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

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ABSTRACT

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