r}{2\lambda}} \left(\frac{r}{\lambda}\right)^l L_{n-l-1}^{2l+D-2}\left(\frac{r}{\lambda}\right) Y_{l,\{\mu\}}(\Omega_D),$$

where $N_{n,l}$ are normalizing constants given by

$$N_{n,l} = \lambda^{-D/2}\left(\frac{(n-l-1)!}{2\eta(n+l+D-3)!}\right)^{1/2},$$

with

$$\eta = n + \frac{D-3}{2}, \qquad \lambda = \frac{\eta}{2}.$$

The quantum numbers $n = 1, 2, 3, \ldots$ and $l = 0, 1, \ldots, n-1$ correspond to the energy

$$E_n = -\frac{1}{2\eta^2}.$$

The associated probability density then is

$$\rho(\vec{r}) = |\Psi_{n,l,\{\mu\}}(\vec{r})|^2$$
$$= N_{n,l}^2 e^{-\frac{r}{\lambda}} \left(\frac{r}{\lambda}\right)^{2l} \left[L_{n-l-1}^{2l+D-2}\left(\frac{r}{\lambda}\right)\right]^2 |Y_{l,\{\mu\}}(\Omega_D)|^2. \tag{18}$$

By using a generalization of the method used by Fock [12] we find that the eigenfunction in the momentum space is

$$\hat{\Psi}_{n,l,\{\mu\}}(\vec{p}) = \frac{(2p_0)^{\frac{D}{2}+1}}{2^{1/2}\left(p^2+p_0^2\right)^{\frac{D+1}{2}}} Y_{n-1,\{\mu\}}\left(\Omega_{D+1}\right),$$

where $p_0^2 = -2E_n = \eta^{-2}$. If we use the known relationship between the hyperspherical harmonics in a $(D+1)$-dimensional space and those in a D-dimensional space, the eigenfunction is also equal to

$$\hat{\Psi}_{n,l,\{\mu\}}(\vec{p}) = K_{n,l} \frac{(\eta p)^l}{(1+\eta^2p^2)^{l+\frac{D+1}{2}}} C_{n-l-1}^{l+\frac{D-1}{2}}\left(\frac{1-\eta^2p^2}{1+\eta^2p^2}\right)$$
$$\times Y_{l,\{\mu\}}(\hat{\Omega}_D),$$

where $C_n^{\alpha}(t)$ is a Gegenbauer polynomial, η has the same meaning as in the position space, and

$$K_{n,l} = \left(\frac{(n-l-1)!}{2\pi(n+l+D-3)!}\right)^{1/2}$$
$$\times 2^{2l+D}\Gamma(l+\frac{D-1}{2})\eta^{\frac{D+1}{2}}.$$

Then, according to Eq. (6), the momentum density is

$$\gamma(\vec{p}) = K_{n,l}^2 \frac{(\eta p)^{2l}}{(1+\eta^2p^2)^{2l+D+1}} \left[C_{n-l-1}^{l+\frac{D-1}{2}}\left(\frac{1-\eta^2p^2}{1+\eta^2p^2}\right)\right]^2$$
$$\times |Y_{l,\{\mu\}}(\hat{\Omega}_D)|^2. \tag{19}$$

It is worth treating the Coulomb potential in one dimension separately, i.e., $V(x) = -\frac{1}{|x|}$. The ground state of this system has a degenerate energy $E_0 = -\infty$ and thus some care has to be taken in analyzing this state; its eigenfunction in the position space is most appropriately given by [15]

$$\Psi(x) = \alpha^{-1/2} e^{-\frac{|x|}{\alpha}}, \qquad \alpha \to 0.$$

By taking the Fourier transform we obtain the eigenfunction in momentum space

$$\hat{\Psi}(p) = \sqrt{\frac{2}{\pi}} \frac{\alpha^{1/2}}{1+\alpha^2p^2}, \qquad \alpha \to 0.$$

Then the ground-state probability densities in both position and momentum spaces are

$$\rho(x) = \alpha^{-1} e^{-2\frac{|x|}{\alpha}}, \qquad \alpha \to 0, \tag{20a}$$

$$\gamma(p) = \frac{2}{\pi} \frac{\alpha}{(1+\alpha^2p^2)^2}, \qquad \alpha \to 0. \tag{20b}$$

The eigenfunctions for the excited states are [15]

$$\Psi_{\text{even}}(x) = \sqrt{\frac{2}{n^5}} e^{-|x|/n} |x| L_{n-1}^1(2|x|/n),$$
$$\Psi_{\text{odd}}(x) = \sqrt{\frac{2}{n^5}} e^{-|x|/n} x L_{n-1}^1(2|x|/n),$$

where $\Psi_{\text{even}}(x)$ is the wave function for the even states and $\Psi_{\text{odd}}(x)$ is the wave function for the odd states. In the momentum space the wave functions are [16]

$$\hat{\Psi}_n(p) = \sqrt{\frac{2n}{\pi}} \frac{e^{\pm 2in\arctan(np)}}{1+n^2p^2},$$

with $n = 1, 2, 3, \ldots$. The state n has the energy $E_n = -1/n^2$. Then one has the expressions

$$\rho(x) = \frac{2}{n^5} e^{-2|x|/n} x^2 \left[L_{n-1}^1(2|x|/n)\right]^2, \tag{21a}$$

$$\gamma(p) = \frac{2n}{\pi} \frac{1}{(1+n^2p^2)^2} \tag{21b}$$

for the densities in position and momentum spaces, respectively.

III. INFORMATION ENTROPIES OF THE HARMONIC OSCILLATOR

Taking into account the densities of the D-dimensional harmonic oscillator in position space (15a) and momentum space (15b) and that

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

we obtain from Eqs. (2) and (3) the following expressions for the information entropies of this system in the position and momentum spaces denoted by S_ρ and S_γ, respectively.

(i) For the ground state

$$S_\rho = -\frac{D}{2}\ln\left(\frac{\lambda}{\pi}\right) + \frac{D}{2}, \tag{22a}$$

$$S_\gamma = \frac{D}{2}\ln(\lambda\pi) + \frac{D}{2}. \tag{22b}$$

It is worth pointing out that the entropy sum saturates the BBM inequality (4), that is, one has

$$S_\rho + S_\gamma = D(1 + \ln\pi). \tag{23}$$

(ii) For the excited state

$$S_\rho = -\ln\left(\frac{2n!}{\Gamma(n+l+D/2)}\right)$$
$$+\frac{D}{2}(1-\ln\lambda) + 2n + l$$
$$-\frac{n!}{\Gamma(n+l+D/2)}(I_1 + I_2) - I_3, \tag{24a}$$

$$S_\gamma = -\ln\left(\frac{2n!}{\Gamma(n+l+D/2)}\right) + \frac{D}{2}(1+\ln\lambda) + 2n + l - \frac{n!}{\Gamma(n+l+D/2)}(I_1+I_2) - I_3, \tag{24b}$$

where

$$I_1 = \int_0^\infty t^{l-1+D/2}e^{-t}\ln t^l[L_n^{l-1+D/2}(t)]^2dt, \tag{25a}$$

$$I_2 = \int_0^\infty t^{l-1+D/2}e^{-t}[L_n^{l-1+D/2}(t)]^2 \times \ln[L_n^{l-1+D/2}(t)]^2dt, \tag{25b}$$

$$I_3 = \int \left|Y_{l,\{\mu\}}(\hat{\Omega}_D)\right|^2 \ln\left|Y_{l,\{\mu\}}(\hat{\Omega}_D)\right|^2 d\Omega_D. \tag{25c}$$

According to Eq. (9) the integrals I_2 and I_3 are the entropy of the orthogonal Laguerre polynomials and in extenso the entropy of the hyperspherical harmonics, respectively. The last integral I_3 can be reduced to

$$I_3 = \ln N_{l,\{\mu\}}^2 + \sum_{j=1}^{D-2}\frac{(\alpha_j+\mu_j)(\mu_j-\mu_{j+1})!\,[\Gamma(\alpha_j+\mu_{j+1})]^2}{\pi 2^{1-2\alpha_j-2\mu_{j+1}}\Gamma(2\alpha_j+\mu_j+\mu_{j+1})} \times (I_4+\mu_{j+1}I_5)\,, \tag{26}$$

where

$$I_4 = \int_{-1}^{+1}(1-t^2)^{\mu_j-\mu_{j+1}-\frac{1}{2}}\left[C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(t)\right]^2 \times \ln\left[C_{\alpha_j+\mu_{j+1}}^{\mu_j-\mu_{j+1}}(t)\right]^2 dt, \tag{27a}$$

$$I_5 = \int_{-1}^{+1}(1-t^2)^{\mu_j-\mu_{j+1}-\frac{1}{2}}\left[C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(t)\right]^2 \times \ln(1-t^2)dt. \tag{27b}$$

According to Eq. (9), the integral I_4 is the entropy of the orthogonal Gegenbauer polynomials. To obtain (26) from (25c) we have used the explicit form (11a) and (11b) of the hyperspherical harmonics and taken into account the orthogonality condition of the Gegenbauer polynomials, namely

$$\int_{-1}^{+1}(1-x^2)^{\nu-\frac{1}{2}}C_m^\nu(x)C_n^\nu(x)dx = \frac{\pi 2^{1-2\nu}\Gamma(2\nu+n)}{n!(n+\nu)\,[\Gamma(\nu)]^2}\delta_{nm}. \tag{28}$$

The expressions (24a) and (24b) allow us to find that the sum of entropies is given by

$$S_\rho + S_\gamma = -2\ln\left(\frac{2n!}{\Gamma(n+l+D/2)}\right) + 4n + 2l + D - \frac{2n!}{\Gamma(n+l+D/2)}(I_1+I_2) - 2I_3, \tag{29}$$

which is independent of the strength λ of the potential. This is because of the scale invariance of the entropy sum, which comes from the special relationship (15b).

In the following we give explicit expressions for the entropies of the one-, two-, and three-dimensional harmonic oscillators for both ground and excited states.

(a) For the one-dimensional oscillator we find in the ground state $n=0$ that

$$S_\rho = \frac{1}{2}\ln(e\pi/\lambda), \tag{30a}$$

$$S_\gamma = \frac{1}{2}\ln(e\pi\lambda), \tag{30b}$$

and for the first excited state $n=1$

$$S_\rho = -\frac{1}{2}\ln\frac{\lambda e}{4\pi} + C, \tag{31a}$$

$$S_\gamma = -\frac{1}{2}\ln\frac{e}{4\pi\lambda} + C, \tag{31b}$$

where $C = 0.577\,215\,664\,9\ldots$ is Euler's constant. For arbitrary states n we have

$$S_\rho = \ln(\sqrt{\pi}2^n n!\lambda^{-\frac{1}{2}}) + n + \frac{1}{2} - \frac{1}{\sqrt{\pi}2^n n!}I_6, \tag{32a}$$

$$S_\gamma = \ln(\sqrt{\pi}2^n n!\lambda^{\frac{1}{2}}) + n + \frac{1}{2} - \frac{1}{\sqrt{\pi}2^n n!}I_6, \tag{32b}$$

where

$$I_6 = \int_{-\infty}^{\infty} e^{-t^2}\,[H_n(t)]^2\ln[H_n(t)]^2\,dt \tag{33}$$

is the entropy of the orthogonal Hermite polynomials. It follows from Eqs. (32a) and (32b) that the sum of entropies $S_\rho + S_\gamma$ is independent of the strength λ of the oscillator potential.

(b) For the harmonic oscillator in two dimensions we have two quantum numbers n and m. The ground state has the usual entropies and the first excited state $n=0$, $|m|=1$ has the entropies

$$S_\rho = \ln(e\pi/\lambda) + C, \tag{34a}$$

$$S_\gamma = \ln(e\pi\lambda) + C. \tag{34b}$$

For arbitrary states n,m the entropies involve the integrals I_1 and I_2 given above, associated with the Laguerre polynomials $L_n^{|m|}(t)$. That is, the corresponding expressions are

$$S_\rho = -\ln\left(\frac{n!}{(n+|m|)!\lambda\pi}\right) + 2n + |m| + 1 - \frac{n!}{(n+|m|)!}(I_1+I_2), \tag{35a}$$

$$S_\gamma = -\ln\left(\frac{n!\lambda}{(n+|m|)!\pi}\right) + 2n + |m| + 1 - \frac{n!}{(n+|m|)!}(I_1+I_2), \tag{35b}$$

where the integrals I_i, $i=1,2,3$ are given by Eqs. (25a)–(25b) with $D=2$ and $l=|m|$. We note that the entropies

S_ρ and S_γ of the states (n, m) and $(n, -m)$ have the same value.

(c) Finally, for the harmonic oscillator in three dimensions we have three quantum numbers n, l, m. For the ground state we have the usual simple expressions (22a) and (22b). The first excited states $n = 0$, $l = 1$ have the entropies $S_\rho^{n,l,|m|}$:

$$S_\rho^{0,1,0} = \ln[2(\pi/\lambda)^{3/2}] + C + 1/2, \tag{36a}$$

$$S_\gamma^{0,1,0} = \ln[2(\pi\lambda)^{3/2}] + C + 1/2, \tag{36b}$$

$$S_\rho^{0,1,1} = \frac{3}{2}\ln[\pi/\lambda] + C + 3/2, \tag{36c}$$

$$S_\gamma^{0,1,1} = \frac{3}{2}\ln[\pi\lambda] + C + 3/2, \tag{36d}$$

where again C is Euler's constant. For arbitrary states we need to use Eqs. (24a) and (24b) with $D = 3$. In this case, the integral I_3 is

$$\begin{aligned} I_3 &= \int |Y_{l,m}(\Omega_3)|^2 \ln |Y_{l,m}(\Omega_3)|^2 d\Omega_3 \\ &= \ln\left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right) + \left(\frac{(2l+1)(l-m)!}{2(l+m)!}\right) \\ &\quad \times \int_{-1}^{+1} [P_l^m(t)]^2 \ln[P_l^m(t)]^2 dt, \end{aligned} \tag{37}$$

where $P_l^m(t)$ are Legendre functions. If we use the relationship with Gegenbauer polynomials

$$(-1)^m \frac{(1-t^2)^{-m/2} m! 2^m}{(2m)!} P_l^m(t) = C_{l-m}^{m+1/2}(t),$$

the expression (37) becomes

$$\begin{aligned} I_3 = {} & \ln\left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right) \\ & + \left(\frac{(2l+1)(l-m)![(2m)!]^2}{2^{2m+1}(l+m)!(m!)^2}\right)(I_4 + I_5) \\ & + 2\ln\left(\frac{(2m)!}{m! 2^m}\right), \end{aligned} \tag{38}$$

with

$$I_4 = \int_{-1}^{+1} [C_{l-m}^{m+1/2}(t)]^2 (1-t^2)^m \ln(1-t^2)^m dt, \tag{39a}$$

$$I_5 = \int_{-1}^{+1} [C_{l-m}^{m+1/2}(t)]^2 (1-t^2)^m \ln[C_{l-m}^{m+1/2}(t)]^2 dt. \tag{39b}$$

Alternatively, the expressions (38) and (39b) follow directly from Eqs. (26) and (27b) in the case $D = 3$. Let us finally comment that again here the entropies S_ρ and S_γ have the same values in the states (n, l, m) and $(n, l, -m)$.

IV. INFORMATION ENTROPIES OF THE HYDROGEN ATOM

Operations similar to those already done in the preceding section lead to the following values for the position and momentum information entropies of the D-dimensional hydrogen atom.

(i) For the ground state

$$S_\rho = D - \ln\left(\frac{2^{2D-1}\Gamma(\frac{D}{2})}{(D-1)^{D+1}(D-2)!\pi^{D/2}}\right), \tag{40a}$$

$$\begin{aligned} S_\gamma = {} & (D+1)\left([(-1)^{D+1}+1]\ln 2 - \sum_{i=1}^{D}\frac{(-1)^{i+D}}{i}\right) \\ & - \ln\left(\frac{(D-1)^{D+1}\Gamma(\frac{D-1}{2})}{2\pi^{\frac{D+1}{2}}}\right). \end{aligned} \tag{40b}$$

The sum of entropies is

$$\begin{aligned} S_\rho + S_\gamma = {} & D\ln(e\pi) + \ln 2 \\ & + \frac{1}{2}(D+1)\left[\psi\left(\frac{D+1}{2}\right) - \psi\left(\frac{D}{2}+1\right)\right], \end{aligned} \tag{41}$$

where $\psi(x)$ is the psi function; note that this sum is always larger than $D(1 + \ln\pi)$, in agreement with the BBM inequality (4). Moreover, the entropy sum is $D(1 + \ln\pi) + O(1)$ for large values of D.

(ii) For the excited states

$$S_\rho = -\ln N_{n,l}^2 + \lambda^D N_{n,l}^2 (J_1 - 2lJ_2 - J_3) - J_4, \tag{42}$$

where

$$\begin{aligned} J_1 = {} & \frac{(n+l+D-1)!}{(n-l-1)!} + 4\frac{(n+l+D-2)!}{(n-l-2)!} \\ & + \frac{(n+l+D-3)!}{(n-l-3)!}, \end{aligned} \tag{43a}$$

$$J_2 = \int_0^\infty t^{\alpha+1} e^{-t} \ln t \, [L_k^\alpha(t)]^2 \, dt, \tag{43b}$$

$$J_3 = \int_0^\infty t^{\alpha+1} e^{-t} [L_k^\alpha(t)]^2 \ln [L_k^\alpha(t)]^2 \, dt, \tag{43c}$$

$$J_4 = \int \left|Y_{l,\{\mu\}}(\hat{\Omega}_D)\right|^2 \ln \left|Y_{l,\{\mu\}}(\hat{\Omega}_D)\right|^2 d\Omega_D = I_3, \tag{43d}$$

with $k = n - l - 1$, $\alpha = 2l + D - 2$, and

$$\begin{aligned} S_\gamma = {} & -\ln K_{n,l}^2 + (2l+D+1)\ln 2 \\ & - \frac{K_{n,l}^2}{\eta^D 2^{2l+D+1}} [lJ_5 + (D+1)J_6 + J_7] - J_4, \end{aligned} \tag{44}$$

where

$$J_5 = \int_{-1}^{+1} \left(1-t^2\right)^{\nu-1/2} \ln\left(1-t^2\right) [C_k^\nu(t)]^2 \, dt, \tag{45a}$$

$$J_6 = \int_{-1}^{+1} \left(1-t^2\right)^{\nu-1/2} (1+t)\ln(1+t) \, [C_k^\nu(t)]^2 \, dt, \tag{45b}$$

$$J_7 = \int_{-1}^{+1} \left(1-t^2\right)^{\nu-1/2} [C_k^\nu(t)]^2 \ln [C_k^\nu(t)]^2 \, dt, \tag{45c}$$

with $k = n - l - 1$ and $\nu = l + (D-1)/2$.

The entropies for the Coulomb potential in two and three dimensions can easily be obtained from the general expressions (42)–(45c) by setting $D = 2$ and $D = 3$, respectively.

For the one-dimensional Coulomb potential we use the densities (20a) and (20b), which, together with the expressions (2) and (3) produce the following values for the position and momentum entropies

(a) In the ground state the entropies for $\alpha > 0$ are given by

$$S_\rho = 1 + \ln\alpha, \tag{46a}$$

$$S_\gamma = \ln\left(\frac{8\pi}{e^2}\right) - \ln\alpha. \tag{46b}$$

Hence the sum of the entropies is

$$S_\rho + S_\gamma = \ln\left(\frac{8\pi}{e}\right), \tag{47}$$

independent of α.

(b) In the excited state

$$S_\rho = \ln\left(\frac{2n^2}{e^{3n}}\right) - \frac{1}{n^2}\left(J_2 + J_3/2\right), \tag{48a}$$

$$S_\gamma = \ln\left(\frac{8\pi}{e^2 n}\right), \tag{48b}$$

where

$$J_2 = \int_0^\infty t^2 e^{-t} \ln t \left[L_{n-1}^1(t)\right]^2 dt, \tag{49a}$$

$$J_3 = \int_0^\infty t^2 e^{-t} \left[L_{n-1}^1(t)\right]^2 \ln \left[L_{n-1}^1(t)\right]^2 dt. \tag{49b}$$

V. ENTROPY OF CHEBYSHEV POLYNOMIALS

In this section we begin with the notation and definition of the Chebyshev polynomials of first and second kind, and then we give the entropies of both polynomials in the form of theorems 1 and 2 below, which are proved in detail by extensive use of the algebraic properties of these polynomials [17–19]. For the harmonic oscillator these entropies appear in (27a) for $\mu_j = \mu_{j+1}$ and $\mu_j = \mu_{j+1} + 1$ and for the hydrogen atom in (43d) for the same parameters.

Chebyshev polynomials of the first kind are

$$T_n(x) = \cos n\theta, \quad x = \cos\theta, \qquad n = 0, 1, 2, \ldots .$$

They satisfy the following orthogonality relation:

$$\frac{1}{\pi}\int_{-1}^{+1} T_n(x) T_m(x) \frac{dx}{\sqrt{1-x^2}} = \frac{1}{2}\delta_{m,n}, \qquad m, n \geq 0, m + n \neq 0$$

and for $m + n = 0$

$$\frac{1}{\pi}\int_{-1}^{+1} T_0^2(x) \frac{dx}{\sqrt{1-x^2}} = 1.$$

The orthonormal polynomials are thus $p_n(x) = \sqrt{2} T_n(x)$ when $n \geq 1$ and $p_0(x) = T_0(x)$.

Chebyshev polynomials of the second kind are

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad x = \cos\theta, \quad n = 0, 1, 2, \ldots .$$

The orthogonality is

$$\frac{2}{\pi}\int_{-1}^{+1} U_n(x) U_m(x) \sqrt{1-x^2}\, dx = \delta_{m,n}, \qquad m, n \geq 0$$

and hence these are orthonormal polynomials.

Theorem 1. The entropy of the orthonormal Chebyshev polynomials of the first kind has the values

$$E_n = -\frac{1}{\pi}\int_{-1}^{+1} p_n^2(x) \ln p_n^2(x) \frac{dx}{\sqrt{1-x^2}} = \begin{cases} \ln 2 - 1 & \text{when } n \geq 1 \\ 0 & \text{when } n = 0. \end{cases} \tag{50}$$

Proof. Use

$$\left[\sqrt{1-x^2}\, U_{n-1}(x)\right]' = -n \frac{T_n(x)}{\sqrt{1-x^2}}$$

to find

$$\frac{1}{\pi}\int_{-1}^{+1} T_n^2(x) \ln T_n^2(x) \frac{dx}{\sqrt{1-x^2}} = -\frac{1}{n\pi}\int_{-1}^{+1} T_n(x) \ln T_n^2(x)\, d\left[\sqrt{1-x^2}\, U_{n-1}(x)\right].$$

Integration by parts gives

$$\frac{1}{\pi}\int_{-1}^{+1} T_n^2(x) \ln T_n^2(x) \frac{dx}{\sqrt{1-x^2}} = \frac{1}{n\pi}\int_{-1}^{+1} \sqrt{1-x^2}\, U_{n-1}(x) T_n'(x) \ln T_n^2(x)\, dx + \frac{2}{n\pi}\int_{-1}^{+1} \sqrt{1-x^2}\, U_{n-1}(x) T_n'(x)\, dx.$$

From $T_n'(x) = nU_{n-1}(x)$ we then find

$$\frac{1}{\pi}\int_{-1}^{+1} T_n^2(x)\ln T_n^2(x)\frac{dx}{\sqrt{1-x^2}} = \frac{1}{\pi}\int_{-1}^{+1} \sqrt{1-x^2}U_{n-1}^2(x)\ln T_n^2(x)dx + \frac{2}{\pi}\int_{-1}^{+1} \sqrt{1-x^2}U_{n-1}^2(x)dx.$$

Euler's formula $(1-x^2)U_{n-1}^2(x) + T_n^2(x) = 1$ gives

$$\begin{aligned}\frac{1}{\pi}\int_{-1}^{+1} T_n^2(x)\ln T_n^2(x)\frac{dx}{\sqrt{1-x^2}} &= \frac{1}{\pi}\int_{-1}^{+1} \ln T_n^2(x)\frac{dx}{\sqrt{1-x^2}} \\ &\quad -\frac{1}{\pi}\int_{-1}^{+1} T_n^2(x)\ln T_n^2(x)\frac{dx}{\sqrt{1-x^2}} + \frac{2}{\pi}\int_{-1}^{+1} \sqrt{1-x^2}U_{n-1}^2(x)dx.\end{aligned}$$

Then, since

$$\frac{2}{\pi}\int_{-1}^{+1} U_{n-1}^2(x)\sqrt{1-x^2}dx = 1, \qquad n \geq 1$$

and

$$\begin{aligned}\frac{1}{\pi}\int_{-1}^{+1} \ln T_n^2(x)\frac{dx}{\sqrt{1-x^2}} &= \frac{1}{\pi}\int_0^{\pi} \ln|\cos n\theta|^2 d\theta \\ &= \frac{1}{2\pi}\int_0^{2\pi} \ln\left|\frac{z^n + z^{-n}}{2}\right|^2 d\theta \qquad (z = e^{i\theta}) \\ &= \frac{1}{2\pi}\int_0^{2\pi} \ln\left|\frac{1+z^{2n}}{2}\right|^2 d\theta = -2\ln 2\end{aligned}$$

(the last equation follows because $\ln\left|\frac{1+z^{2n}}{2}\right|^2$ is harmonic in $|z| < 1$, so that the integral over the unit circle is equal to the value of the integrand at 0), we find for $n \geq 1$

$$\frac{2}{\pi}\int_{-1}^{+1} T_n^2(x)\ln T_n^2(x)\frac{dx}{\sqrt{1-x^2}} = -2\ln 2 + 1.$$

For the orthonormal polynomials we just set $p_n(x) = \sqrt{2}T_n(x)$ to find the desired result (50) for $n \geq 1$. The result for $n = 0$ is checked immediately.

For the Chebyshev polynomials of the second kind we can also make an exact computation.

Theorem 2. The entropy of the Chebyshev polynomials of the second kind has the values

$$E_n = -\frac{2}{\pi}\int_{-1}^{+1} p_n^2(x)\ln p_n^2(x)\sqrt{1-x^2}dx = \frac{1}{n+1} - 1, \qquad n \geq 0. \tag{51}$$

Proof. Use $T_{n+1}'(x) = (n+1)U_n(x)$ to find

$$\frac{2}{\pi}\int_{-1}^{+1} U_n^2(x)\ln U_n^2(x)\sqrt{1-x^2}dx = \frac{2}{\pi(n+1)}\int_{-1}^{+1} U_n(x)\ln U_n^2(x)\sqrt{1-x^2}dT_{n+1}(x).$$

Integration by parts gives

$$\begin{aligned}\frac{2}{\pi}\int_{-1}^{+1} U_n^2(x)\ln U_n^2(x)\sqrt{1-x^2}dx &= -\frac{4}{\pi(n+1)}\int_{-1}^{+1} T_{n+1}(x)U_n'(x)\sqrt{1-x^2}dx \\ &\quad -\frac{2}{\pi(n+1)}\int_{-1}^{+1} T_{n+1}(x)\left[U_n(x)\sqrt{1-x^2}\right]'\ln U_n^2(x)dx.\end{aligned}$$

The use of

$$\left[\sqrt{1-x^2}U_n(x)\right]' = -(n+1)\frac{T_{n+1}(x)}{\sqrt{1-x^2}} = \frac{-x}{\sqrt{1-x^2}}U_n(x) + \sqrt{1-x^2}U_n'(x)$$

allows us to find

$$\frac{2}{\pi}\int_{-1}^{+1} U_n^2(x)\ln U_n^2(x)\sqrt{1-x^2}\,dx = \frac{2}{\pi}\int_{-1}^{+1} T_{n+1}^2(x)\ln U_n^2(x)\frac{dx}{\sqrt{1-x^2}}$$
$$+\frac{4}{\pi}\int_{-1}^{+1} T_{n+1}^2(x)\frac{dx}{\sqrt{1-x^2}} - \frac{4}{\pi(n+1)}\int_{-1}^{+1} xT_{n+1}(x)U_n(x)\frac{dx}{\sqrt{1-x^2}}.$$

Euler's formula $(1-x^2)U_{n-1}^2(x)+T_n^2(x)=1$ gives

$$\frac{2}{\pi}\int_{-1}^{+1} U_n^2(x)\ln U_n^2(x)\sqrt{1-x^2}\,dx = \frac{2}{\pi}\int_{-1}^{+1} \ln U_n^2(x)\frac{dx}{\sqrt{1-x^2}} - \frac{2}{\pi}\int_{-1}^{+1} U_n^2(x)\ln U_n^2(x)\sqrt{1-x^2}\,dx$$
$$+\frac{4}{\pi}\int_{-1}^{+1} T_{n+1}^2(x)\frac{dx}{\sqrt{1-x^2}} - \frac{4}{\pi(n+1)}\int_{-1}^{+1} xT_{n+1}(x)U_n(x)\frac{dx}{\sqrt{1-x^2}}.$$

The third and fourth terms on the right-hand side can be computed by

$$\frac{2}{\pi}\int_{-1}^{+1} T_{n+1}^2\frac{dx}{\sqrt{1-x^2}} = 1,$$
$$\frac{2}{\pi}\int_{-1}^{+1} xT_{n+1}(x)U_n(x)\frac{dx}{\sqrt{1-x^2}} = 1,$$

and furthermore

$$\frac{2}{\pi}\int_{-1}^{+1} \ln U_n^2(x)\frac{dx}{\sqrt{1-x^2}} = \frac{1}{\pi}\int_0^{2\pi} \ln|\sin(n+1)\theta|^2 d\theta - \frac{1}{\pi}\int_0^{2\pi}\ln|\sin\theta|^2 d\theta$$
$$= \frac{1}{\pi}\int_0^{2\pi}\ln\left|\frac{z^{n+1}-z^{-n-1}}{2i}\right|^2 d\theta - \frac{1}{\pi}\int_0^{2\pi}\ln\left|\frac{z-z^{-1}}{2i}\right|^2 d\theta$$
$$= \frac{1}{\pi}\int_0^{2\pi}\ln\left|\frac{z^{2n+2}-1}{2}\right|^2 d\theta - \frac{1}{\pi}\int_0^{2\pi}\ln\left|\frac{z^2-1}{2}\right|^2 d\theta = 2\ln\frac{1}{4} - 2\ln\frac{1}{4} = 0,$$

where we have used the mean value property of harmonic functions. This gives the desired result (51).

VI. ENTROPY OF GEGENBAUER POLYNOMIALS

Let us calculate the entropy of the Gegenbauer polynomials (also called ultraspherical polynomials) $C_n^\lambda(x)$, $\lambda > -\frac{1}{2}$. This entropy, as well as some related integrals which involve the same polynomials, appears when one computes the angular part of the information entropies of the hydrogen atom and harmonic oscillator in both position and momentum spaces; see, e.g., Eq. (45c) as well as Eqs. (27), (39), (45a), and (45b).

The Gegenbauer polynomials are symmetric Jacobi polynomials [18–20]; they satisfy the following orthogonality relation:

$$\frac{1}{\pi}\int_{-1}^{+1} C_n^\lambda(x)C_m^\lambda(x)(1-x^2)^{\lambda-\frac{1}{2}}dx = \frac{2^{1-2\lambda}\Gamma(n+2\lambda)}{\Gamma^2(\lambda)(n+\lambda)n!}\delta_{m,n}. \quad (52)$$

By taking into account the expression

$$(1-x^2)^{\lambda-\frac{1}{2}}C_n^\lambda(x) = -\frac{2\lambda}{(2\lambda+n)n}\left[(1-x^2)^{\lambda+\frac{1}{2}}C_{n-1}^{\lambda+1}(x)\right]'$$

(which follows from the Rodrigues formula) we find

$$\int_{-1}^{+1}[C_n^\lambda(x)]^2\ln[C_n^\lambda(x)]^2(1-x^2)^{\lambda-\frac{1}{2}}dx$$
$$= -\frac{2\lambda}{(2\lambda+n)n}\int_{-1}^{+1} C_n^\lambda(x)\ln[C_n^\lambda(x)]^2$$
$$\times d\left[(1-x^2)^{\lambda+\frac{1}{2}}C_{n-1}^{\lambda+1}(x)\right].$$

Integration by parts and the difference-differential relation

$$\left[C_n^\lambda(x)\right]' = 2\lambda C_{n-1}^{\lambda+1}(x)$$

gives

$$\begin{aligned}\int_{-1}^{+1}&[C_n^{\lambda}(x)]^2\ln[C_n^{\lambda}(x)]^2(1-x^2)^{\lambda-\frac{1}{2}}dx\\ &=\frac{2(2\lambda)^2}{(2\lambda+n)n}\int_{-1}^{+1}[C_{n-1}^{\lambda+1}(x)]^2(1-x^2)^{\lambda+\frac{1}{2}}dx\\ &\quad+\frac{(2\lambda)^2}{(2\lambda+n)n}\int_{-1}^{+1}[C_{n-1}^{\lambda+1}(x)]^2\\ &\quad\times\ln[C_n^{\lambda}(x)]^2(1-x^2)^{\lambda+\frac{1}{2}}dx. \qquad (53)\end{aligned}$$

The first term on the right-hand side can be computed by (52) and is

$$\frac{2(2\lambda)^2}{(2\lambda+n)n}\int_{-1}^{+1}[C_{n-1}^{\lambda+1}(x)]^2(1-x^2)^{\lambda+\frac{1}{2}}dx =\frac{2\pi 2^{1-2\lambda}\Gamma(2\lambda+n)}{\Gamma^2(\lambda)(n+\lambda)n!}.$$

In the case of Chebyshev polynomials we were able to make the explicit computation by using Euler's formula. An analog of this important formula can be obtained via orthogonal polynomials on the unit circle. Let $p_n(x)$ be the orthonormal polynomials on $[-1,+1]$ with weight function $\omega(x)$ and $q_n(x)$ those with weight function $(1-x^2)\omega(x)$. If $\phi_n(x)$ are the orthonormal polynomials on the unit circle with weight $\omega(\cos\theta)|\sin\theta|$, then (see [20] Sec. 11.5)

$$\begin{aligned}A_np_n(x)&=z^{-n}\phi_{2n}(z)+z^n\phi_{2n}(1/z),\\ \frac{z-z^{-1}}{2}B_nq_{n-1}(x)&=z^{-n}\phi_{2n}(z)-z^n\phi_{2n}(1/z),\end{aligned}$$

where $z=e^{i\theta}$,

$$A_n=\sqrt{2\pi}\sqrt{1+\frac{\phi_{2n}(0)}{\kappa_{2n}}},\qquad B_n=\sqrt{2\pi}\sqrt{1-\frac{\phi_{2n}(0)}{\kappa_{2n}}},$$

and κ_{2n} is the leading coefficient of $\phi_{2n}(z)$. From this, we find for $x=\cos\theta$ and $z=e^{i\theta}$

$$\begin{aligned}A_np_n(x)+iB_n\sin\theta q_{n-1}(x)&=2z^{-n}\phi_{2n}(z),\\ A_np_n(x)-iB_n\sin\theta q_{n-1}(x)&=2z^n\phi_{2n}(1/z),\end{aligned}$$

so that

$$A_n^2p_n^2(x)+(1-x^2)B_n^2q_{n-1}^2(x)=4|\phi_{2n}(z)|^2, \qquad (54)$$

which is the desired generalization of Euler's formula. If we take $\omega=(1-x^2)^{\lambda-\frac{1}{2}}$, then by (52) the orthonormal polynomials are

$$\begin{aligned}p_n(x)&=\Gamma(\lambda)\left(\frac{(n+\lambda)n!}{2^{1-2\lambda}\pi\Gamma(n+2\lambda)}\right)^{1/2}C_n^{\lambda}(x),\\ q_{n-1}(x)&=\Gamma(\lambda+1)\left(\frac{(n+\lambda)(n-1)!}{2^{-1-2\lambda}\pi\Gamma(n+2\lambda+1)}\right)^{1/2}\\ &\quad\times C_{n-1}^{\lambda+1}(x),\end{aligned}$$

and for the weight function $|\sin\theta|^{2\lambda}$ on the unit circle one has $\phi_{2n}(0)/\kappa_{2n}=\lambda/(n+\lambda)$ [21,22] so that

$$A_n^2=2\pi\frac{n+2\lambda}{n+\lambda},\qquad B_n^2=2\pi\frac{n}{n+\lambda},$$

and (54) becomes

$$\begin{aligned}[C_n^{\lambda}(x)]^2&+(1-x^2)\frac{4\lambda^2}{(n+2\lambda)^2}[C_{n-1}^{\lambda+1}(x)]^2\\ &=\frac{4\Gamma(n+2\lambda)}{2^{2\lambda}n!(n+2\lambda)\Gamma^2(\lambda)}|\phi_{2n}(z)|^2. \qquad (55)\end{aligned}$$

Insert this into (53) to find

$$\begin{aligned}\int_{-1}^{+1}&[C_n^{\lambda}(x)]^2\ln[C_n^{\lambda}(x)]^2(1-x^2)^{\lambda-\frac{1}{2}}dx\\ &=\frac{2^{1-2\lambda}\Gamma(n+2\lambda)}{\Gamma^2(\lambda)(n+\lambda)n!}\left(\frac{n+\lambda}{n}+\frac{1}{\pi}\int_{-1}^{+1}|\phi_{2n}(z)|^2\right.\\ &\quad\left.\times\ln[C_n^{\lambda}(x)]^2(1-x^2)^{\lambda-\frac{1}{2}}dx\right).\end{aligned}$$

Furthermore,

$$\begin{aligned}\frac{1}{\pi}\int_{-1}^{+1}&|\phi_{2n}(z)|^2\ln[C_n^{\lambda}(x)]^2(1-x^2)^{\lambda-\frac{1}{2}}dx\\ &=\frac{1}{2\pi}\int_0^{2\pi}|\phi_{2n}(z)|^2\ln\left|z^nC_n^{\lambda}\left(\frac{z+z^{-1}}{2}\right)\right|^2|\sin\theta|^{2\lambda}d\theta\ \ (z=e^{i\theta})\\ &=\frac{1}{2\pi}\int_0^{2\pi}\ln\left|z^nC_n^{\lambda}\left(\frac{z+z^{-1}}{2}\right)\right|^2d\theta+\frac{1}{2\pi}\int_0^{2\pi}\left[|\phi_{2n}(z)|^2|\sin\theta|^{2\lambda}-1\right]\ln\left|z^nC_n^{\lambda}\left(\frac{z+z^{-1}}{2}\right)\right|^2d\theta.\end{aligned}$$

The first integral on the right-hand side can be computed by the mean value theorem for harmonic functions and is equal to $2\ln c_n/2^n$, where c_n is the leading coefficient of $C_n^{\lambda}(x)$. By [20], Sec. (4.7.9), this gives

$$\frac{1}{2\pi}\int_0^{2\pi}\ln\left|z^nC_n^{\lambda}\left(\frac{z+z^{-1}}{2}\right)\right|^2d\theta=2\ln\frac{\Gamma(n+\lambda)}{\Gamma(\lambda)n!}.$$

From the result in [23] Corollary 2.2, p. 243, we know that

$$\lim_{n\to\infty}\frac{1}{2\pi}\int_0^{2\pi}\left||\phi_n(z)|^2|\sin\theta|^{2\lambda}-1\right|d\theta=0$$

and thus

$$\frac{1}{\pi}\int_{-1}^{+1}[C_n^\lambda(x)]^2\ln[C_n^\lambda(x)]^2(1-x^2)^{\lambda-\frac{1}{2}}dx$$

$$=\frac{2^{1-2\lambda}\Gamma(n+2\lambda)}{\Gamma^2(\lambda)(n+\lambda)n!}\left(\frac{n}{n+\lambda}+2\ln\frac{\Gamma(n+\lambda)}{\Gamma(\lambda)n!}[1+o(1)]\right).$$

For the normalized entropy integral we use the probability weight function

$$\omega_\lambda(x)=\frac{\Gamma^2(\lambda)\lambda}{2^{1-2\lambda}\Gamma(2\lambda)\pi}(1-x^2)^{\lambda-\frac{1}{2}},$$

with orthonormal polynomials

$$p_n(x)=\left(\Gamma(2\lambda)\frac{(n+\lambda)n!}{\lambda\Gamma(n+2\lambda)}\right)^{1/2}C_n^\lambda(x).$$

Straightforward calculus gives the following values for the entropy of the Gegenbauer polynomial:

$$\begin{aligned}E_n&=-\int_{-1}^{+1}p_n^2(x)\ln p_n^2(x)\omega_\lambda(x)dx=-\frac{n}{n+\lambda}-2\ln\frac{\Gamma(n+\lambda)}{\Gamma(\lambda)n!}[1+o(1)]-\ln\frac{\Gamma(2\lambda)(n+\lambda)n!}{\lambda\Gamma(n+2\lambda)}\\&=-\frac{n}{n+\lambda}+\ln\frac{\Gamma(\lambda)\Gamma(\lambda+1)}{\Gamma(2\lambda)}+\frac{\lambda(\lambda-1)}{n}+o(\ln n),\end{aligned}\tag{56}$$

where we have used Stirling's formula for the last equality.

VII. PHYSICAL ENTROPIES: NUMERICAL VALUES

For the ground state we have calculated the exact values of the entropies of the two D-dimensional systems under consideration in both position and momentum spaces as shown by Eqs. (22a) and (22b) for the oscillator case and Eqs. (40a) and (40b) for the hydrogen atom. In the oscillator case we observe from Eqs. (22a) and (22b) that both position and momentum entropies (i) increase linearly with the dimension D for a fixed strength λ and (ii) have a logarithmic dependence on λ, though of opposite sign, for a fixed dimensionality. Then the sum of entropies of the ground-state harmonic oscillator has a linear dependence on D and it is independent of the potential strength; it reaches the saturation value of the BBM inequality.

Figure 1 shows the dimensionality dependence of the position S_ρ and momentum S_γ entropies of the hydrogen atom in its ground state for the range $D=2-60$. We observe that S_ρ and S_γ present an opposite nonlinear behavior with increasing dimension such that its sum has a dimensionality dependence of practically linear type.

For the excited states we have not calculated the exact values of the two complementary physical entropies of both D-dimensional systems because we cannot yet evaluate the necessary entropy integrals (9) of the involved classical orthogonal polynomials. Because of this and to study the variation of these physical entropies with the dimensionality of the system and with the quantum numbers which characterize a state, we have computed numerically the values of the entropies of the one-, two-, and three-dimensional harmonic oscillator and hydrogen atom in various excited states. The results are shown in Figs. 2–5 and 6 for the oscillator case and in Figs. 7–9 for the hydrogen atom.

Figure 2 gives the values of the entropies S_ρ and S_γ of the one-dimensional harmonic oscillator (with strength $\lambda=\frac{1}{2}$) given by Eqs. (32a) and (32b), as well as its sum $S_\rho+S_\gamma$, in various excited states: those with the quantum number $n=0-60$. Both quantities S_ρ and S_γ increase rapidly for small values of n (say, $n\leq 15$) and at a much slower rate for larger n. They might be asymptotically

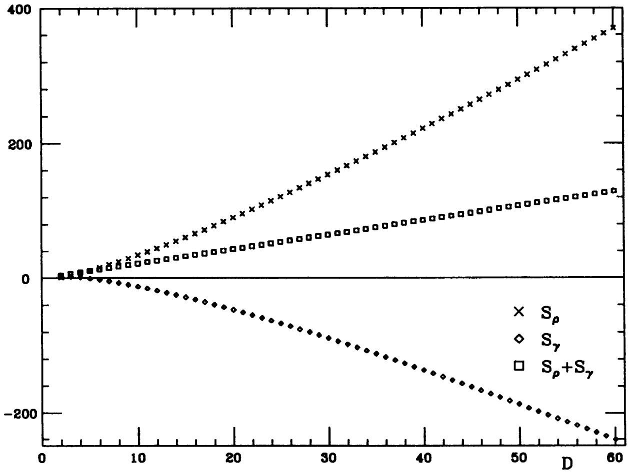

FIG. 1. Dimensionality dependence of the ground-state information entropies in the position space S_ρ and in the momentum space S_γ as well as of the entropy sum $S_\rho+S_\gamma$ for the hydrogen atom in the range $D=2-60$. All values are in atomic units.

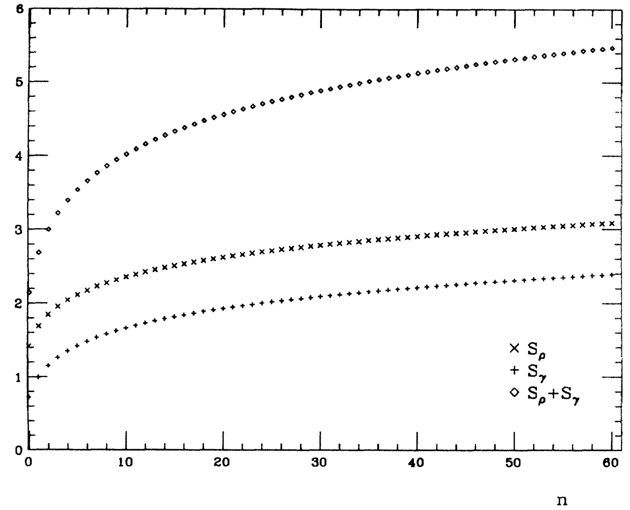

FIG. 2. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the one-dimensional harmonic oscillator with strength $\lambda = \frac{1}{2}$ in the excited states with $n = 0 - 60$. All values are in atomic units.

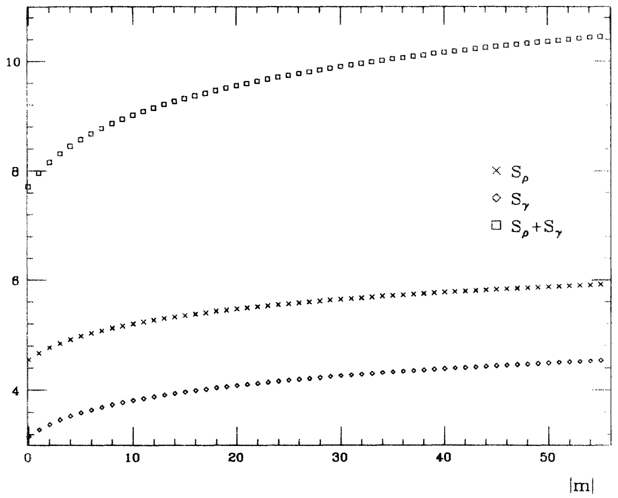

FIG. 4. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the two-dimensional harmonic oscillator with strength $\lambda = \frac{1}{2}$ in the excited states $(n = 4, |m|)$ with $|m| = 0 - 55$. All values are in atomic units.

convergent, but to know this we need to calculate the asymptotic value of the entropy integral of the Hermite polynomials (33). The entropy sum has a increasing behavior with n. This trend was pointed out by Gadre *et al.* [9] in a numerical examination of the five lowest excited states of this one-dimensional system. This should be expected since $\exp(S_\rho + S_\gamma)$ is proportional to the uncertainty product $\Delta x \Delta p$, which is equal to $n + \frac{1}{2}$ as it follows immediately from the virial theorem [14].

Figures 3 and 4 gives the values of the entropies S_ρ and S_γ of the two-dimensional harmonic oscillator (with strength $\lambda = \frac{1}{2}$) given by Eqs. (35a) and (35b), as well as its sum $S_\rho + S_\gamma$, in the excited states characterized by the quantum numbers $(n, |m| = 3)$ with $n = 0 - 60$ and $(n = 4, |m|)$ with $|m| = 0 - 55$, respectively. In both figures we observe a global dependence on n and $|m|$ similar to the dependence of the same quantities of the one-dimensional system with respect to n. One should remember in order to understand both phenomena that the energy of the physical states increases linearly with n in both systems and also with $|m|$ in the two-dimensional case as given by Eqs. (16) and (14) for the one- and two-dimensional harmonic oscillators, respectively.

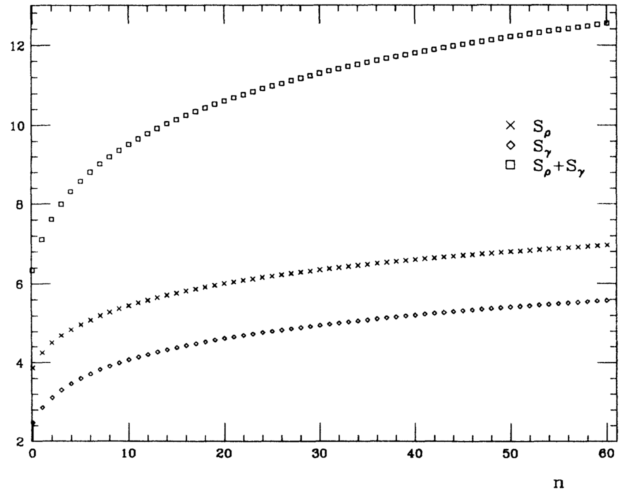

FIG. 3. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the two-dimensional harmonic oscillator with strength $\lambda = \frac{1}{2}$ in the excited states $(n, |m| = 3)$ with $n = 0 - 60$. All values are in atomic units.

Figure 5 gives the dependence on n of the entropies S_ρ and S_γ, as well as their sum, for the three-dimensional harmonic oscillator with strength $\lambda = \frac{1}{2}$ in the excited states $(n, l = 3, |m| = 2)$ with $n = 0 - 50$. Again here we observe a behavior similar to that previously described, possibly due to the fact that the energy of this system increases also linearly with increasing n. Most interesting in this case is the behavior of the entropies with the magnetic quantum number m since the energy is degenerated in m (i.e., it does not depend on it). This is analyzed in Fig. 6, where the values of the position and momentum entropies and its sum are shown for the excited states $(n = 4, l, |m|)$ with $l = 0 - 10$ and $|m| = 0 - l$. Deliberately there are no units on the abscissa axis, where the values of l and $|m|$ are assumed; one should keep in mind that for each l there are $l+1$ values of $|m|$ and then there appears $l+1$ values of the corresponding entropies which have an arc form. According to Eqs. (35a) and (35b) with $D = 3$, this arc behavior corresponds to the dependence on m of the entropy integral I_3 given by Eq. (37) to be called entropy of spherical harmonics $Y_{l,m}(\Omega_3)$ or just spatial entropy. The numerical results shown in Fig. 6 seem to indicate that both entropies reach the highest

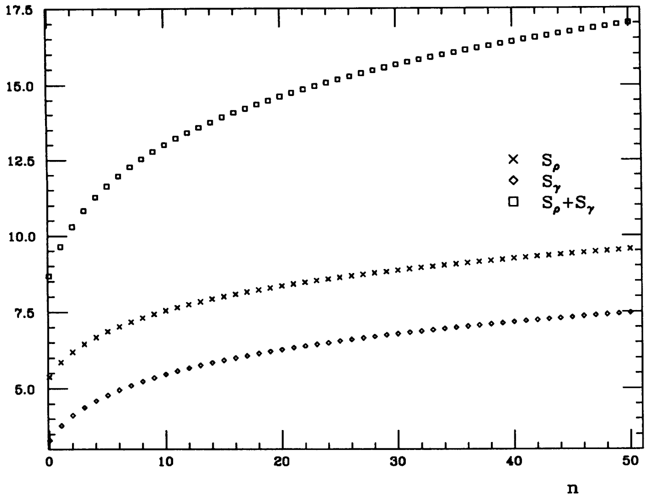

FIG. 5. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the three-dimensional harmonic oscillator with strength $\lambda = \frac{1}{2}$ in the excited states $(n, l = 3, |m| = 2)$ with $n = 0 - 50$. All values are in atomic units.

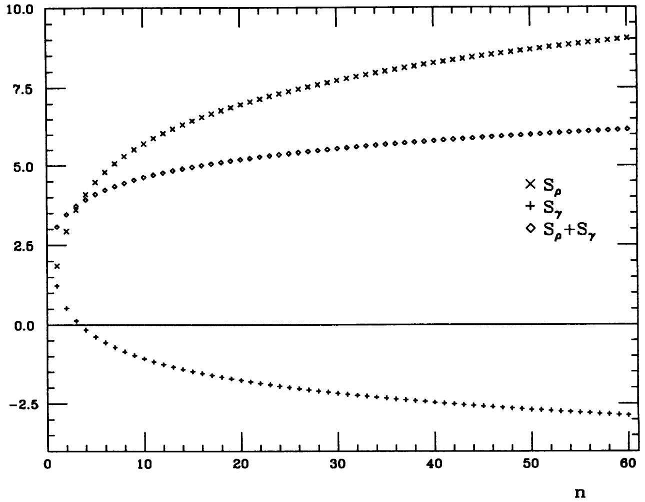

FIG. 7. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the one-dimensional hydrogen atom in the excited states with $n = 1 - 60$. All values are in atomic units.

value at $|m| = [(l+1)/2]$ in the multiplet characterized by the quantum numbers (n, l), where $[a]$ is the largest integer $\leq a$.

The information entropies S_ρ and S_γ, as well as their sum, for the one-dimensional hydrogen atom are displayed in Fig. 7 for the excited states with $n = 1 - 60$. We observe that both entropies have a monotonic behavior of increasing and decreasing type, respectively, with this quantum number, so that the entropy sum enhances with n. The same behavior with the principal quantum number n is observed for the corresponding quantities in various excited states of the two- and three-dimensional hydrogen atoms as shown in Figs. 8 and 9, respectively. This behavior was pointed out by Gadre *et al.* [9] in their numerical analysis of the states $(n, l = 0)$ with $n = 1 - 4$ in the three-dimensional system. The present work extends this analysis not only because of the consideration

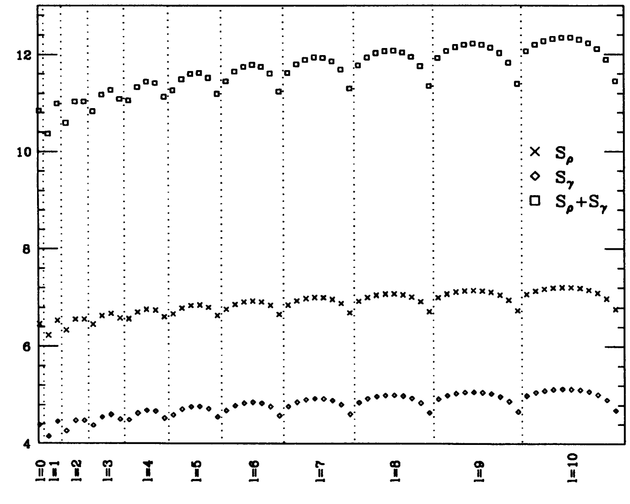

FIG. 6. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the three-dimensional harmonic oscillator with strength $\lambda = \frac{1}{2}$ in the excited states $(n = 4, l, |m|)$ with $l = 0{-}10$ and $|m| = 0{-}l$. Vertical dotted lines are drawn to separate entropy values of the states with the same quantum number l. All values are in atomic units.

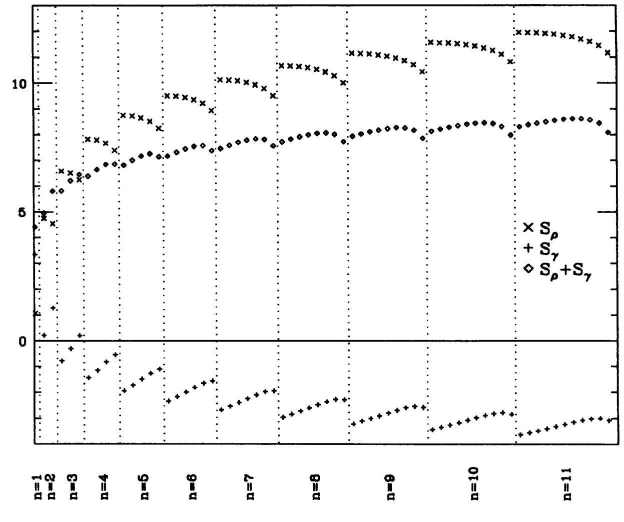

FIG. 8. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the two-dimensional hydrogen atom in the excited states characterized by the quantum numbers $(n, |m|)$ with $n = 1 - 11$ and $|m| = 0 - (n-1)$. Vertical dotted lines are drawn to separate entropy values of the states with the same quantum number n. All values are in atomic units.

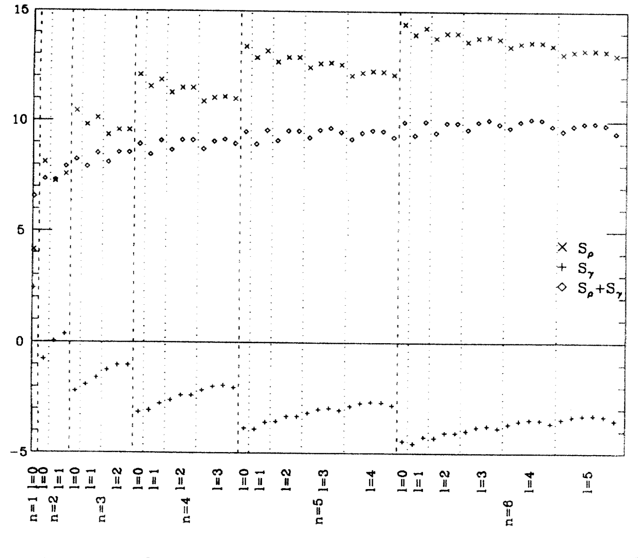

FIG. 9. Information entropies in position space S_ρ and momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the three-dimensional hydrogen atom in the excited states characterized by the quantum numbers $(n, l, |m|)$ with $n = 1 - 6$, $l = 0 - (n-1)$, and $|m| = 0 - l$. Vertical dashed and dotted lines are drawn to separate entropy values of the states with the same n and same l for given n, respectively. All values are in atomic units.

of the one- and two-dimensional atoms but also because we analyzed the trend of the entropies with not only the principal quantum number n but also with the orbital and magnetic quantum number l and m, respectively, in a much larger class of states (n, l, m) of the three-dimensional hydrogen atom.

Indeed, Fig. 8 gives the position and momentum information entropies of the two-dimensional hydrogen atom in the excited states $(n, |m|)$ with $n = 1 - 11$ and all possible values of $|m|$, i.e., $|m| = 0 - (n-1)$. In addition to the above mentioned behavior with n of S_ρ and S_γ, these entropies are such that for a given n the position entropy decreases with $|m|$ and the momentum entropy first enhances up to a maximum and then decreases with increasing $|m|$. This unimodal $|m|$ dependence of S_γ, which is specially apparent for states with a large principal quantum number, is even more striking in the entropy sum $S_\rho + S_\gamma$.

Finally, we display in Fig. 9 the position and momentum information entropies of the three-dimensional hydrogen atom in the excited states $(n, l, |m|)$ with $n = 1 - 6$, $l = 0 - (n-1)$, and $|m| = 0 - l$. Vertical dashed and dotted lines have been drawn to separate out the entropy values of the states with the same principal quantum number n and, for a given n, the same orbital quantum number l, respectively. In addition to the above mentioned behavior with n of S_ρ and S_γ, we observe that (i) the position entropy globally decreases with l for fixed n and has a dependence on m, for fixed (n, l) values, of arc form; (ii) the momentum entropy enhances with l for fixed n and has also a unimodal or arc behavior with m for fixed (n, l) values; and (iii) the values of the entropy sum $S_\rho + S_\gamma$ show a light enhancement with excitation of the system in the region of quantum numbers $(n, l, |m|)$ considered in the present work, always in agreement with the BBM inequality.

VIII. SUMMARY AND OPEN PROBLEMS

The present work is the first step in the analytical determination of the position and momentum information entropies of the D-dimensional $(D \geq 1)$ harmonic oscillator and hydrogen atom for both ground and excited states in terms of the strength of the potential and the quantum numbers which characterize the states under consideration. Each of these entropies are known to decrease without bound when the corresponding probability density becomes more concentrated, that is, when (technically speaking) information increases. However, according to the BBM inequality (4), the sum of both entropies and then the total uncertainty in positions and momenta cannot be decreased beyond a certain value. We have shown that the evaluation of these entropies can be reduced to the calculation of the entropy integrals (9), which involve the classical orthogonal polynomials of Gegenbauer, Hermite, and Laguerre. We have called these integrals entropies of orthogonal polynomials, denoted by E_n, where n is the degree of the involved polynomials.

The complete evaluation of E_n for the classical Jacobi polynomials is an open problem which requires a deep knowledge of the algebraic aspects of the theory of orthogonal polynomials and other analytical methods such as, e.g., potential theory. Here we have illustrated this statement with the calculation of the exact values of the entropies of Chebyshev polynomials $T_n(x) = \lim_{\lambda \to 0} \frac{n}{2} C_n^\lambda(x)$; this has been possible because the algebraic properties of these polynomials are particularly simple and well known. The problem becomes much more complicated for the Gegenbauer polynomials $C_n^\lambda(x)$, where we have calculated the entropies only in an approximate way. Thus the present work urges for the determination of the entropies E_n of general orthogonal polynomials on both compact and noncompact sets as well as its asymptotic (n large) limit. Let us point out that only recently [24] an asymptotic formula for the entropy of general orthogonal polynomials on finite intervals has been obtained by means of the relative entropy of the equilibrium measure and the weight function of these polynomials. This has been possible because the theory of orthogonal polynomials in compact intervals is well established [20]. This is not true in the noncompact case where much more effort is required [25,26].

Finally we have numerically evaluated the information entropies in position space S_ρ and in momentum space S_γ, as well as their sum $S_\rho + S_\gamma$, of the harmonic oscillator and the hydrogen atom to know (i) the dimensionality dependence of the ground-state entropies and (ii) the dependence of these entropies with the excitation of the specific one-, two-, and three-dimensional systems. Let us highlight the following findings.

The position space entropy enhances with the dimensionality of the two quantum-mechanical systems under consideration. The momentum-space entropy has a dimensionally increasing behavior in the oscillator case while it has the opposite one in hydrogen. However, the entropy sum has the same, approximately linear, increasing dependence on the dimensionality in both ground-state systems.

The position-space entropy globally enhances with the excitation of the two systems at any dimensionality. It increases monotonically with increasing values of the principal quantum number n (Figs. 2, 3, 5, and 7). A similar behavior is observed with the second quantum number $|m|$ for the two-dimensional oscillator (Fig. 4).

The momentum-space entropy behaves differently with the excitation in the two systems considered in this work. For the oscillator, it increases monotonically with the principal quantum number n at any dimension and with the quantum number $|m|$ in the two-dimensional case. For hydrogen, S_γ decreases monotonically with increasing values of the principal quantum number.

Both position and momentum entropies present a global dependence on $(l, |m|)$ of unimodal and/or arc form in the three-dimensional oscillator and hydrogen systems.

The total uncertainty or entropy sum $S_\rho + S_\gamma$ enhances with the principal quantum number at any dimensionality and also with $|m|$ in the two-dimensional oscillator case, having a dependence on $(l, |m|)$ of unimodal and/or arc form in the two- and three-dimensional cases.

The theoretical interpretation of all these phenomena requires the evaluation of the entropies of the Gegenbauer, Hermite, and Laguerre polynomials, as well as their asymptotic limits [24–26].

ACKNOWLEDGMENTS

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