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ORIGINAL PAPER

Position and momentum information-theoretic measures of a *D*-dimensional particle-in-a-box

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Abstract The main information-theoretic measures of a one-dimensional particle-in-a-box (also known as the infinite potential well or the infinite square well) in both position and momentum spaces, as well as their associated uncertainty relations, are calculated and discussed. The power and entropic moments, the Shannon, Renyi and Tsallis entropies and the Fisher information together with two composite measures (Fisher–Shannon and LMC shape complexities) are considered. Moreover, the associated information-theoretic spreading lengths, which characterize the spread/delocalization of the particle beyond (but complementarily) the standard deviation, and their corresponding uncertainty relations are given and mutually compared. It is found, in particular, that the Fisher length is the proper measure of uncertainty for the infinite

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well, mainly because it grasps the oscillatory nature of the wavefunctions. Finally, this study is extended to a D-dimensional box.

Keywords Infinite well potential · Information theory · Entropic moments · Renyi entropy · Tsallis entropy · Shannon entropy · Fisher information · LMC shape complexity · Rydberg states · Information-theoretic lengths

1 Introduction

The one dimensional particle-in-a-box model (see e.g. [14,15,26,27] is an ideal system composed by a single point particle moving in an infinite potential well; i.e. on a line segment (the box) where it experiences no force whatsoever (i.e., it is at zero potential energy), except at the endpoints of the segment where the potential rises to infinity; so, forming impenetrable walls. This model is the simplest and, together with the isotropic harmonic oscillator and Coulomb potentials, the most versatile prototype of physical systems and phenomena. Indeed, this ideal system is used in virtually every introductory text on quantum mechanics to illustrate for the first time the main characteristics of the quantum behaviour of a particle (i.e., energy quantization, non-vanishing zero-point energy, spatial nodes), manifesting their sharp contrast with the predictions of classical mechanics [36]. The reason is that the fundamental equation of motion (i.e., Schrödinger equation) of the particle in an infinite potential well can be analytically solved by elementary differential calculus. This is so in one and D-dimensions ($D > 1$). On the other hand, this theoretical model has been frequently used to meet and interpret for the first time numerous real physico-chemical phenomena in atomic and molecular physics [4,31,42], nanotechnology [19,38,42], nuclear physics [6,20], polymer science [22,33], mathematical physics [7], supersymmetric quantum mechanics [10,11] and chaos [21], among others. Recently an experimental realization of the "particle-in-a-box" has been developed by means of a unique system that includes a tightly confined Bose-Einstein condensate in a one-dimensional potential [43].

In this work the particle-in-a-box model is used to illustrate the uncertainty and spreading fundamental variables of the information theory of quantum-mechanical systems. In spite of the fact that this theory is (a) closely related to other theoretical methods such as the density functional theory [32], and (b) on the basis of the modern quantum computation and information [29], this theory is in a state of flux; that is, it has still many open questions. We want to contribute to the knowledge of this theory and to gain insight into its fundamental variables by means of the analysis of the power and entropic moments (and the associated Heisenberg measure and linear entropy) of the quantum-mechanical density of this canonical model and its information-theoretic measures of global (Shannon, Renyi, Tsallis) and local (Fisher) types, as well as some related composite measures, like the Heisenberg-Fisher and Fisher–Shannon products and the LMC shape complexity. Moreover, the uncertainty relations associated to these measures are also discussed.

This paper is structured as follows. First, in Sect. 2, the well-known eigensolutions of the stationary states of the infinite well potential are described in position and momentum spaces. Second, in Sect. 3, the power and entropic moments are explicitly determined for both ground and excited states of the particle-in-a-box in the two reciprocal spaces; let us highlight the values obtained for the momentum entropic moments of the highly excited (Rydberg) states. In Sect. 4 the Shannon, Renyi and Tsallis entropies together with the Fisher information and the Fisher–Shannon and LMC shape complexities of our model are shown. Then, in Sect. 5 the direct spreading measures of the particle confined in the box (i.e. the Heisenberg measure and the information-theoretic lengths of Shannon, Renyi and Fisher types) and their corresponding uncertainty relations are discussed. Finally, the generalization to the D-dimensional box is done in Sect. 6, and some conclusions are given.

2 The infinite potential well: basics

The eigensolutions of the infinite well potential $V(x) = 0$ for $|x| \leq a$ and infinite otherwise, are known to have the expressions [26,27] (units $\hbar = 1$ will be used throughout the paper)

$$\psi_n(x) = \begin{cases} \frac{1}{\sqrt{a}} \sin\left[\frac{\pi n}{2a}(x-a)\right] & \text{for} \quad |x| \leq a \\ 0 & \text{for} \quad |x| > a \end{cases},$$

and

$$E_n = \frac{\pi^2}{8a^2} n^2, \quad n = 1, 2, 3, \ldots, \tag{1}$$

for the position-space eigenfunctions and the energetic eigenvalues, respectively, and

$$\phi_n(p) = \left(\frac{\pi n^2 a}{2}\right)^{1/2} \frac{\sin\left(ap - \frac{\pi n}{2}\right)}{\left(a^2 p^2 - \frac{\pi^2 n^2}{4}\right)} \exp\left(-\frac{\pi n}{2} i\right)$$

for the corresponding eigenfunctions in momentum space. Then, the quantum-mechanical probability density is given by

$$\rho_n(x) = |\psi_n(x)|^2 = \begin{cases} \frac{1}{a} \sin^2\left[\frac{\pi n}{2a}(x-a)\right] & \text{for} \quad |x| \leq a \\ 0 & \text{for} \quad |x| > a \end{cases},$$

in position space and

$$\gamma_n(p) = |\phi_n(p)|^2 = \frac{\pi n^2 a}{2} \frac{\sin^2\left(ap - \frac{\pi n}{2}\right)}{\left(a^2 p^2 - \frac{\pi^2 n^2}{4}\right)^2}, \quad p \in (-\infty, \infty),$$

in momentum space. The comparison with the corresponding classical values has been discussed by Robinett [36].

3 Power and entropic moments

In this section we show the values of the ordinary or power moments $(\langle x^m\rangle_n, \langle p^m\rangle_n)$ and the frequency or entropic moments $\left(\langle\rho_n^k\rangle, \langle\gamma_n^k\rangle\right)$ of the ground and excited states of the infinite well potential. These two set of moments do not only characterize the density but also they describe some fundamental quantities of the system.

3.1 Power moments

The position and momentum probability densities of the physical state characterized by the quantum number n can be completely characterized by the ordinary power moments

$$\langle x^m\rangle_n := \int_{-a}^{a} x^m \rho_n(x)\mathrm{d}x$$

and

$$\langle p^m\rangle_n := \int_{-\infty}^{+\infty} p^m \gamma_n(p)\mathrm{d}p,$$

respectively. We have found that these quantities have the values

$$\begin{aligned}\langle x^{2k}\rangle_n &= \frac{a^{2k}}{2k+1}\left[1+(-1)^{n+1}{}_1F_2\left(\begin{matrix}k+\frac{1}{2}\\ \frac{1}{2}, k+\frac{3}{2}\end{matrix}\middle| -\frac{n^2\pi^2}{4}\right)\right],\\ \langle x^{2k-1}\rangle_n &= 0; \quad k=1,2,\ldots,\end{aligned} \tag{2}$$

in position space, and

$$\begin{aligned}\langle p^{2k}\rangle_n &= \pi n^2 a\int_0^{\infty} p^{2k}\frac{\sin^2\left(ap-\frac{\pi n}{2}\right)}{\left(a^2p^2-\frac{\pi^2n^2}{4}\right)^2}\mathrm{d}p,\\ \langle p^{2k-1}\rangle_n &= 0; \quad k=1,2,\ldots,\end{aligned} \tag{3}$$

in momentum space. We should point out that the expectation values $\langle p^m\rangle$ only exist for $-1 < m < 3$. In particular, Eqs. (2) and (3) give for, the case $k=1$, the values

$$\left\langle x^2\right\rangle = \frac{a^2}{3}\left(1-\frac{6}{\pi^2n^2}\right) \quad \text{and} \quad \left\langle p^2\right\rangle = \left(\frac{\pi n}{2a}\right)^2 \tag{4}$$

for the second-order position and momentum power moments. Remark that $\langle x^2\rangle\langle p^2\rangle = \frac{\pi^2}{12}\left(n^2-\frac{6}{\pi^2}\right) \geq \frac{\pi^2-6}{12} \simeq 0.3216$ so fulfilling the known position-momentum uncertainty relation $\langle x^2\rangle\langle p^2\rangle \geq 1/4$. Moreover, this uncertainty product does not depend on the potential width.

3.2 Entropic moments

The position and momentum probability densities can be alternatively characterized by their corresponding frequency moments (also called entropic moments) defined by

$$\langle \rho_n^{k-1}\rangle := \int_{-a}^{a} [\rho_n(x)]^k \, \mathrm{d}x, \quad k \geq 1,$$

and

$$\langle \gamma_n^{k-1}\rangle := \int_{-\infty}^{+\infty} \left[\gamma_n(p)\right]^k \, \mathrm{d}p, \quad k \geq 1,$$

respectively. We have found the values

$$\begin{aligned}\langle \rho_n^{k-1}\rangle &= \frac{1}{a^k}\int_{-a}^{+a}\left[\sin\left(\frac{\pi n}{2a}(x-a)\right)\right]^{2k} \mathrm{d}x = \frac{1}{2^{2k-1}a^{k-1}}\binom{2k}{k}\\ &= \frac{2\Gamma\left(k+\frac{1}{2}\right)}{a^{k-1}\sqrt{\pi}\,\Gamma(k+1)}\end{aligned} \tag{5}$$

for the position entropic moments, which does not depend on n. From Eqs. (2) and (5) it is worth noting that, contrary to the usual situations for physical systems other than the box, the position entropic moments have a much simpler expression than the power moments. In addition, let us quote that for $k = 1$, $\langle \rho_n^0\rangle = 1$ as expected, and for $k = 2$ we have that the averaging position density is given by the second entropic moment

$$\langle \rho_n\rangle = \frac{3}{4a}. \tag{6}$$

For the momentum entropic moments we have

$$\langle \gamma_n^{k-1}\rangle = \left(\frac{\pi n^2}{2}\right)^k a^{k-1}\mathcal{I}_{n,k}, \tag{7}$$

where the Dirichlet-like trigonometric functional $\mathcal{I}_{n,k}$ is given by

$$\mathcal{I}_{n,k} = \int_{-\infty}^{+\infty} \left[\frac{\sin^2\left(t - \frac{\pi n}{2}\right)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2} \right]^k \mathrm{d}t. \tag{8}$$

This integral can be calculated for a given k, obtaining the values

$$\begin{aligned}
\mathcal{I}_{n,1} &= \frac{2}{\pi n^2}, \\
\mathcal{I}_{n,2} &= \frac{4}{3\pi^3 n^4}\left(1 + \frac{15}{2\pi^2 n^2}\right), \\
\mathcal{I}_{n,3} &= \frac{1}{10\pi^5 n^6}\left(11 + \frac{105}{\pi^2 n^2} + \frac{945}{\pi^4 n^4}\right), \\
\mathcal{I}_{n,4} &= \frac{1}{630\pi^7 n^8}\left(604 + \frac{7560}{\pi^2 n^2} + \frac{69300}{\pi^4 n^4} + \frac{675675}{\pi^6 n^6}\right), \\
\mathcal{I}_{n,5} &= \frac{1}{18144\pi^9 n^{10}}\left(15619 + \frac{242550}{\pi^2 n^2} + \frac{2567565}{\pi^4 n^4} + \frac{23648625}{\pi^6 n^6} + \frac{241215975}{\pi^8 n^8}\right),
\end{aligned} \tag{9}$$

for $k = 1, 2, 3, 4$ and 5, respectively. It is worth noting that $\langle \gamma_n^0 \rangle = 1$, as expected, and that the averaging momentum density $\langle \gamma_n \rangle$ has the value

$$\langle \gamma_n \rangle = \frac{a}{3\pi}\left(1 + \frac{15}{2\pi^2 n^2}\right), \tag{10}$$

according to Eqs. (7) and (9) for $k = 2$. Moreover, we have found that

$$\mathcal{I}_{n,k} \simeq \frac{b_k}{\pi^{2k-1} n^{2k}} \tag{11}$$

for large values of n, where

$$b_k = 4k \sum_{j=0}^{k-1} \frac{(-1)^j (k-j)^{2k-1}}{j!(2k-j)!}; k \geq 1.$$

This result is obtained by making the change of variable $t - \pi n/2 = u$ in the expression (8), that yields

$$\mathcal{I}_{n,k} = 2 \int_{0}^{+\infty} \left[\frac{\sin^2\left(t - \frac{\pi n}{2}\right)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2} \right]^k \mathrm{d}t = 2 \int_{-\frac{\pi n}{2}}^{+\infty} \left[\frac{\sin^2 u}{u^2 (u + \pi n)^2} \right]^k \mathrm{d}u.$$

Since $u + \pi n \simeq \pi n$ for large values of n, we obtain

$$\mathcal{I}_{n,k} \simeq \frac{2}{(\pi n)^{2k}} \int_{-\frac{\pi n}{2}}^{+\infty} \left(\frac{\sin^2 u}{u^2} \right)^k \mathrm{d}u,$$

and, as $-\pi n/2 \to -\infty$,

$$\mathcal{I}_{n,k} \simeq \frac{2}{(\pi n)^{2k}} \int_{-\infty}^{+\infty} \left(\frac{\sin^2 u}{u^2} \right)^k \mathrm{d}u = \frac{4}{(\pi n)^{2k}} \int_{0}^{+\infty} \left(\frac{\sin^2 u}{u^2} \right)^k \mathrm{d}u$$
$$= \frac{4k}{\pi^{2k-1} n^{2k}} \sum_{j=0}^{k-1} \frac{(-1)^j (k-j)^{2k-1}}{j!(2k-j)!},$$

where we have used the relation [3.836.2] of Gradshteyn and Ryzhik [16] in the last equality. Then, the asymptotic behaviour of the momentum entropic moments is given by

$$\langle \gamma_n^{k-1} \rangle \simeq \frac{b_k a^{k-1}}{2^k \pi^{k-1}};\ k \geq 1, n \to +\infty.$$

Moreover, the value of the integral $\mathcal{I}_{n,k}$ is not yet known for n fixed and k generic. Finally, let us point out that the position-momentum product

$$\langle \rho_n^{k-1} \rangle \langle \gamma_n^{k-1} \rangle = \frac{(\pi n^2)^k}{2^{3k-1}} \binom{2k}{k} \mathcal{I}_{n,k}$$

does not depend on the potential width. For highly excited states (i.e. when $n \to \infty$), this product reduces as

$$\langle \rho_n^{k-1} \rangle \langle \gamma_n^{k-1} \rangle \simeq \frac{b_k}{2^{3k-1} \pi^{k-1}} \binom{2k}{k},$$

which does not depend on n. This expression has been shown to satisfy the general Maassen-Uffink-Rajagopal uncertainty relation [25,35] for position and momentum entropic moments.

4 Single and composite information-theoretic measures

Here we give the values of the most relevant single and composite information-theoretic measures of the $1D$ particle-in-a-box in the two reciprocal spaces. First we will consider the (global) Shannon, Renyi and Tsallis entropies together with the (local) Fisher information. Then we will analyze the Fisher–Shannon and LMC shape complexities, which are measures composed by two single information-theoretic quantities, so describing the quantum-mechanical probability spreading of the system in a complementary and more complete manner than their individual components; they have the property to have their minimal values on the extreme ordered and disordered limits.

The *Shannon entropy* of this system in position space $S[\rho_n]$ has been shown [39] to have the value

$$S[\rho_n] := -\int_{-a}^{a} \rho_n(x) \ln \rho_n(x) \mathrm{d}x = \ln(4a) - 1, \tag{12}$$

which does not depend on n. This is because of the periodicity of the density ρ_n as a function of x, i.e. $\rho_n(x) = f(n(x-a))$. The momentum Shannon entropy $S[\gamma_n]$ was monographically discussed by Majernik et al. [26]. They found that

$$S[\gamma_n] := -\int_{-\infty}^{+\infty} \gamma_n(p) \ln \gamma_n(p) \mathrm{d}p = -\ln(4a) + K(n), \tag{13}$$

where $K(n)$ denotes the following trigonometric functional

$$K(n) = \ln\left(\frac{8}{\pi}\right) - \pi \int_{-\frac{\pi n}{2}}^{+\infty} n^2 \frac{\sin^2 t}{(t^2 + \pi n t)^2} \ln\left[n^2 \frac{\sin^2 t}{(t^2 + \pi n t)^2}\right] \mathrm{d}t, \tag{14}$$

which has not yet been exactly calculated up until now. It is known, however, that its asymptotical value is [26]:

$$\lim_{n\to\infty} K(n) = \ln(8\pi) + 2(1-\gamma), \tag{15}$$

where γ is the Euler-Mascheroni constant. Moreover, $K(n)$ has been numerically shown [26] that it increases when n is increasing. Then, the Shannon entropy sum of the particle-in-a-box has the value

$$S[\rho_n] + S[\gamma_n] = K(n) - 1,$$

for $n = 1, 2, 3, \ldots$ For highly excited (Rydberg) states, (i.e. for $n \gg 1$) this entropic sum reduces as

$$S[\rho_n] + S[\gamma_n] \simeq \ln(8\pi) + 1 - 2\gamma \simeq 3.0697, \; n \gg 1.$$

Moreover, the Shannon entropy sum is numerically known to range from 2.212 up to the value 3.0697, so that it fulfils the entropic uncertainty relation $S[\rho] + S[\gamma] \geq \ln \pi + 1 \simeq 2.145$.

The position *Renyi entropy* $R_\alpha[\rho_n]$ of the particle-in-a-box is given by

$$R_\alpha[\rho_n] := \frac{1}{1-\alpha}\ln\left(\int_{-a}^{a}[\rho_n(x)]^\alpha\,\mathrm{d}x\right) \equiv \frac{1}{1-\alpha}\ln\langle\rho_n^{\alpha-1}\rangle$$
$$= \ln a + \frac{1}{1-\alpha}\ln\left(\frac{2\Gamma\left(\alpha+\frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\alpha+1)}\right), \tag{16}$$

where Eq. (5) was taken into account. This quantity was first calculated and extensively discussed by Sánchez-Ruiz [40]. In momentum space, the Renyi entropy of our system is

$$R_\beta[\gamma_n] = \frac{1}{1-\beta}\ln\left(\int_{-\infty}^{+\infty}\left[\gamma_n(x)\right]^\beta\,\mathrm{d}x\right) = \frac{1}{1-\beta}\ln\langle\gamma_n^{\beta-1}\rangle$$
$$= -\ln a + \frac{1}{1-\beta}\ln\left(\left(\frac{\pi n^2}{2}\right)^\beta \mathcal{I}_{n,\beta}\right), \tag{17}$$

where Eqs. (7) and (8) have been taken into account. It follows that the sum of the position and momentum Renyi entropies does not depend on the potential width. Moreover, taking into account (16) and (17) and (11) one has that the Renyi entropy sum for the Rydberg states (i.e. for large n) simplifies as

$$R_\alpha[\rho_n] + R_\beta[\gamma_n] \simeq \ln\left\{\left[\frac{2\Gamma\left(\alpha+\frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\alpha+1)}\right]^{\frac{1}{1-\alpha}}\left(\frac{b_\beta}{2^\beta\pi^{\beta-1}}\right)^{\frac{1}{1-\beta}}\right\},$$

so that it does not depend on the quantum number n, at least for its leading term. The reader can easily check that this expression satisfies the uncertainty relation for Renyi entropies found independently by Bialynicki-Birula [5] and Zozor and Vignat [47] (see also [46]) which is given by

$$R_\alpha[\rho_n] + R_\beta[\gamma_n] \geq \ln\left[\left(\frac{\beta}{\pi}\right)^{\frac{1}{2(1-\beta)}}\left(\frac{\alpha}{\pi}\right)^{-\frac{1}{2(1-\alpha)}}\right],$$

valid for general densities and $\beta > \alpha$.

The position *Tsallis entropy* of the particle-in-a-box is given by

$$T_q[\rho_n] := \frac{1}{q-1}\left[1-\int_{-a}^{a}[\rho_n(x)]^q\,\mathrm{d}x\right] \equiv \frac{1}{q-1}\left[1-\langle\rho_n^{q-1}\rangle\right]$$
$$= \frac{1}{q-1}\left[1-\frac{2}{a^{q-1}\sqrt{\pi}}\frac{\Gamma\left(q+\frac{1}{2}\right)}{\Gamma(q+1)}\right], \tag{18}$$

where the expression (5) for the position entropic moments was used. Similarly, from (7), it is straightforward to write the following expression for the momentum Tsallis entropy of our system:

$$T_q[\gamma_n] := \frac{1}{q-1}\left[1-\left\langle \gamma_n^{q-1}\right\rangle\right] = \frac{1}{q-1}\left[1-\left(\frac{\pi n^2}{2}\right)^q a^{q-1}\mathcal{I}_{n,q}\right], \qquad (19)$$

where $\mathcal{I}_{n,q}$ is the Dirichlet-like trigonometric functional discussed above (8). Remark that the position and momentum Tsallis entropies satisfy the expression

$$\{1+(1-q)T_q[\rho_n]\}\{1+(1-q)T_q[\gamma_n]\} = \frac{2\Gamma\left(q+\frac{1}{2}\right)}{\sqrt{\pi}\Gamma(q+1)}\left(\frac{\pi n^2}{2}\right)^q \mathcal{I}_{n,q},$$

for both ground and excited states. Moreover, for Rydberg states this expression simplifies as

$$\{1+(1-q)T_q[\rho_n]\}\{1+(1-q)T_q[\gamma_n]\} \simeq \frac{\Gamma\left(q+\frac{1}{2}\right)}{\sqrt{\pi}\Gamma(q+1)}\frac{b_q}{(2\pi)^{q-1}},$$

which does not depend on the potential width a nor the quantum number n. These two expressions can be shown to fulfil the known Maasen-Uffink-Rajagopal uncertainty relation [25,35] satisfied by the position and momentum Tsallis entropies of general systems.

It is interesting to highlight from the comparison of Eqs. (5) and (7), (12) and (13), (16) and (17), and (18) and (19), that the momentum entropic moments and Shannon, Renyi and Tsallis entropies do depend on the quantum number n which characterizes the quantum state under consideration while the corresponding position entropies do not.

Let us now consider the *Fisher information* of the particle-in-a-box. In position space this quantity is defined by

$$F[\rho_n] := \left\langle \left[\frac{d}{dx}\ln\rho_n(x)\right]^2 \right\rangle = \int_{-\infty}^{+\infty} \frac{\left[\rho_n'(x)\right]^2}{\rho_n(x)} dx$$

$$= 4\int_{-\infty}^{+\infty}\left[\frac{d}{dx}\sqrt{\rho_n(x)}\right]^2 dx = 4\int_{-\infty}^{+\infty}\left[\psi_n'(x)\right]^2 dx \qquad (20)$$

$$= 4\langle p^2\rangle = \frac{\pi^2 n^2}{a^2}. \qquad (21)$$

Then, the Fisher information $F[\rho_n]$ measures the gradient content of the position probability density. Since the main contributions to the integral (20) come from the regions where the density is wigglier (i.e. when the density has more nodes per unit argument of x), this quantity (a) provides an estimation of the oscillatory character of the wavefunctions and the density, and (b) has the property of locality since it has the bias to particular points of the configuration space on the system, i.e. the interval $[-a, +a]$ in our case. From Eqs. (1) and (21) one realizes that $E_n = \frac{1}{8}F[\rho_n]$, indicating, in particular, that the state with the least gradient contain (so, the least curvature; so, with no nodes save the zeros at the two borders of the box) in position space lies lowest. Moreover, in general, the Fisher information controls the energy spectrum of the system.

In momentum space the Fisher information $F[\gamma_n]$ of the particle-in-a-box model can be obtained in a parallel way. We have

$$F\left[\gamma_n\right] = \int_{-\infty}^{+\infty} \frac{\left[\gamma_n^{'}(p)\right]^2}{\gamma_n(p)} \mathrm{d}p = 4 \int_{-\infty}^{+\infty} \left[\phi_n^{'}(p)\right]^2 \mathrm{d}p$$
$$= 4\langle x^2 \rangle = \frac{4a^2}{3}\left(1 - \frac{6}{\pi^2 n^2}\right), \tag{22}$$

where the reciprocity between position and momentum spaces has been taken into account in writing the third equality, and Eq. (4) in the fourth equality. From Eqs. (21) and (22) we have that the Fisher-information product becomes

$$F[\rho_n]F[\gamma_n] = 4\left(\frac{\pi^2 n^2}{3} - 2\right) \geq 4\left(\frac{\pi^2}{3} - 2\right) \simeq 5.15947,$$

which is bounded from below by the constant value 5.15947, so fulfilling the uncertainty relation $F[\rho]F[\gamma] \geq 4$ recently found by Dehesa et al. [12] for all symmetric one-dimensional quantum-mechanical potentials.

Let us now calculate the Fisher–Shannon and LMC shape complexities of our system. The *Fisher–Shannon complexity* [2,3,37] of the probability density $\rho_n(x)$ is defined by

$$C_{FS}[\rho_n] := F[\rho_n]J[\rho_n], \tag{23}$$

where

$$J[\rho_n] := \frac{1}{2\pi e}\exp(2S[\rho_n]) = \frac{8a^2}{\pi e^3} \tag{24}$$

gives the Shannon entropic power of the $1D$ particle-in-a-box. Remark that we have used Eq. (12) for the second equality. Moreover, from Eqs. (21), (23) and (24) we find the value

$$C_{FS}[\rho_n] = \frac{8\pi n^2}{e^3}, \quad n = 1, 2, \ldots,$$

for the position Fisher–Shannon complexity of the system. Similarly, from Eqs. (13), (14) and (22) we obtain the value

$$C_{FS}[\gamma_n] := F[\gamma_n]J[\gamma_n] = \frac{\exp(2K(n))}{24\pi e}\left(1 - \frac{6}{\pi^2 n^2}\right) \geq \frac{\pi^2 - 6}{24\pi^3 e}\exp(K(1)),$$

where $K(1) \simeq 3.212\ldots$, for the momentum Fisher–Shannon complexity of the system. It is interesting to point out that, taking into account Eq. (15), this quantity simplifies for Rydberg states (i.e. for large n) as

$$C_{FS}[\gamma_n] \simeq \frac{8\pi}{3e}e^{4(1-\gamma)},$$

which does not depend on the quantum number n.

The *LMC shape complexity* [8,23] of the particle in a box is given by the known [24] value

$$C_{LMC}[\rho_n] := \langle\rho_n\rangle e^{S[\rho_n]} = \frac{3}{e}$$

in position space, where we have taken into account Eqs. (6) and (12) for the averaging density and the Shannon entropy respectively. Remark that it does not depend on n. Similarly, we find from Eqs. (10) and (13) the value

$$C_{LMC}[\gamma_n] := \langle\gamma_n\rangle e^{S[\gamma_n]} = \frac{e^{K(n)}}{12\pi}\left(1 + \frac{15}{2\pi^2 n^2}\right)$$

for the momentum shape complexity of the system. Here again we observe that for Rydberg states

$$C_{LMC}[\gamma_n] \simeq \frac{2}{3}e^{2(1-\gamma)}, \quad n \gg 1$$

where Eq. (15) was taken into account.

5 Direct spreading measures

Here we will discuss the direct spreading measures (standard deviation or Heisenberg measure and the information-theoretic lengths of Renyi, Shannon and Fisher) of the $1D$ particle in a box. They quantify the spreading of the probability density most appropriately. Indeed, contrary to the information-theoretic measures discussed in the previous section, the direct spreading measures have the same units as the random variable and they satisfy the three following properties: translation and reflection invariance, linear scaling and vanishing as the density approaches to a Dirac delta. These quantities will be calculated by use of the expressions found in Sect. 3 for the ordinary and entropic moments.

The familiar *Heisenberg uncertainty measure* (i.e, the standard deviation) in both reciprocal spaces, which quantifies the spreading of the probability cloud around the centroid (in our case the origin, since $\langle x\rangle = 0$), has the values

$$\triangle x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\langle x^2\rangle} = \frac{a}{\sqrt{3}}\sqrt{1 - \frac{6}{\pi^2 n^2}}, \tag{25}$$

and

$$\triangle p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\langle p^2\rangle} = \frac{\pi n}{2a},$$

in position and momentum spaces, respectively, as it is already known [9,34]. It is worth noticing that for large values of the quantum number n, the momentum Heisenberg measure increases linearly while the corresponding position measure tends towards the constant value $a/\sqrt{3}$. The former can be explained because the momentum probability is mainly concentrated around two symmetrical peaks with respect to the origin, whose mutual distance increases with n.

In addition it is observed that the position-momentum uncertainty product

$$\triangle x \triangle p = \frac{1}{2\sqrt{3}}\sqrt{\pi^2 n^2 - 6}, \qquad n = 1, 2, \ldots,$$

which satisfies the inequality $\triangle x \triangle p \geq \frac{\sqrt{\pi^2-6}}{2\sqrt{3}} = 0.5679$, so fulfilling the celebrated Heisenberg uncertainty relation $\triangle x \triangle p \geq \frac{1}{2}$. In addition, this product does not depend on the width of the box [26]. This property, according to which the position-momentum uncertainty product does not depend on the parameters of the potential well, has been also shown for the class of homogeneous quantum-mechanical potentials [41,42]; moreover, it is possibly universally valid for all the position-momentum uncertainty relations. This is true not only for the information-theoretic measures considered in this work as it is shown later on, but also for many quantum-mechanical potentials other than the infinite square well.

Let us now calculate the information-theoretic lengths which, in contrast to the standard deviation, do not depend on any specific point of the interval $[-a, +a]$ where the particle is moving in. From Eqs. (12), (13) and (14) we have the following expressions

$$L^S[\rho_n] = \exp(S[\rho_n]) = \frac{4a}{e},$$

and

$$L^S[\gamma_n] = \exp(S[\gamma_n]) = \frac{\exp(K(n))}{4a},$$

for the position and momentum *Shannon length*, respectively, where $K(n)$ is given by Eq. (14). Then, the position-momentum Shannon product is

$$L^S[\rho_n]L^S[\gamma_n] = C_n,$$

where $C_n = \exp[K(n) - 1]$ for a generic quantum state and $C_n = 8\pi \exp(1 - 2\gamma)$ for Rydberg states, where γ is the Euler-Mascheroni constant, according to Eq. (15). Remark that in both cases it is fulfilled the general Shannon-length-based uncertainty relation $L^S[\rho_n]L^S[\gamma_n] \geq \pi e$.

On the other hand, Hall [17] has defined the *Renyi lengths* of order α as

$$\begin{aligned} L_\alpha^R[\rho_n] &:= \exp(R_\alpha[\rho_n]) = \langle[\rho_n]^{\alpha-1}\rangle^{-\frac{1}{\alpha-1}} \\ &= \left\{\int_{-\infty}^{+\infty} [\rho_n(x)]^\alpha \, dx\right\}^{-\frac{1}{\alpha-1}}; \quad (\alpha > 0, \alpha \neq 1). \end{aligned}$$

Remark that the Onicescu or Heller length corresponds to the first order Renyi length. The reciprocals of these quantities have been used as indirect measures of the uncertainty by Maasen and Uffink [25,44]. Moreover, they are closely connected to other measures of uncertainties of quantum systems [13,45]. We obtain, taking into account (5) and (7), the values

$$L_\alpha^R[\rho_n] = 2^{2+\frac{1}{\alpha-1}} a \binom{2\alpha}{\alpha}^{-\frac{1}{\alpha-1}}$$

and

$$L_\beta^R[\gamma_n] = \left\langle[\gamma_n]^{\beta-1}\right\rangle^{-\frac{1}{\beta-1}} = \frac{1}{a}\left[\left(\frac{\pi n^2}{2}\right)^\beta \mathcal{I}_{n,\beta}\right]^{-\frac{1}{\beta-1}},$$

for the position and momentum Renyi lengths, respectively. Then, the product of these two Renyi lengths is

$$L_\alpha^R[\rho_n]L_\beta^R[\gamma_n] = A_{\alpha,\beta}(n),$$

with

$$A_{\alpha,\beta}(n) = 2^{2+\frac{1}{\alpha-1}} \binom{2\alpha}{\alpha}^{-\frac{1}{\alpha-1}} \left[\left(\frac{\pi n^2}{2}\right)^\beta \mathcal{I}_{n,\beta}\right]^{-\frac{1}{\beta-1}},$$

for a given quantum state, and

$$A_{\alpha,\beta}(n) \simeq 2^{3+\frac{1}{\alpha-1}+\frac{1}{\beta-1}} \pi \binom{2\alpha}{\alpha}^{-\frac{1}{\alpha-1}} b_\beta^{-\frac{1}{\beta-1}},$$

for Rydberg states, which fulfils the general Renyi-length-based uncertainty relation [13,17].

A particularly relevant case is the Renyi length of first order (also called Onicescu or Heller length, linear entropy, collision length, inverse participation ratio or inverse averaging density in other contexts) is defined by the inverse of the entropic moment of second order [30]; that is,

$$L^O\left[\rho_n\right] = L_2^R\left[\rho_n\right] = \frac{1}{\langle \rho_n \rangle} = \frac{4}{3}a,$$

in position space, and

$$L^O\left[\gamma_n\right] = L_2^R\left[\gamma_n\right] = \frac{1}{\langle \gamma_n \rangle} = \frac{1}{a}\frac{3\pi}{\frac{15}{2\pi^2 n^2}+1},$$

in momentum space, where we have used Eqs. (6) and (10), respectively. Notice that the position Onicescu-Heller length does not depend on the quantum number n in contrast to the corresponding Heisenberg measure. Moreover, the momentum length tends to the constant value $3\pi/a$ for large values of n.

The associated position-momentum product has the expression

$$L^O\left[\rho_n\right] L^O\left[\gamma_n\right] = \frac{4\pi}{\frac{15}{2\pi^2 n^2}+1},$$

which does not depend on the width a, fulfils that $L^O\left[\rho_n\right] L^O\left[\gamma_n\right] \geq \frac{8\pi^3}{2\pi^2+15} = 7.1404$, and tends to the constant value 4π when n goes to infinity. Let us remark that there does not exist a general uncertainty relation for the Onicescu-Heller measures similar to the Heisenberg relation for the standard deviation.

The position *Fisher length* of the particle is thus given by

$$(\delta x)_n := \frac{1}{\sqrt{F[\rho_n]}} = \frac{a}{\pi n}, \tag{26}$$

where we have used Eq. (21).

It is worth noticing that the three Heisenberg $(\triangle x)$, Onicescu-Heller (L_n) and the Fisher (δx) measures of the particle delocalization depend on the potential width, and that they satisfy the inequalities

$$(\delta x)_n < (\triangle x)_n < L_{\alpha_1}^R[\rho_n] < L_{\alpha_2}^R[\rho_n] \quad \text{for } \alpha_1 > \alpha_2, \tag{27}$$

where, as $\lim_{\alpha\to 1} L_\alpha^R[\rho_n] = L^S[\rho_n]$, the Shannon length would be equivalent to the Renyi length of order 1: $L_1^R[\rho_n] \equiv L^S[\rho_n]$. This chain of inequalities clearly indicates that the Fisher length is a more appropriate measure of uncertainty for the infinite potential well than the standard-deviation-based Heisenberg and Renyi lengths. Moreover, Eq. (26) shows that in the high energy limit (i.e. when n becomes large) the Fisher length tends to zero indicating that the particle becomes completely localized since then the particle behaves classically. Then, the momentum Fisher length is defined as

$$(\delta p)_n = \frac{1}{\sqrt{F[\gamma_n]}} = \frac{\sqrt{3}}{2a} \frac{1}{\sqrt{1 - \frac{6}{\pi^2 n^2}}}, \tag{28}$$

which tends to the constant value $\frac{\sqrt{3}}{2a}$ when n goes to infinity.

The uncertainty relation fulfilled by these Fisher measures is given by

$$(\delta x)_n \, (\delta p)_n = \frac{\sqrt{3}}{2\sqrt{\pi^2 n^2 - 6}},$$

which again does not depend on the potential width, and satisfies the inequalities

$$0 \leq (\delta x)_n \, (\delta p)_n \leq \frac{\sqrt{3}}{2\sqrt{\pi^2 - 6}} = 0.4402.$$

More interesting is the combination of Eqs. (25) and (28), which yields the following exact uncertainty relation

$$(\triangle x)_n \, (\delta p)_n = \frac{1}{2},$$

which has general validity [18].

6 Generalization to *D* dimensions

In D-dimensions, the infinity well potential has the form

$$V(\vec{r}) = \begin{cases} 0, & \text{if } \vec{r} \in \mathcal{B} \\ +\infty, & \text{if } \vec{r} \notin \mathcal{B} \end{cases},$$

where, in Cartesian coordinates, $\vec{r} = (x_1, x_2, \ldots, x_D)$, and $\mathcal{B} = \{\vec{r} \in \mathbb{R}^D; |x_i| \leq a, \forall i, 1 \leq i \leq D\}$.

In these coordinates the position and momentum eigenfunctions can be fairly easily obtained from the corresponding ones of the one dimensional case. We have the eigenfunctions

$$\psi_{\{n\}}(\vec{r}) = \begin{cases} \frac{1}{a^{D/2}} \prod_{i=1}^{D} \sin\left[\frac{\pi n_i}{2a}(x_i - a)\right], & \text{if } \vec{r} \in \mathcal{B} \\ 0, & \text{if } \vec{r} \notin \mathcal{B} \end{cases},$$

in position space, and

$$\phi_{\{n\}}(\vec{p}) = \left(\frac{\pi a}{2}\right)^{D/2} \prod_{i=1}^{D} n_i \frac{\sin\left(ap_i - \frac{\pi n_i}{2}\right)}{\left(a^2 p_i^2 - \frac{\pi^2 n_i^2}{4}\right)} \exp\left(-\frac{\pi n_i}{2} i\right), \quad \vec{p} \in \mathbb{R}^D,$$

in momentum space, where $\vec{p} = (p_1, p_2, \ldots, p_D)$. The symbol $\{n\} \equiv \{n_1, n_2, \ldots, n_D\}$ denotes the set of quantum numbers associated to each coordinate, which characterize a generic quantum-mechanical state of the D-dimensional box.

Then, the quantum-mechanical probability densities are given by

$$\rho_{\{n\}}(\vec{r}) = |\psi_{\{n\}}(\vec{r})|^2 = \begin{cases} \frac{1}{a^D} \prod_{i=1}^{D} \sin^2\left[\frac{\pi n_i}{2a}(x_i - a)\right], & \text{if } \vec{r} \in \mathcal{B} \\ 0, & \text{if } \vec{r} \notin \mathcal{B} \end{cases},$$

and

$$\gamma_{\{n\}}(\vec{p}) = |\phi_{\{n\}}(\vec{p})|^2 = \left(\frac{\pi a}{2}\right)^D \prod_{i=1}^{D} n_i^2 \frac{\sin^2\left(ap_i - \frac{\pi n_i}{2}\right)}{\left(a^2 p_i^2 - \frac{\pi^2 n_i^2}{4}\right)^2}, \quad \vec{p} \in \mathbb{R}^D,$$

in position space and momentum spaces, respectively.

6.1 Power and entropic moments

The advantage of working in Cartesian coordinates is that, once known the results in the one-dimensional case, we can obtain directly the results in D-dimensions. The position and momentum power moments in D-dimensions can be defined as

$$\langle r^m \rangle_{\{n\}} := \int_{\mathcal{B}} r^m \rho_{\{n\}}(\vec{r}) \mathrm{d}^D r,$$
$$\langle p^m \rangle_{\{n\}} = \int_{\mathcal{R}^D} p^m \gamma_{\{n\}}(\vec{p}) \mathrm{d}^D p,$$

respectively. Taking into account that $r = (x_1^2 + x_2^2 + \cdots + x_D^2)^{1/2}$ and $p = (p_1^2 + p_2^2 + \cdots + p_D^2)^{1/2}$, we have the following expressions

$$\langle r^{2k} \rangle_{\{n\}} = \sum_{k_1, k_2, \ldots k_D} \frac{2}{a^D} \frac{k!}{k_1! k_2! \cdots k_D!} \prod_{i=1}^{D} \int_0^a x_i^{2k_i} \sin^2\left(\frac{\pi n_i}{2a}(x_i - a)\right) \mathrm{d}x_i$$
$$= k! \sum_{k_1, k_2, \ldots, k_D} \prod_{i=1}^{D} \frac{a^{2k_i}}{(2k_i + 1) k_i!}$$
$$\times \left[1 + (-1)^{n_i+1} {}_1F_2\left(\begin{matrix} k_i + 1/2 \\ 1/2, k_i + 3/2 \end{matrix} \middle| -\frac{\pi^2 n_i^2}{4}\right)\right], \quad k = 1, 2, \ldots,$$

and

$$\langle p^{2k}\rangle_{\{n\}} = \sum_{k_1,k_1,\ldots k_D} \frac{2}{a^D}\frac{k!}{k_1!k_2!\cdots k_D!}\prod_{i=1}^{D}\frac{\pi a n_i^2}{2}\int_0^{+\infty} p_i^{2k_i}\frac{\sin^2\left(ap_i-\frac{\pi n_i}{2}\right)}{\left(a^2p_i^2-\frac{\pi^2 n_i^2}{4}\right)^2}\mathrm{d}p_i,$$
$$k = 1, 2, \ldots,$$

for the position and momentum power moments, respectively. For completeness, let us point out that the power moments of order $2k-1$ are not obtained in such a simple way, because they require a more elaborated discussion. The sums run over the indices $k_1,\ldots,k_D$ such that $k_1+k_2+\cdots+k_D = k$. In these expressions we have used the multinomial theorem

$$(a_1+a_2+\cdots+a_m)^n = n!\sum_{k_1,k_2,\ldots,k_m}\left(\prod_{i=1}^{m}\frac{a_i^{k_i}}{k_i!}\right),\quad k_1+k_2+\cdots+k_m = n,$$

in the first equality. Remark that, as in the one-dimensional case, $\langle p^m\rangle$ only exists for $-1 < m < 3$. In particular, for $k = 1$ one has the values

$$\left\langle r^2\right\rangle_{\{n\}} = \frac{a^2}{3}\sum_{i=1}^{D}\left(1-\frac{6}{\pi^2 n_i^2}\right) \quad\text{and}\quad \left\langle p^2\right\rangle = \frac{\pi^2}{4a^2}\sum_{i=1}^{D} n_i^2,$$

for the second-order power moments in position and momentum spaces, respectively.

On the other hand, the frequency or *entropic moments* in position and momentum spaces of a D-dimensional particle in a box are given by

$$\langle\rho_{\{n\}}^{k-1}\rangle := \int\left[\rho_{\{n\}}(\vec{r})\right]^k \mathrm{d}^D r = \prod_{i=1}^{D}\frac{1}{a^k}\int_{-a}^{+a}\sin^{2k}\left(\frac{\pi n_i}{2a}(x_i-a)\right)\mathrm{d}x_i$$
$$= \left[\frac{1}{2^{2k-1}a^{k-1}}\binom{2k}{k}\right]^D, \tag{29}$$

and

$$\langle\gamma_{\{n\}}^{k-1}\rangle := \int\left[\gamma_{\{n\}}(\vec{p})\right]^k \mathrm{d}^D p = \prod_{i=1}^{D}\left(\frac{\pi a}{2}\right)^k n_i^{2k}\int_{-\infty}^{+\infty}\frac{\sin^{2k}\left(ap_i-\frac{\pi n_i}{2}\right)}{\left(a^2p_i^2-\frac{\pi^2 n_i^2}{4}\right)^{2k}}\mathrm{d}p_i$$
$$= \prod_{i=1}^{D}\left(\frac{\pi n_i^2}{2}\right)^k a^{k-1}\mathcal{I}_{n_i,k}, \tag{30}$$

respectively. Remark that the integrals $\mathcal{I}_{n_i,k}$ were explicitly expressed and discussed in Sect 3.2. The use of those expressions allows us to obtain, in particular, the value

$$\langle \gamma_{\{n\}} \rangle = \left(\frac{a}{3\pi}\right)^D \prod_{i=1}^{D} \left(1 + \frac{15}{2\pi^2 n_i^2}\right),$$

for the momentum second order entropic moment of a generic quantum state $\{n\}$, and the value

$$\langle \gamma_{\{n\}}^{k-1} \rangle \simeq \left(\frac{b_k a^{k-1}}{2^k \pi^{k-1}}\right)^D, \; k \geq 1, \; n_i \to \infty \text{ for all } i = 1, \ldots, D,$$

for the Rydberg states of the particle in a D-dimensional box. Moreover, the product of the position and momentum entropic moments of this system satisfies the relation

$$\langle \rho_{\{n\}}^{k-1} \rangle \langle \gamma_{\{n\}}^{k-1} \rangle = \left(\frac{\pi^k}{2^{3k-1}} \binom{2k}{k}\right)^D \prod_{i=1}^{D} n_i^{2k} \mathcal{I}_{n_i,k},$$

which for Rydberg states simplifies as

$$\langle \rho_{\{n\}}^{k-1} \rangle \langle \gamma_{\{n\}}^{k-1} \rangle \simeq \left[\frac{b_k}{2^{3k-1} \pi^{k-1}} \binom{2k}{k}\right]^D.$$

It is worth noting again that this expression does not depend on the box length a nor on the principal quantum numbers n_i.

6.2 Information-theoretic measures

As in the case of one-dimensional box, we can calculate the Shannon, Renyi and Tsallis entropies, and the Fisher information for the particle confined in a D-dimensional box. Let us begin with the *Shannon entropy*, which has the expression

$$\begin{aligned}
S\left[\rho_{\{n\}}\right] &= -\int_{\mathcal{B}} \rho_{\{n\}}(\vec{r}) \ln \rho_{\{n\}}(\vec{r}) \mathrm{d}^D r \\
&= -\sum_{i=1}^{D} \left\{ \frac{1}{a} \int_{-a}^{+a} \sin^2\left(\frac{\pi n_i}{2a}(x_i - a)\right) \ln\left(\frac{1}{a} \sin^2\left(\frac{\pi n_i}{2a}(x_i - a)\right)\right) \mathrm{d}x_i \right\} \\
&= \sum_{i=0}^{D} (\ln 4a - 1) = D\left(\ln 4a - 1\right),
\end{aligned}$$

for the position spaces. In momentum space we obtain that

$$S[\gamma_{\{n\}}] = -D\ln(4a) + \sum_{i=1}^{D} K(n_i),$$

where $K(n_i)$ is given by Eq. (14). Then, the Shannon entropy sum

$$S[\rho_{\{n\}}] + S[\gamma_{\{n\}}] = \sum_{i=1}^{D} K(n_i) - D,$$

which has a constant value, non-dependent on a, for a given set of quantum numbers $\{n\}$, i.e. for each quantum state of the system.

In terms of the entropic moments (29), it is straightforward to obtain the position *Renyi entropy* as

$$R_\alpha\left[\rho_{\{n\}}\right] = \frac{1}{1-\alpha}\ln\langle\rho_{\{n\}}^{\alpha-1}\rangle = D\ln a + \frac{D}{1-\alpha}\ln\left(\frac{2\Gamma\left(\alpha+\frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\alpha+1)}\right),$$

which was first pointed out in Ref. [40]. For the value $\alpha = 2$, this measure has a very simple form

$$R_2\left[\rho_{\{n\}}\right] = D\ln\left(\frac{4a}{3}\right),$$

which only depends on the width of the box a, and does not depend on the quantum numbers $\{n\}$.

From Eq. (30) we can obtain similarly the momentum Renyi entropy $R_\beta[\gamma_{\{n\}}]$ in terms of the integrals $\mathcal{I}_{n_i}$ already analyzed in Sect. 3.2. In particular, for $\beta = 2$ we have

$$R_2\left[\gamma_{\{n\}}\right] = -\ln\langle\gamma_{\{n\}}\rangle = D\ln\left(\frac{3\pi}{a}\right) - \sum_{i=1}^{D}\ln\left(\frac{15}{2\pi^2 n_i^2} + 1\right).$$

Remark that, from Eqs. (29) and (30), the Renyi entropy sum is

$$R_2[\rho_{\{n\}}] + R_2[\gamma_{\{n\}}] = D\ln(4\pi) - \sum_{i=1}^{D}\ln\left(\frac{15}{2\pi^2 n_i^2} + 1\right)$$

which, here again, does not depend on a. Extension of this expression to the general (α, β)-Renyi uncertainty relation is straightforward.

The *Tsallis entropy* is found to have the expression

$$T_q\left[\rho_{\{n\}}\right]=\frac{1}{q-1}\left[1-\int[\rho_{\{n\}}(\vec{r})]^q \mathrm{d}^D r\right]=\frac{1}{q-1}\left[1-\langle\rho_n^{q-1}\rangle\right]$$
$$=\frac{1}{q-1}\left[1-\left(\frac{2}{a^{q-1}\sqrt{\pi}}\frac{\Gamma\left(q+\frac{1}{2}\right)}{\Gamma\left(q+1\right)}\right)^D\right], \tag{31}$$

in position space. For $q=2$, we obtain $T_2(\rho_n)=1-\left(\frac{3}{4a}\right)^D$. As in the case of the previous information measure, T_2 does not depend on the quantum numbers $\{n\}$.

In momentum space, we can easily express the momentum Tsallis entropy $T_q[\gamma_{\{n\}}]$ in terms of the Dirichlet-type functionals $\mathcal{I}_{n_i,q}$ previously calculated in Sect. 3.2 by use of Eq. (30). From this expression and Eq. (31) one can directly obtain the corresponding (q,p)-Tsallis uncertainty relation of the D-dimensional quantum box.

In position space the *Fisher information* is given by

$$F\left[\rho_{\{n\}}\right]:=\left\langle\left[\vec{\nabla}\ln\rho_{\{n\}}(\vec{r})\right]^2\right\rangle=\int\frac{\left[\vec{\nabla}\rho_{\{n\}}(\vec{r})\right]^2}{\rho_{\{n\}}(\vec{r})}\mathrm{d}^D r$$
$$=4\langle p^2\rangle=\frac{\pi^2}{a^2}\sum_{i=1}^{D}n_i^2, \tag{32}$$

and, in a parallel way, we can obtain this quantity in momentum space

$$F\left[\gamma_{\{n\}}\right]=\left\langle\left[\vec{\nabla}\ln\gamma_{\{n\}}(\vec{p})\right]^2\right\rangle=\int\frac{\left[\vec{\nabla}\gamma_{\{n\}}(\vec{p})\right]^2}{\gamma_{\{n\}}(\vec{p})}\mathrm{d}^D p$$
$$=4\langle r^2\rangle=\frac{4a^2}{3}\sum_{i=1}^{D}\left(1-\frac{6}{\pi^2 n_i^2}\right). \tag{33}$$

Then, from Eqs. (32) and (33), we have that the product of the position and momentum Fisher informations is

$$F[\rho_{\{n\}}]F[\gamma_{\{n\}}]=\frac{4\pi^2}{3}\left(\sum_{i=1}^{D}n_i^2\right)\sum_{i=1}^{D}\left(1-\frac{6}{\pi^2 n_i^2}\right),$$

which does not depend on the width a, either.

Finally let us now point out that the *Fisher–Shannon and LMC shape complexities* of our system can be also be computed. Indeed, we find the values

$$C_{FS}[\rho_{\{n\}}]=F[\rho_{\{n\}}]J[\rho_{\{n\}}]=\pi a^{2D-2}2^{4D-1}e^{-2D-1}\sum_{i=1}^{D}n_i^2,$$

in position space, and

$$C_{FS}[\gamma_{\{n\}}] = F[\gamma_{\{n\}}]J[\gamma_{\{n\}}] = \frac{2^{1-4D}a^{2-2D}}{3\pi e}\left(\prod_{i=1}^{D} e^{K(n_i)}\right)\sum_{i=1}^{D}\left(1-\frac{6}{\pi^2 n_i^2}\right),$$

in momentum space for the Fisher–Shannon complexity. Notice that these quantities, contrary to the one-dimensional case, depend on the size a of the box. Moreover, for the LMC shape complexities we have obtained the values

$$C_{LMC}[\rho_{\{n\}}] = \langle\rho_{\{n\}}\rangle e^{S[\rho_{\{n\}}]} = \left(\frac{3}{e}\right)^{D},$$

in position space (see [24]), and

$$C_{LMC}[\gamma_{\{n\}}] = \langle\gamma_{\{n\}}\rangle e^{S[\gamma_{\{n\}}]} = (12\pi)^{-D}\prod_{i=1}^{D}\left(1+\frac{15}{2\pi^2 n_i^2}\right)e^{K(n_i)},$$

in momentum space. Let us also point out that for a three-dimensional box we have that the LMC shape complexity is equal to $(3/e)^3 = 1.3207\ldots$ for any quantum state, not only the ground state as given by Ref. [28].

7 Conclusions and open problems

The particle in a box is a useful prototype for the description of "nearly free" particles in atomic nuclei, atomic clusters, molecules and solids, especially because the wave-functions of its stationary states are sufficiently simple that they can be expressed by means of trigonometric functions. Yet, its solutions possess a number of important properties of a general nature (some of them not yet analyzed) which appear over and over again in numerous fields ranging from density functional theory of many-electron systems till the modern quantum information and computation.

In this work we have studied the quantities which measure the spread of the probability cloud of a particle in a box far beyond than the standard deviation or Heisenberg measure. We have considered not only the power moments but also the frequency or entropic moments of this canonical model together with their associated Shannon, Renyi and Tsallis entropies and Fisher information. We have observed that the entropic moments and the Shannon entropy in position space (and consequently the Renyi and Tsallis entropies and the LMC shape complexity) do not depend on the quantum number which characterizes the physical states of the box. Also, it is found that the Shannon, Renyi, Tsallis and Fisher uncertainty relations do not depend on the width a of the box.

We would like to highlight the results obtained here for the direct spreading measures of the model which are described by the information-theoretic lengths of Shannon, Renyi and Fisher types together with the standard deviation because these four measures share the following properties: same units as the variable, translation and reflection invariance, linear scaling and vanishing when the density tends to a Dirac delta. The mutual comparison among them has allowed us to conclude that the Fisher length (26) is the proper uncertainty measure for the infinite well potential. Moreover, the uncertainty relations to all the spreading measures have been given and their explicit expressions for highly excited states have been also pointed out. The generalization to D dimensions has been also considered and discussed.

Another possible extension, not yet accomplished, is the inclusion of relativistic effects [1] but this lies beyond the scope of the present work. Let us also point out that the explicit expression of the Dirichlet-type functionals $\mathcal{I}_{n,k}$ (as well as a recurrence relation) would be desirable to know for a generic k because it would open the way to deeply examine the Renyi and Tsallis entropies of the particle-in-a-box. Finally, it is worth to highlight the relevance of computing of the Hall's spreading or ensemble volumes [17] of the D-dimensional box (so, generalizing to D-dimensions the spreading length of the one-dimensional box), which is a difficult open problem by itself.

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