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Entropy and complexity analysis of Dirac-delta-like quantum potentials

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A B S T R A C T

The Dirac-delta-like quantum-mechanical potentials are frequently used to describe and interpret numerous phenomena in many scientific fields including atomic and molecular physics, condensed matter and quantum computation. The entropy and complexity properties of potentials with one and two Dirac-delta functions are here analytically calculated and numerically discussed in both position and momentum spaces. We have studied the information-theoretic lengths of Fisher, Rényi and Shannon types as well as the Cramér–Rao, Fisher–Shannon and LMC shape complexities of the lowest-lying stationary states of one-delta and twin-delta. They allow us to grasp and quantify different facets of the spreading of the charge and momentum of the system far beyond the celebrated standard deviation.

1. Introduction

The elementary one-dimensional potentials $V(x)$ are interesting *per se* and because they provide approximate models for the physically correct three-dimensional quantum-mechanical potentials of physical systems. Moreover, they are very useful for the interpretation of numerous microscopic and macroscopic properties of natural systems, mainly because their associated quantum-mechanical equation of motion can be exactly solved, so that their physical solutions (wavefunctions) are known to be expressed in terms of special functions of applied mathematics and mathematical physics [1,2]. This is the case for the piecewise-constant potentials (finite and infinite wells), harmonic oscillator ($V \sim x^2$), Coulomb potential ($V \sim 1/|x|$) and delta-function potential ($V = \delta(x)$), to mention just a few although they do not abound.

Recently the emerging information theory of quantum systems, which is at the basis of the modern quantum information and quantum computation, provides the best methodology to quantify the various facets of the charge and momentum spreading all over the confinement region of the system, far beyond the well-known standard deviation or Heisenberg measure. This quantification is carried out by means of various information-theoretic functionals (such as the Fisher information, the Rényi and Shannon entropies, and the associated information-theoretic lengths) and complexity measures (such as the Cramér–Rao, Fisher–Shannon and LMC ones). Such a work has been partially done for the infinite well [3–6], finite well [7], the harmonic oscillator [8,9] and Coulomb potential [8,9], and other potentials [10,11] but the Dirac-delta-like ones still remain to be explored within that framework, to the best of our knowledge. Here we want to contribute to fill this lacuna.

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The one-dimensional Dirac-delta-function potential $\delta(x)$, where x is the Cartesian coordinate, $-\infty < x < \infty$, has been shown to be very useful to describe a number of properties not only for the three-dimensional hydrogen atom and molecule ion [12–15] but also in D-dimensional physics [16,17]. Moreover, this function has been proved to describe short-range potentials such as the interaction between the electrons and fixed ions in a lattice crystal. The use of potentials composed by an array of N-delta functions is very frequent in atomic and molecular physics [18,19,12,15,14], condensed matter [20–22] and quantum computation [23]. Let us just mention the useful Kronig–Penney model to study the physical and chemical properties of solids (see e.g. [20]) and the numerous works done to describe the behavior of impurities in solid-state systems, particularly quantum wires (see e.g. [24,21,25] and references therein) and to characterize the instantaneous interaction between flying and static qubits (see e.g. [23] and references therein).

In this paper we will first calculate the position and momentum entropy and complexity measures of the bound-state wavefunctions of the one-dimensional hydrogen atom with a delta-function interaction, which has been used to study different phenomena of bosonic [26,27], fermionic [18,14,15,12] and anionic [17] systems. In addition, we will compute these quantities for the wavefunctions of the single-particle systems with a twin delta-function potential, which has been used to approximate the helium atom [19,12], the hydrogen molecule ion [14,12,15] and some scattering [28] and solid-state [22] phenomena.

The structure of the paper is the following. First, in Section 2, we give the definitions and meaning of the information-theoretic measures of a general probability density which will be used later in this work to characterize the spreading and the complexity of the quantum-mechanical probability density of the wavefunctions for the one-delta and twin-delta potentials. Then, in Section 3, we obtain the direct spreading measures and the complexity measures of the one-dimensional hydrogen atom with a single-delta potential; namely, the standard deviation and the Fisher, Rényi and Shannon information-theoretic lengths in the two reciprocal spaces. In Section 4, we carry out a similar study for a single-particle system with a twin-delta interaction. The previous analytical results are numerically analyzed in Section 5. Finally we give some conclusions and open problems.

2. Information-theoretic description of a probability density

The information theory for a one-dimensional continuous probability distribution $\rho(x)$ corresponding to some random variable X (e.g. position, momentum, phase, …) provides a number of measures to quantify the spread (or uncertainty) of X over an interval $\Delta \subseteq \Re$ [29,30] far beyond the statistical root-mean-square or standard deviation

$$\Delta x \equiv \left(\langle x^2\rangle - \langle x\rangle^2\right)^{\frac{1}{2}} \tag{1}$$

where $\langle f(x)\rangle$ denotes the expectation value given by

$$\langle f(x)\rangle = \int_\Delta f(x)\rho(x)\mathrm{d}x. \tag{2}$$

The choice $f(x) = x^q$ (i.e., $\langle x^q\rangle$) provides the so-called moment of order q of the probability distribution $\rho(x)$. The most relevant information-theory-based spreading measures of $\rho(x)$ seem to be up until now the Rényi and Shannon entropies and the Fisher information. The Rényi entropy $R_q[\rho]$ (for $q > 0$, and $q \neq 1$) of the normalized-to-unity probability density $\rho(x)$ is defined [29] by

$$R_q[\rho] \equiv \frac{1}{1-q}\ln \omega_q[\rho] = \frac{1}{1-q}\ln \int_\Delta [\rho(x)]^q\,\mathrm{d}x \tag{3}$$

where $\omega_q[\rho]$ denotes the qth order frequency or entropic moment of $\rho(x)$. The limiting value $q \to 1$, taking into account the normalization condition $\omega_1[\rho] = 1$, yields the Shannon entropy [29]

$$S[\rho] \equiv \lim_{q\to 1} R_q[\rho] = -\int_\Delta \rho(x)\ln\rho(x)\mathrm{d}x. \tag{4}$$

The Fisher information of $\rho(x)$ is defined as [31,32]

$$F[\rho] \equiv \int_\Delta \frac{\left[\frac{\mathrm{d}}{\mathrm{d}x}\rho(x)\right]^2}{\rho(x)}\mathrm{d}x. \tag{5}$$

It should be noted that these information-theoretic measures (Shannon entropy and Fisher information) are translationally invariant. Let us remark that the Fisher quantity has a property of locality because it is a functional of the derivative of the density, so that it is very sensitive to the fluctuations of $\rho(x)$. In contrast, the Rényi and Shannon entropies are global measures of spreading, as well as the standard deviation, because they are power and logarithmic functionals of ρ, respectively. Moreover, let us highlight that the Rényi, Shannon and Fisher quantities have an important advantage with respect to Δx: they do not depend on any specific point of the domain Δ, while the standard deviation quantifies the spread with respect to a particular point of the distribution, namely the mean value or centroid $\langle x\rangle$. They have, however, a disadvantage: each one has its own units which differ among each other, what bears a difficulty for their mutual comparison. To overcome this difficulty it is more convenient to use instead the Rényi and Shannon lengths [33,30] defined by

$$L_q^R[\rho] \equiv \exp\left(R_q[\rho]\right) = \left\{\omega_q[\rho]\right\}^{\frac{1}{1-q}} \tag{6}$$

and

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

respectively, and the Fisher length [34,35] given by

$$\delta x \equiv \frac{1}{\sqrt{F[\rho]}}. \tag{8}$$

The standard deviation and these three information-theoretic lengths are *direct* spreading measures of $\rho(x)$ in the sense that they have the same units as X. Moreover, all four quantities share the following relevant properties: translation and reflection invariance, linear scaling with X (e.g., $\Delta Y = \lambda \Delta X$ for $Y = \lambda X$ in the case of standard deviation) and vanishing in the limit for which the random variable has some definite value, that is when $\rho(x)$ approaches a Dirac-delta function. It is worth noting that while the standard deviation quantifies the separation of the region(s) of the probability concentration with respect to the mean value, the Rényi and Shannon entropies are (global) measures of the extent to which the density is in fact concentrated. On the other hand, the Fisher length measures the pointwise concentration of the probability density over its support interval.

Let us also mention that these four direct measures of spreading are complementary in the sense that they grasp different facets of the distribution of the probability density $\rho(x)$ all over its support interval. Moreover, all of them enjoy an uncertainty property: see e.g. Refs. [33,36] for the global quantities (standard deviation, Rényi and Shannon entropies) and [5,37] for the (local) Fisher measure.

Finally let us collect here three two-component composite information-theoretic measures which have been recently shown to be very useful to quantify the complexity of $\rho(x)$. The term 'complexity' refers to the difficulty of modeling a distribution, according to the number and intricacy of functions needed to do it. This will be clearly illustrated in the discussion of the numerical results in Section 5. The main two-component measures of complexity are given by

$$C_{CR}[\rho] \equiv F[\rho] \cdot (\Delta x)^2 \tag{9}$$

for the Cramér–Rao complexity [29,38],

$$C_{FS}[\rho] \equiv F[\rho] \cdot \frac{1}{2\pi e} e^{2S[\rho]} \tag{10}$$

for the Fisher–Shannon complexity [39,40], and

$$C_{LMC} \equiv \omega_2[\rho] \cdot N[\rho] \tag{11}$$

for the López–Ruíz, Mancini and Calbet (LMC) shape complexity [41].

Each complexity encompasses two different facets of the probability distribution. The LMC complexity measures the combined balance of the average height of the probability density $\rho(x)$ (as given by the second-order moment ω_2, also called disequilibrium) and its total bulk extent (as given by the Shannon entropy power). The Cramér–Rao complexity quantifies the gradient content of $\rho(x)$ together with the probability distribution with respect to its mean value (centroid). The Fisher–Shannon complexity measures the gradient content or oscillatory degree of $\rho(x)$ combined with its total extent. Moreover, according to the units in which each individual component is measured, it is straightforwardly observed that the above complexities are dimensionless quantities. It is also worthy to mention that the three complexities are known to be bounded from below by unity for one-dimensional distributions [42,43].

3. Information theory of a single-delta potential

The time-dependent Schrödinger equation of a particle with mass m moving under the action of a single attractive singular potential of Dirac-delta type, $V(x) = -g\delta(x)$ with $g > 0$ a real constant, is given by

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - g\delta(x)\right]\Psi(x,t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x,t). \tag{12}$$

Note that when the particle is an electron and $g = Ze^2/4\pi\epsilon_0$, this system may be considered as the one-dimensional hydrogenic atom (in particular $Z = 1$ for neutral hydrogen) with δ-function interaction. It is well-known that this system has a unique bound state for $E = -|E| < 0$ and a continuum of unbound states for $E > 0$. Moreover, the wavefunction of the bound state is given by [14,13,44] by

$$\Psi(x,t) = \psi(x)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et} \tag{13}$$

with the expressions

$$E = -\frac{mg^2}{2\hbar^2} \quad \text{and} \quad \psi(x) = \sqrt{k}\mathrm{e}^{-k|x|}; \quad k \equiv \frac{mg}{\hbar^2} \tag{14}$$

for its energy and normalized-to-unity eigenfunction, respectively. Notice that $k = a_0^{-1}$ in the hydrogen case, where $a_0 = \hbar^2/me^2$ is the Bohr radius.

Moreover, the momentum space wavefunction $\Phi(p,t) = \phi(p)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Et}$, where the momentum eigenfunction $\phi(p)$ is given [14] by the Fourier transform of the position eigenfunction $\psi(x)$ so that

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{-\infty} \psi(x)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}\mathrm{d}x = \sqrt{\frac{2p_0}{\pi}} \frac{p_0}{p^2 + p_0^2}, \tag{15}$$

with $p_0 \equiv \hbar k$, has a Lorentzian form.

In this section we will compute the information-theoretic measures of the position and momentum spreading of this system, which are characterized by the position and momentum probability densities

$$\rho(x) = k\mathrm{e}^{-2k|x|} \tag{16}$$

and

$$\Pi(p) = \frac{2p_0^3/\pi}{\left(p^2 + p_0^2\right)^2}, \tag{17}$$

respectively. Emphasis will be made on the direct spreading measures in both position and momentum spaces which include the standard deviation and the Fisher, Rényi and Shannon lengths.

(a) In position space we first obtain from Eqs. (1), (2) and (16) the value

$$\Delta x = \frac{\sqrt{2}}{2k} \tag{18}$$

for the standard deviation in a straightforward manner, because $\langle x \rangle = 0$ and $\langle x^2 \rangle = 1/(2k^2)$. Moreover from Eqs. (3)–(5) and (16) we obtain the values

$$\omega_q[\rho] = \frac{1}{q}k^{q-1}; \qquad R_q[\rho] = -\left(\ln k + \frac{\ln q}{1-q}\right) \tag{19}$$

$$S[\rho] = 1 - \ln k \quad \text{and} \quad F[\rho] = 4k^2 \tag{20}$$

for the entropic moments, the Rényi and Shannon entropies and the Fisher information, respectively. Then, from Eqs. (6)–(8), (19) and (20) we obtain the values

$$L_q^R[\rho] = \frac{1}{kq}, \qquad N[\rho] = \frac{e}{k} \quad \text{and} \quad \delta x = \frac{1}{2k} \tag{21}$$

for the Rényi, Shannon and Fisher information-theoretic lengths. The mutual comparison of Eqs. (18) and (21) indicates that $\delta x = \Delta x/\sqrt{2} \cong 0.7071\Delta x$ and $N[\rho] = 2e\delta x$, so that

$$\delta x < \Delta x < N[\rho] \tag{22}$$

In addition, it is useful to calculate, in order to quantify the complexity of the distribution, the two-component composite measures of Cramér–Rao, Fisher–Shannon and LMC types defined by Eqs. (9)–(11) respectively. From those expressions and Eq. (21), we have the values

$$C_{CR}[\rho] = 2, \qquad C_{FS}[\rho] = \frac{2e}{\pi} \quad \text{and} \quad C_{LMC}[\rho] = \frac{e}{2} \tag{23}$$

for the corresponding complexities. It is worthy to remark that, in spite of the dependence of the individual components on the potential strength g, the above complexity values do not depend on such a parameter. It is worth noting that the same phenomenon holds for homogeneous potentials [11]. Additionally, all of them are above unity as should be expected [42,43].

(b) In momentum space we first observe that the moments $\langle p^n \rangle$ of the momentum density in Eq. (17) diverge for $n \geq 3$ due to the long-range behavior of the density $\Pi(p)$. The only finite moments of integer order are $\langle p^0 \rangle = 1$, $\langle p \rangle = 0$ and $\langle p^2 \rangle = p_0^2$.

The entropic moments have the values

$$\omega_q[\Pi] = \int_{-\infty}^{\infty} [\Pi(p)]^q \mathrm{d}p = \left(\frac{2}{\pi p_0}\right)^q p_0 \frac{\Gamma\left(2q - \frac{1}{2}\right)\sqrt{\pi}}{\Gamma(2q)} \tag{24}$$

with $q > \frac{1}{4}$ as imposed by the convergence of the integral defining $\omega_q[\Pi]$. Additionally, the momentum standard deviation is given by

$$\Delta p = \left(\langle p^2\rangle - \langle p\rangle^2\right)^{\frac{1}{2}} = p_0 \tag{25}$$

and the Rényi entropies have the values

$$R_q[\Pi] = \frac{1}{1-q}\ln\omega_q[\Pi] = \frac{1}{1-q}\ln\left(p_0\sqrt{\pi}\left(\frac{2}{\pi p_0}\right)^q \frac{\Gamma\left(2q-\frac{1}{2}\right)}{\Gamma(2q)}\right), \quad q > \frac{1}{4}. \tag{26}$$

Moreover, taking into account Eqs. (17) and (24) one has that the momentum Shannon entropy is

$$S[\Pi] = -\frac{\mathrm{d}}{\mathrm{d}q}\ln\omega_q[\Pi]\bigg|_{q=1} = \ln\frac{8\pi p_0}{e^2} \tag{27}$$

and the momentum Fisher information is

$$F[\Pi] = \int_{-\infty}^{\infty}\frac{[\Pi'(p)]^2}{\Pi(p)}\mathrm{d}p = \frac{2}{p_0^2}. \tag{28}$$

Then, the Rényi, Shannon and Fisher information-theoretic lengths (6)–(8) are

$$L_q^R[\Pi] = \left[p_0\sqrt{\pi}\left(\frac{2}{\pi p_0}\right)^q \frac{\Gamma\left(2q-\frac{1}{2}\right)}{\Gamma(2q)}\right]^{\frac{1}{1-q}}, \quad q > \frac{1}{4} \tag{29}$$

$$N[\Pi] = \frac{8\pi p_0}{e^2} \tag{30}$$

and

$$\delta p = \frac{\sqrt{2}}{2}p_0 \tag{31}$$

respectively. The mutual comparison of Eqs. (25), (30) and (31) shows that $\delta p = \Delta p/\sqrt{2} \cong 0.7071\Delta p$ and $N[\Pi] = \frac{8\pi}{e^2}\Delta p$, so that

$$\delta p < \Delta p < N[\Pi]. \tag{32}$$

In addition, we obtain the values

$$C_{CR}[\Pi] = 2, \qquad C_{FS}[\Pi] = \frac{64\pi}{e^5} \quad \text{and} \quad C_{LMC}[\Pi] = \frac{10}{e^2} \tag{33}$$

for the Cramér–Rao, Fisher–Shannon and LMC complexities of the system in momentum space, where we have taken into account Eqs. (9)–(11) together with Eq. (24) for $q = 2$, and Eqs. (25), (28) and (30). It is important to note that: (i) the Cramér–Rao complexity in both position and momentum spaces are equal; this is because when the wavefunction is real and its moment of order 1 vanishes, the relationships $F_\rho = \frac{4}{\hbar^2}V_\Pi$ and $F_\Pi = \frac{4}{\hbar^2}V_\rho$ between Fisher information and variance are fulfilled; and (ii) these three complexity measures are independent of the parameter k, highlighting that the difficulty of modeling the distributions $\rho(x)$ and $\Pi(p)$ is determined by the presence of a unique parameter, but not by its specific value.

(c) Finally, the expressions given by Eqs. (18), (21), (25), (30) and (31) yield the following uncertainty products:

$$\Delta x\cdot\Delta p = \frac{\hbar}{\sqrt{2}} = 0.7071\hbar \tag{34}$$

$$\delta x\cdot\delta p = \frac{\sqrt{2}}{4}\hbar = 0.3536\hbar \tag{35}$$

$$N[\rho]\cdot N[\Pi] = \frac{8\pi}{e}\hbar = 9.2458\hbar \tag{36}$$

respectively. The above products do not depend on the g parameter value and they certainly fulfill the Heisenberg [45], Fisher-information-based [5,37] and Shannon-entropy-based or entropic [46,36,47] uncertainty relations given by

$$\Delta x\cdot\Delta p \geq \frac{\hbar}{2} \tag{37}$$

$$\delta x\cdot\delta p \leq \frac{\hbar}{2} \tag{38}$$

$$N[\rho]\cdot N[\Pi] \geq e\pi\hbar \tag{39}$$

respectively.

4. Information theory of a twin-delta potential

Let us here consider the non-relativistic motion of a particle with mass m in a potential having not one (as in the previous section) but two attractive centers separated by a distance $2a$, i.e. in the twin-δ-function potential defined as

$$V(x) = -g[\delta(x+a) + \delta(x-a)].$$

This potential with $g = e^2/4\pi\epsilon_0$ describes not only the one-dimensional hydrogen molecule with δ-function interactions (see [14,12,15] and references therein) and approximates the helium atom [19,12], but also it has been used to interpret some scattering [28] and solid-state [22] phenomena. Because of its symmetry, this potential has two types of solutions which correspond to even and odd eigenfunctions [14,13].

The even bound-state ($E = -|E|$) solution has the eigenfunction

$$\psi_+(x) = \begin{cases} Ae^{kx}, & x < -a \\ B\cosh(kx), & -a < x < a \\ Ae^{-kx}, & x > a \end{cases} \tag{40}$$

and the energy E is given by the eigenvalue condition

$$\gamma(1 + \tanh\gamma) = 2\frac{a}{a_0} \tag{41}$$

with $\gamma = ka$, $k = \frac{\sqrt{2m|E|}}{\hbar}$ and $a_0 = \frac{\hbar^2}{mg}$. The parameters A and B are given by

$$A = Be^{\gamma}\cosh\gamma \quad \text{and} \quad B = \left(\frac{2\gamma}{a}\right)^{1/2}\left(e^{2\gamma} + 2\gamma + 1\right)^{-1/2}, \tag{42}$$

as imposed by the continuity and the normalization conditions.

The odd solution has the eigenfunction

$$\psi_-(x) = \begin{cases} Ce^{kx}, & x < -a \\ D\sinh(kx), & -a < x < a \\ -Ce^{-kx}, & x > a \end{cases} \tag{43}$$

where

$$C = -De^{\gamma}\sinh\gamma \quad \text{and} \quad D = \left(\frac{2\gamma}{a}\right)^{1/2}\left(e^{2\gamma} - 2\gamma - 1\right)^{-1/2}, \tag{44}$$

and the corresponding eigenvalue equation being

$$\gamma(1 + \text{cotanh}\gamma) = 2\frac{a}{a_0}. \tag{45}$$

A detailed analysis of the energy eigenvalue conditions (41) and (45) shows [13] that (i) for $a \gg a_0/2$ (i.e., in the limit of large separation) there are two degenerated eigenfunctions, one even and the other odd, at the energy given by Eq. (14) of the single-delta case, (ii) for $a < a_0/2$ there are no odd solutions and, most important, (iii) the odd solution, whenever exists, lies energetically above the corresponding even solution; i.e. it is less bounded. So, we will restrict ourselves to the even bound-state eigenstate given by Eqs. (40) and (42) in position space. The corresponding Fourier transformation provides the expression

$$\phi_+(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi_+(x)e^{-\frac{i}{\hbar}px} = B\sqrt{\frac{2\hbar}{\pi}}\frac{p_0 e^{\frac{p_0 a}{\hbar}}\cos\frac{pa}{\hbar}}{p^2 + p_0^2}, \tag{46}$$

where $p_0 \equiv \hbar k$. In this Section we will quantify the position and momentum spreading of this system in its ground state as described by the eigenfunctions (40) and (46), respectively. This will be done not only by means of the standard deviation (already done by Lapidus [14]) but also by the following information-theoretic measures: Rényi and Shannon entropies and Fisher information and, most appropriately, their corresponding lengths. To do that, and according to the procedure used in Section 3, we start with the expressions $\rho_+(x) = |\psi_+(x)|^2$ and $\Pi_+(p) = |\Phi_+(p)|^2$ for the position and momentum space quantum-mechanical probability densities of this state, respectively.

(a) In position space, we first check that $\langle x^0\rangle_+ = 1$ so that the density $\rho_+(x)$ is normalized to unity. Then, since $\langle x\rangle_+ = 0$ because of symmetry, one obtains that the standard deviation $(\Delta x)_+$ is given by

$$(\Delta x)_+^2 = \langle x^2\rangle_+ = \frac{a^2}{2\gamma^2} + a^2\frac{e^{2\gamma} + \frac{2}{3}\gamma + 1}{e^{2\gamma} + 2\gamma + 1} \tag{47}$$

which provides the Heisenberg uncertainty measure of the system. Moreover, one can also obtain the even-order moments of $\rho_+(x)$ as

$$\langle x^{2n}\rangle_+ = 2\int_0^\infty x^{2n}\rho_+(x)\mathrm{d}x = \frac{a^{2n}}{(2\gamma)^{2n}(\mathrm{e}^{2\gamma}+2\gamma+1)}\left[\left(\frac{\mathrm{e}^{4\gamma}}{2}+\mathrm{e}^{2\gamma}\right)\Gamma(2n+1,2\gamma)+\frac{\Gamma(2n+1,-2\gamma)}{2}+\frac{(2\gamma)^{2n+1}}{2n+1}\right] \tag{48}$$

for $n = 0, 1, 2, \ldots$, where the symbol $\Gamma(\alpha,\beta)$ denotes the incomplete gamma function. In addition, the Fisher information (5) of the system is computed as

$$F[\rho_+] = \int_{-\infty}^{\infty}\frac{\left[\frac{\mathrm{d}}{\mathrm{d}x}\rho_+(x)\right]^2}{\rho_+(x)}\mathrm{d}x = 2\int_0^a\frac{\left[\rho_+'(x)\right]^2}{\rho_+(x)}\mathrm{d}x + 2\int_a^\infty\frac{\left[\rho_+'(x)\right]^2}{\rho_+(x)}\mathrm{d}x = \frac{4B^2}{a}\gamma\left[\mathrm{e}^\gamma\cosh\gamma-\gamma\right] = \frac{4\gamma^2}{a^2}\cdot\frac{\mathrm{e}^{2\gamma}-2\gamma+1}{\mathrm{e}^{2\gamma}+2\gamma+1} \tag{49}$$

so that the Fisher measure $(\delta x)_+$ of the system, as defined by Eq. (8), is given by the Fisher length

$$(\delta x)_+ = \frac{1}{\sqrt{F[\rho_+]}} = \frac{a}{2\gamma}\left(\frac{\mathrm{e}^{2\gamma}+2\gamma+1}{\mathrm{e}^{2\gamma}-2\gamma+1}\right)^{1/2}. \tag{50}$$

Working similarly, one can calculate the frequency or entropic moments

$$\omega_q[\rho_+] = 2\int_0^\infty[\rho_+(x)]^q\mathrm{d}x = 2\left\{B^{2q}\int_0^a[\cosh(kx)]^{2q}\mathrm{d}x + A^{2q}\int_a^\infty \mathrm{e}^{-2kqx}\mathrm{d}x\right\}. \tag{51}$$

According to the integral expressions

$$\int_a^\infty \mathrm{e}^{-2kqx}\mathrm{d}x = \frac{a\mathrm{e}^{-2q\gamma}}{2q\gamma}$$

and

$$\int_0^a[\cosh(kx)]^{2n}\mathrm{d}x = \frac{a}{2^{2n}\gamma}\left[\binom{2n}{n}\gamma+\sum_{m=1}^{n}\binom{2n}{n-m}\frac{\sinh(2m\gamma)}{m}\right]$$

for any integer n, one has that the entropic moments $\omega_q[\rho_+]$ with integer order $q = n$ have the values

$$\omega_n[\rho_+] = \frac{2\gamma^{n-1}}{(2a)^{n-1}(\mathrm{e}^{2\gamma}+2\gamma+1)^n}\left\{\binom{2n}{n}\left(2\gamma+\frac{1}{n}\right)+\sum_{\substack{m=-n\\ m\neq 0}}^{n}\binom{2n}{n-m}\left(\frac{1}{n}+\frac{1}{m}\right)\mathrm{e}^{2m\gamma}\right\}. \tag{52}$$

For the lowest n's we have that $\omega_1[\rho_+] = 1$ and

$$\omega_2[\rho_+] = \frac{\gamma}{4a}\cdot\frac{\mathrm{e}^{4\gamma}+6\mathrm{e}^{2\gamma}-2\mathrm{e}^{-2\gamma}+12\gamma+3}{(\mathrm{e}^{2\gamma}+2\gamma+1)^2}, \tag{53}$$

which gives the so-called "disequilibrium" [48] of the system. It is also worth noting that in the limit $a \to 0$ we obtain the single-delta-potential value k^{n-1}/n as given by Eq. (19). From the expressions (6) and (52) we obtain the Rényi uncertainty measure as given by the Rényi lengths

$$L_n^R[\rho_+] = (\omega_n[\rho_+])^{\frac{1}{1-n}}.$$

For $n = 2$ we have the Onicescu–Heller measure [48]

$$L_2^R[\rho_+] = \frac{4a}{\gamma}\cdot\frac{(\mathrm{e}^{2\gamma}+2\gamma+1)^2}{\mathrm{e}^{4\gamma}+6\mathrm{e}^{2\gamma}-2\mathrm{e}^{-2\gamma}+12\gamma+3}.$$

Let us now compute the position Shannon entropy of the ground state density $\rho_+(x)$. According to its definition (4), one has

$$S[\rho_+] = -\int_{-\infty}^{\infty}\rho_+(x)\ln\rho_+(x)\mathrm{d}x = -2\left\{\int_0^a\rho_+(x)\ln\rho_+(x)\mathrm{d}x+\int_a^\infty\rho_+(x)\ln\rho_+(x)\mathrm{d}x\right\}$$

$$= \frac{e^{2\gamma}-2\gamma+1}{e^{2\gamma}+2\gamma+1} + 2\left[\frac{\gamma^2-\frac{\pi^2}{12}+2\gamma\ln(1+e^{2\gamma})}{e^{2\gamma}+2\gamma+1} - \frac{Li_2(-e^{-2\gamma})}{e^{2\gamma}+2\gamma+1} - \ln\cosh\gamma\right] - \ln\left(\frac{2\gamma/a}{e^{2\gamma}+2\gamma+1}\right) \tag{54}$$

where $Li_s(x) = \sum_{k=1}^{\infty}\frac{x^k}{k^s}$ is the polylogarithm function.

(b) In momentum space we first observe that the density $\Pi_+(p) = |\phi_+(p)|^2$ has all the odd moments $\langle p^{2n+1}\rangle_+ = 0$ for $n = 0, 1, 2, \ldots$ because of symmetry. Moreover, all the even moments $\langle p^{2n}\rangle_+$ diverge except for $n = 0$ and 1: $\langle p^0\rangle_+ = 1$ and

$$\langle p^2\rangle_+ = \frac{\hbar^2\gamma^2}{a^2}\cdot\frac{e^{2\gamma}-2\gamma+1}{e^{2\gamma}+2\gamma+1}. \tag{55}$$

So, the Heisenberg uncertainty measure of the system in momentum space is given by the standard deviation

$$(\Delta p)_+ = \langle p^2\rangle_+^{1/2} = \frac{\hbar\gamma}{a}\left(\frac{e^{2\gamma}-2\gamma+1}{e^{2\gamma}+2\gamma+1}\right)^{1/2}. \tag{56}$$

The Fisher information (5) of the momentum ground state density $\Pi_+(p)$ has the value

$$F[\Pi_+] = \int_{-\infty}^{\infty}\frac{\left[\Pi_+'(p)\right]^2}{\Pi_+(p)}dp = 4\int_{-\infty}^{\infty}[\phi_+'(p)]^2dp = -4\int_{-\infty}^{\infty}\phi_+(p)\phi_+''(p)dp = \frac{4}{\hbar^2}\langle x^2\rangle_+ \tag{57}$$

which was calculated in Eq. (47). Then, the Fisher uncertainty measure $(\delta p)_+$ has, according to Eq. (8), the value

$$(\delta p)_+ = \frac{1}{\sqrt{F[\gamma_+]}} = \frac{\hbar}{2}\langle x^2\rangle_+^{-1/2}. \tag{58}$$

Working similarly, the frequency or entropic moments $\omega_n[\Pi_+]$ with integer n of the momentum density $\Pi_+(p)$ are given by

$$\omega_n[\Pi_+] = \int_{-\infty}^{\infty}[\Pi_+(p)]^n dp = \frac{n}{(4\pi p_0)^{n-1}}\frac{e^{2n\gamma}}{(e^{2\gamma}+2\gamma+1)^n} \times\left[\frac{(4n-3)!!}{(n!)^2} + 2^{2-2n}\sum_{l=1}^{n}\frac{e^{-2l\gamma}}{(n-l)!(n+l)!}\cdot\sum_{j=0}^{2n-1}\frac{(4n-j-2)!(4l\gamma)^j}{j!(2n-j-1)!}\right] \tag{59}$$

with $p_0 = \hbar k = \frac{\hbar\gamma}{a}$. It is interesting to check the normalization condition $\omega_1[\Pi_+] = 1$, and to compute the second-order entropic moment or disequilibrium:

$$\omega_2[\Pi_+] = \frac{a}{8\pi\hbar\gamma(e^{2\gamma}+2\gamma+1)}\left\{15e^{4\gamma} + 4e^{2\gamma}\left(\frac{8}{3}\gamma^3+8\gamma^2+10\gamma+5\right) + \frac{64}{3}\gamma^3+32\gamma^2+20\gamma+5\right\}. \tag{60}$$

From Eqs. (3), (6), (59) and (60) the Rényi entropies and lengths of the system are obtained as

$$R_n[\Pi_+] = \frac{1}{1-n}\ln\omega_n[\Pi_+] \quad\text{and}\quad L_n^R[\Pi_+] = (\omega_n[\Pi_+])^{\frac{1}{1-n}} \tag{61}$$

in a straightforward manner. Moreover, from Eq. (4) and the expression of $\Pi_+(p)$ one obtains that the momentum Shannon entropy of the twin-delta potential can be expressed as

$$S[\Pi_+] = -\int_{-\infty}^{\infty}\Pi_+(p)\ln\Pi_+(p)dp = -2M\left\{\frac{\pi\ln M/p_0^4}{8p_0^3}[1+e^{-2\gamma}(1+2\gamma)] + J_1(a,p_0) - 2J_2(a,p_0)\right\} \tag{62}$$

with

$$M = \frac{4p_0^3}{\pi}\frac{e^{2\gamma}}{e^{2\gamma}+2\gamma+1}$$

and the integrals

$$J_1(a,p_0) = \int_0^{\infty}\frac{\cos^2\left(\frac{pa}{\hbar}\right)\ln\cos^2\left(\frac{pa}{\hbar}\right)}{(p^2+p_0^2)^2}dp$$

Table 1
Standard deviation, Shannon length and Fisher length for different values of the parameter k (position space) and p_0 (momentum space) for the single-delta position and momentum space densities, $\rho(x)$ and $\Pi(p)$ respectively. Atomic units ($a_0 = 1$) are used.

Position space			
k	$(\Delta x) \times 10^{-2}$	$N[\rho] \times 10^{-2}$	$(\delta x) \times 10^{-2}$
1	70.711	271.828	49.991
20	3.536	13.591	2.491
50	1.414	5.437	0.991
90	0.786	3.020	0.556
Momentum space			
p_0	$(\Delta p) \times 10^{-2}$	$N[\Pi] \times 10^{-2}$	$(\delta p) \times 10^{-2}$
1	0.730	2.482	0.516
20	14.595	49.642	10.320
50	36.487	124.104	25.800
90	65.676	223.387	46.440

$$J_2(a, p_0) = \int_0^\infty \frac{\cos^2\left(\frac{pa}{\hbar}\right)\ln(p^2 + p_0^2)}{(p^2 + p_0^2)^2} \mathrm{d}p$$

which cannot be solved analytically up until now. The corresponding Shannon length (7) is given by

$$N[\Pi_+] = \exp\{S[\Pi_+]\}. \tag{63}$$

We can go forward by calculating the momentum two-component complexities of Cramér–Rao, Fisher–Shannon and LMC types by use of Eqs. (9)–(11) together with Eqs. (56), (60), (62) and (63). From the information-theoretic quantities previously considered in this section, plenty of results can be derived. Let us here only point out the Heisenberg–Fisher uncertainty products

$$(\Delta x)_+(\delta p)_+ = (\delta x)_+(\Delta p)_+ = \frac{\hbar}{2} \tag{64}$$

and the connection between the Cramér–Rao complexity and the Heisenberg product given by

$$\begin{aligned} C_{CR}[\rho_+] = C_{CR}[\Pi_+] &= \frac{4}{\hbar^2}\left[(\Delta x)_+(\Delta p)_+\right]^2 \\ &= 4\gamma^2 \frac{e^{2\gamma} - 2\gamma + 1}{e^{2\gamma} + 2\gamma + 1}\left(\frac{1}{2\gamma^2} + \frac{e^{2\gamma} + \frac{2}{3}\gamma + 1}{e^{2\gamma} + 2\gamma + 1}\right). \end{aligned} \tag{65}$$

The reason for these two complexity measures to be equal in both conjugated spaces is the same as described in the previous section. Note that in this case, however, the three complexity measures depend on the parameters k or a through $\gamma = ka$. It is worthy remarking that the complexity measures obtained for the even solution tend to the complexity values of the single-delta when a approaches zero. We continue with a more detailed description of this phenomenon in the next section.

5. Numerical results

In this Section the information-theoretic measures (lengths and complexities) of the stationary states of the single- and twin-delta potentials, previously obtained in an analytical way, are numerically analyzed and discussed in terms of their characteristic parameter in both position and momentum space.

5.1. Single-delta potential: lengths and complexities

Each of the densities given in Eqs. (16) and (17), corresponding to position and momentum spaces respectively, is characterized by a parameter which is determined, in fact, by the energy of the bounded state. The characteristic parameter is k in position space and p_0 in the momentum one.

Let us analyze the Shannon- and Fisher-type information measures, as well as the standard deviation, by means of their corresponding lengths. In doing so, different values of k and p_0 will be considered. Those values are given in Table 1, for the aforementioned parameters and lengths.

Some comments are in order. It is firstly observed the decreasing trend of all spreading measures, in position space, as the parameter k increases. In fact, and according to Eqs. (21) and (29) with $q = 2$, (30) and (31), the three measures are essentially the inverse of k in position space and proportional to p_0 in momentum space. Let us remind the functional expression of $\rho(x)$, an exponential on each of the half-axes with a decreasing rate determined by k. Consequently, increasing the value of k provokes a higher concentration of the density around the origin, where its value becomes higher as far as k increases. On the other hand, diminishing the k value makes the density to progressively spread over the whole real line. This means that, as k decreases, (i) the variance, a measure of the mean deviation from the centroid at the origin, increases because the density enhances its contribution in regions far from the origin, (ii) the Shannon length, a measure of spread over the whole real line, also increases because of its progressive approach to a uniform distribution, and (iii) the Fisher information, a measure of the 'content of gradient', decreases notably with a consequent increase of its inverse, the square of the Fisher length; the reason is that the density approaches a Dirac delta for extremely large k, with a very high value of the derivative (its absolute value) around the origin.

In what concerns the momentum density, similar interpretations can be done, according to the value of p_0, the parameter which determines the structural characteristics of the momentum density $\Pi(p)$. An increasing trend of each measure as functions of p_0 (notice that $p_0 = \hbar k$) is now displayed. The functional dependence of $\Pi(p)$ on p_0, as shown in Eq. (17), makes the density to spread over its domain and to reduce its content of gradient as far as p_0 increases. This behavior appears opposite to that of the position space density, and consequently the same occurs with the information measures considered, namely standard deviation and Shannon and Fisher lengths, as clearly observed in Table 1.

Considering the LMC, Fisher–Shannon and Cramér–Rao complexities values, let us remember their values, provided in Eqs. (23) and (33). The numerical values are:

$$C_{CR}[\rho] = 2.0000, \qquad C_{FS}[\rho] = 1.7305 \quad \text{and} \quad C_{LMC}[\rho] = 1.3591 \tag{66}$$

in position space, and

$$C_{CR}[\gamma] = 2.0000, \qquad C_{FS}[\gamma] = 1.3547 \quad \text{and} \quad C_{LMC}[\gamma] = 1.3534 \tag{67}$$

in momentum space, all of them above unity as emphasized in Section 3.

5.2. Twin-delta potential: lengths

The interpretation of the different information lengths in the twin-delta problem is based on identical arguments for both the symmetric and antisymmetric solutions. For the sake of simplicity and brevity, we will restrict the discussion to the symmetric solution, keeping in mind that similar conclusions in opposite spaces are obtained from the analysis of the antisymmetric wavefunction. The densities $\rho_+(x)$ and $\Pi_+(p)$ will be denoted by $\rho(x)$ and $\Pi(p)$ in what follows.

In position space, we observe that the density $\rho(x)$ has two different components: (i) an hyperbolic function within the interval $(-a, a)$ determined by the location of the two attractive centers, and (ii) a decreasing exponential out of the aforementioned interval.

The parameter k, which determines the decreasing rate of the exponential component as well as the curvature of the hyperbolic one, is determined by the half-width a of the interval through the eigenvalue equation (41). The analysis of their mutual relationship allows to assert that the parameter k is a decreasing function of a. Consequently, considering wider intervals $(-a, a)$ implies to deal with lower values of k.

In Fig. 1(a), the standard deviation and the Shannon, Fisher and second-order Rényi lengths (denoted by $N[\rho]$, δx and $R_2[\rho]$, respectively) are displayed for different values of the interval half-width a. It is remarkable that the three curves display an unimodal shape: they increase until reaching their absolute maximum, and then slowly decreasing towards an asymptotic value for large a. Opposite behavior is observed in momentum space (Fig. 1(b)): the curves first decrease and then tend to a constant long-range limit.

Let us interpret the above comments according to the structural properties of the densities $\rho(x)$ and $\Pi(p)$, as displayed in Fig. 2 for different values of their characteristic parameters. In what concerns the position space density (Fig. 2(a)) and starting with a very narrow interval, amplifying the small-sized hyperbolic interval increases the global spreading, not only due to the lower curvature and exponential decreasing rate as determined by k, but also because the contribution of the exponential component diminishes as compared to the hyperbolic one. On the other hand, the extremely high gradient at the points $x = \pm a$ decreases as far as a increases, what justifies the enhancement of the Fisher length.

However, after reaching the interval a large enough width, the aforementioned lengths display a decreasing trend. The reason is that the hyperbolic component mainly governs the length values as compared to the exponential contribution. In this sense, the global spread as measured by the variance and the Shannon, Rényi and Fisher lengths remains almost constant, because the density approaches a unique-component distribution, namely the hyperbolic one with very low curvature.

Concerning the momentum space density, we firstly observe that its analytical expression in Eq. (46) consists of an (oscillatory) cosine-like numerator and a decreasing factor as given by the denominator. The behavior of both factors is determined by the parameter p_0: the numerator becomes increasingly oscillatory as far as p_0 increases, while the complementary factor (denominator) governs the rate of global decrease. In this sense, higher values of p_0 give rise to highly oscillatory momentum densities but also with a higher global spreading. Again we observe a counterbalance of both contributions for large enough p_0, as displayed in Fig. 2(b) for the momentum density and Fig. 1(b) for the momentum space lengths.

It is also interesting to analyze the dependence of the Rényi lengths on the order parameter q. This will be done attending to the curves displayed in Fig. 3 for a fixed interval extremum a. The decreasing behavior observed for the symmetric solution as also occurs with the antisymmetric one, independently of dealing with position or momentum space densities, can be

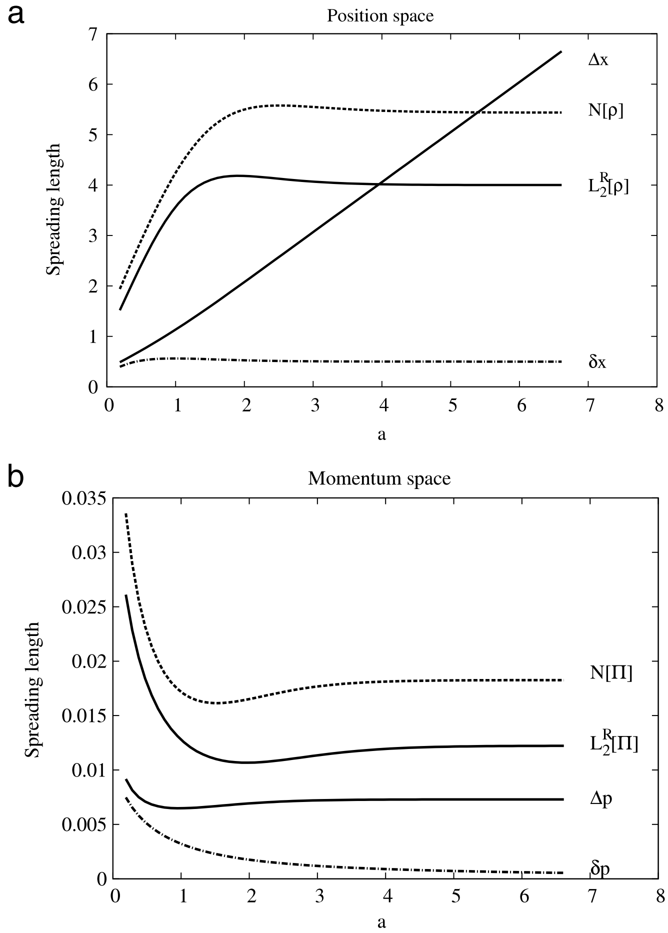


Fig. 1. Standard deviation and Shannon, Fisher and second-order Rényi lengths for the symmetric solution of the twin-potential problem, in (a) position and (b) momentum spaces. Atomic units ($a_0 = 1$) are used.

justified as follows. The effect of increasing q translates into a 'more concentrated' integrand within the expression (3) defining the frequency moments and their corresponding Rényi lengths. So, increasing q makes the relative contribution from the exponential component in position space to become almost negligible as compared to the hyperbolic one, as corresponds to a density highly concentrated around the origin and, consequently, less sparse. Concerning the momentum space density, an enhancement of both the strength of oscillations as well as a global concentration around the origin arises as q increases. The consequence is the same as in position space, that is, lower values of the Rényi length, indicating a higher level of concentration, especially around the origin but also at the extrema of the oscillatory curve.

5.3. Twin-delta potential: complexities

According to the general interpretation of the 'complexity' concept, as a measure of the difficulty of modeling the distribution, it is clear that the distance between the locations of the delta functions or, equivalently, the width of the interval $(-a, a)$, will be essential in determining the level of complexity. This is shown in Fig. 4, where the LMC, Fisher–Shannon and Cramér–Rao complexities are displayed as functions of the half-distance a between delta attractors. Let us analyze the results in position (Fig. 4(a)) and momentum (Fig. 4(b)) spaces.

In doing so, let us firstly think on the process of 'separation of deltas' (increase of a). For large enough separation, the quantum-mechanical problem can be approximated by an 'overlap' of two independent single-delta equations, dealt in detail in Section 3. For the single-delta case we obtained constant values of all complexities; in our case we observe that the LMC and Fisher–Shannon complexities displayed in Fig. 4(a) are constant unless dealing with very small values of a. This is a consequence of the behavior of the factors composing those complexities, as observed in Fig. 2(a). Increasing a makes the Shannon, Fisher and second-order Rényi lengths to become almost constant, because each of the single-delta components corresponding to potentials centered at $x = \pm a$ gives rise to a density approaching uniformity as far as a increases. The situation is very different, however, regarding the variance or the standard deviation, which monotonically increases as the

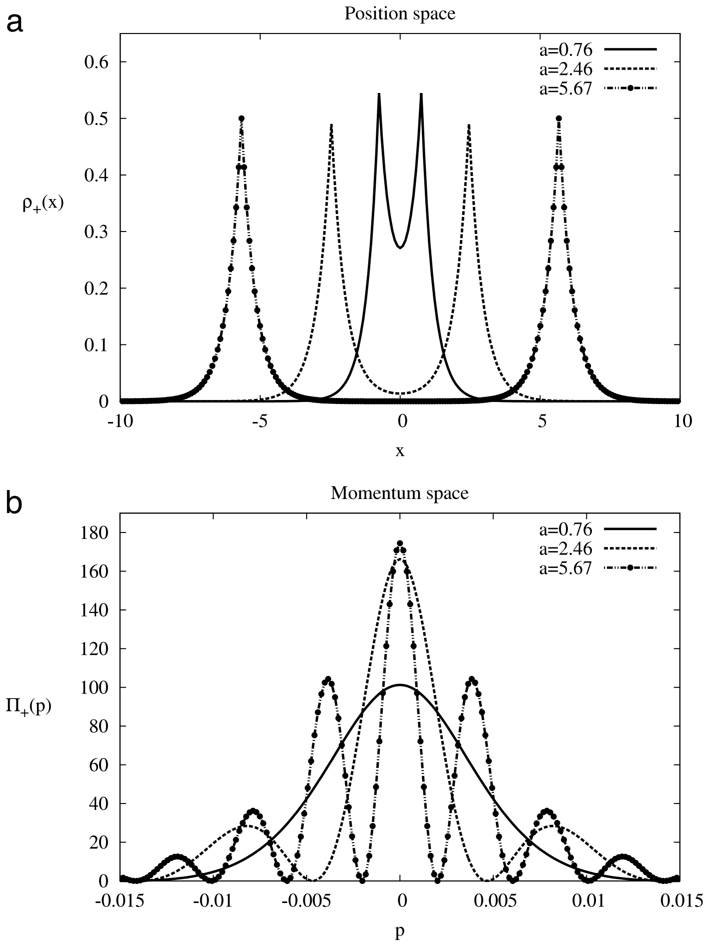


Fig. 2. Density function for the symmetric solution of the twin-potential problem, in (a) position and (b) momentum spaces. Atomic units ($a_0 = 1$) are used.

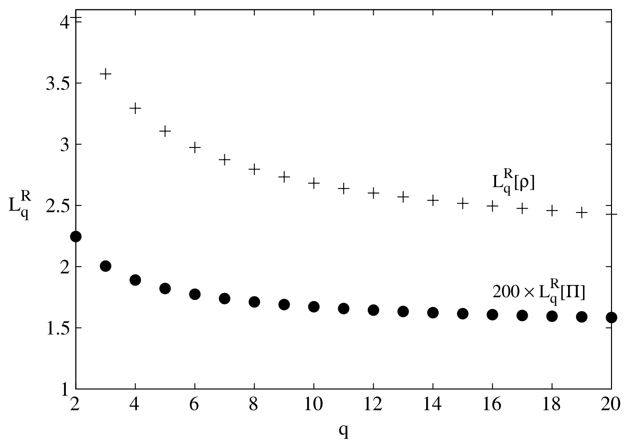
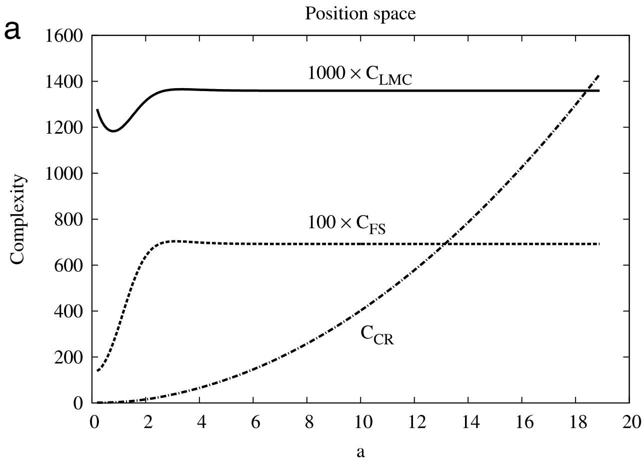


Fig. 3. Rényi length, as a function of its order q, for the symmetric solution of the twin-potential problem with a fixed value $a = 1.4$ in position and momentum spaces. Atomic units ($a_0 = 1$) are used.

centers separate among themselves. The key point here is the definition of variance as a measure of spreading with respect to the centroid, the origin in the present problem. So, the highest values of the density, which occur around the attractive centers, are progressively more distant from the centroid at the origin. This makes the variance to increase because of its



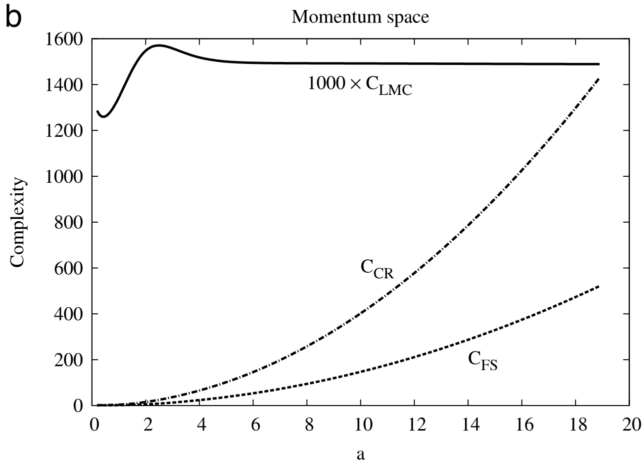


Fig. 4. Complexities LMC, Fisher–Shannon (FS) and Cramér–Rao (CR) for the symmetric solution of the twin-potential problem, in (a) position and (b) momentum spaces. Atomic units ($a_0 = 1$) are used.

reference with respect to the origin, contrary to the other information measures and lengths which have no reference points, being determined instead according to the behavior of the density over its whole domain.

Concerning the momentum space complexities (Fig. 4(b)), the essential difference among themselves is the presence or not of the Fisher information factor, which appears in the Fisher–Shannon and Cramér–Rao cases but not in the LMC one. It is observed that (i) the LMC complexity in momentum space displays a very similar shape to the corresponding one in position space, and (ii) the Fisher–Shannon and Cramér–Rao momentum complexities are increasing functions, in a similar fashion as the Crámer–Rao one in position space. It is worthy remembering the presence of an oscillatory factor in the momentum density, the frequency of the oscillations being determined by the half-distance a. Such an oscillatory behavior mainly affects the Fisher information factor, whose increase with a translates into that of the associated complexities. Such is not the case of the LMC complexity, for which a 'counterbalance effect' of each factor restricts the LMC complexity value for arbitrary a to a much narrower interval.

6. Conclusions and open problems

In this paper we have studied both analytically and numerically the single information-theoretic (Fisher, Shannon and Rényi) lengths and complexity (Cramér–Rao, Fisher–Shannon and LMC) measures of the lowest-lying stationary state of the single-delta and twin-delta potentials in terms of their energies and characteristic parameters. These quantities are discussed in both position and momentum spaces. They grasp various individual and combined spreading facets of the charge and momentum of the particle far beyond that described by the celebrated standard deviation.

Finally, let us point out some open problems. First, to study the information and complexity properties of (i) the excited states resulting from the single- and multiple-delta functions in one dimension, and (ii) the bound states of the one-dimensional hydrogen atom as well as the helium and hydrogen molecule ion with a single- and twin-delta potential, respectively, confined in a box [49,50] or under the action of external electric and/or magnetic fields. Second, to extend the results of this work to N-delta one-dimensional arrays because of their use to approximate and describe numerous scientific and technological properties of quantum wires and other semiconductor nanostructures. Third, to study the related information-theoretic and complexity measures of higher dimensionality delta potentials, which do not have the same properties as those in one dimension. It is known that delta potentials in more than one dimension do not allow bound states and scattering but, nevertheless, once regularized they are very instructive for illustrating basic concepts of quantum field theory [51]. Fourth, to investigate the relativistic effects in the aforementioned information-theoretic properties of delta-like potentials. It is planned the inclusion, in all of the above points, of information lengths based on a so relevant information quantifier as the Tsallis entropy [52], a non-extensive measure which characteristic parameter measures the departure from extensivity. Numerous applications of this entropy in non-extensive thermodynamics or statistical mechanics and many other scientific fields have been carried out [53].

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