ORIGINAL PAPER

Rényi entropy of the infinite well potential in momentum space and Dirichlet-like trigonometric functionals

A. I. Aptekarev · J. S. Dehesa · P. Sánchez-Moreno · D. N. Tulyakov

Received: 21 October 2011 / Accepted: 30 November 2011 / Published online: 13 December 2011 © Springer Science+Business Media, LLC 2011

Abstract The momentum entropic moments and Rényi entropies of a onedimensional particle in an infinite well potential are found by means of explicit calculations of some Dirichlet-like trigonometric integrals. The associated spreading lengths and quantum uncertainty-like sums are also provided.

Keywords Information-theoretic measures · Quantum infinite well · Rényi entropy · Rényi spreading length

1 Introduction

A major goal of the information theory of quantum systems is the determination of the uncertainty fundamental quantities beyond the well-known standard deviation

A. I. Aptekarev · D. N. Tulyakov

D. N. Tulyakov e-mail: dnt@mail.nnov.ru

J. S. Dehesa · P. Sánchez-Moreno (⊠) Institute "Carlos I" for Computational and Theoretical Physics, University of Granada, Granada, Spain e-mail: pablos@ugr.es

J. S. Dehesa e-mail: dehesa@ugr.es

J. S. Dehesa Department of Atomic, Molecular and Nuclear Physics, University of Granada, Granada, Spain

P. Sánchez-Moreno Department of Applied Mathematics, University of Granada, Granada, Spain

Keldysh Institute for Applied Mathematics, Russian Academy of Sciences, Moscow State University, Moscow, Russia e-mail: aptekaa@keldysh.ru

(or its square, the variance) in both position and momentum spaces [1-4]. They include the spreading measures of global (entropic moments, the Rényi, Shannon and Tsallis' entropies and lengths) and local (Fisher's information) character [5-7,3]. These information-theoretic measures quantify the spread of the position and momentum one-particle densities of the system (which are the basic variables according to the Density Functional Theory [8]) in various complementary ways and, in contrast to the variance, without reference to any specific point of the corresponding Hilbert space. Moreover, they are closely related to various energetic and experimentally measurable quantities of the system [3,8-11].

However, they have not yet been or cannot be analytically calculated; not even for the one-dimensional systems with a Coulomb, oscillator or infinite well potential despite they are very often used to explain and predict numerous physico-mathematical phenomena in science and technology. The present knowledge of the information-theoretic measures of the hydrogenic, oscillator-like and particle-in-a-box systems is described in Refs. [9, 10, 12] and [13], respectively. Therein we realize that the entropic moments and the Rényi, Shannon and Tsallis entropies are not yet known except for the lowest-and highest-lying states, mainly because they are power (entropic moments, Rényi and Tsallis entropies) or logarithmic (Shannon entropy) functionals of the corresponding densities. The calculation of the Fisher information is somewhat easier because of its close connection with the kinetic energy.

In this paper we will center around the particle-in-a-box system, which is composed by a particle moving in the infinite well potential V(x) = 0 for |x| < a and ∞ otherwise. This canonical system has been used to simplify the description of numerous scientific phenomena in nuclei [14], polymers [15] and various nanosystems [16,17] as well as in chaos [18], among others. The quantum-mechanical states of this system are characterized [13,19,20] by the energies

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

and the densities

$$\rho_n(x) = \begin{cases} \frac{1}{a} \sin^2 \left[\frac{\pi n}{2a} (x-a) \right]; \ |x| \le a \\ 0; \qquad \qquad |x| > a \end{cases}$$

and

$$\gamma_n(p) = \frac{\pi n^2}{2} \frac{\sin^2 \left[ap - \frac{\pi n}{2}\right]}{\left(a^2 p^2 - \frac{\pi^2 n^2}{4}\right)^2}; \quad p \in (-\infty, +\infty), \tag{1}$$

in position and momentum spaces, respectively. Recently, the power moments $\langle x^k \rangle$ and the entropic moments $W_k[\rho_n] = \langle \rho_n^{k-1} \rangle$ in position space have been determined [13,21,22] what has allowed us to find the values for the position variance, Rényi, Shannon and Tsallis entropies; in addition the position Fisher information $F[\rho_n]$ is also known [13]. In momentum space, however, the situation is very different; while

the second-order moment $\langle p^2 \rangle$ and the Fisher information $F[\gamma_n]$ have known values [13], the entropic moments and consequently the Rényi and Tsallis entropies have not yet been able to be calculated, mainly because all these three quantities depend [13] on the Dirichlet-like trigonometric integrals [23]

$$I_{n,k} = \int_{-\infty}^{+\infty} \left[\frac{\sin^2 \left(t - \frac{\pi n}{2} \right)}{\left(t^2 - \frac{\pi^2 n^2}{4} \right)^2} \right]^k dt,$$
(2)

(compare with (1)).

This functional has been recently computed only in the two following cases [13]: (a) *n* fixed and the first few values of *k*, and (b) *k* fixed and very large *n*. A main purpose of this paper is to calculate this functional for the generic pair (n, k), and then to find the values of all entropic moments, the Rényi entropies and lengths, the Tsallis entropies and the associated uncertainty relations in momentum space. This opens the way to calculate various complexity measures not only in position space but also in momentum space. This is the case of the López-Ruiz-Mancini-Calbet (LMC, in short) [24] and the Fisher-Rényi [25] complexities, where the Rényi entropy plays an important role; in particular, the LMC complexity of the particle-in-a-box has been numerically studied in [26,27] and mathematically considered in [13]. It has been recently reviewed the high relevance of these statistical complexity measures in analysing a great diversity of physical phenomena related with the internal disorder of the intrinsic structure of many-electron systems [28].

The paper is structured as follows. Firstly, in Sect. 2 the information-theoretic measures of a one-dimensional probability distribution needed in this work are briefly discussed. Then, in Sect. 3, the calculation of the trigonometric integral $I_{n,k}$ is explicitly carried out. The resulting expression is used in Sect. 4 to find the values of the entropic moments, Rényi's measures and Tsallis' entropies in momentum space, as well as the associated uncertainty-like expressions which combines them with the corresponding quantities in position space with integer orders. Finally, the conclusions and some open problems are given.

2 Information-theoretic measures of a probability density: Basics

The uncertainty measures of a random variable *X* are given by the spreading measures of the corresponding probability density $\rho(x), x \in (-\infty, +\infty)$. These measures are defined either in terms of the moments-around-the-origin (or simply, power moments) $\langle x^k \rangle$ (such as, e.g., the variance $V[\rho] = \langle x^2 \rangle - \langle x \rangle^2$) or in terms of the frequency or entropic moments $W_k[\rho]$ of $\rho(x)$, which are defined by

$$\langle x^k \rangle = \int_{-\infty}^{+\infty} x^k \rho(x) dx,$$

and

$$W_k[\rho] = \left\langle \rho^{k-1} \right\rangle = \int_{-\infty}^{+\infty} [\rho(x)]^k \, dx, \tag{3}$$

respectively. From the latter quantities various information-theoretic measures have been defined, such as the Rényi entropy [5]

$$R_{\alpha}[\rho] = \frac{1}{1-\alpha} \ln W_{\alpha}[\rho] = \frac{1}{1-\alpha} \ln \left\langle \rho^{\alpha-1} \right\rangle, \quad \alpha > 0, \tag{4}$$

and the Tsallis entropy [7]

$$T_{\alpha}[\rho] = \frac{1}{\alpha - 1} \left(1 - W_{\alpha}[\rho] \right) = \frac{1}{\alpha - 1} \left(1 - \left\langle \rho^{\alpha - 1} \right\rangle \right), \quad \alpha > 0.$$
 (5)

The limiting case $\alpha \to 1$ of these two quantities is the celebrated Shannon entropy [6]

$$S[\rho] = -\int_{-\infty}^{+\infty} \rho(x) \ln \rho(x) dx.$$

In contrast to these three entropy quantities which measure in various (but complementary) ways the total extent in which the random variable is distributed, there exists a qualitatively different spreading quantity: the Fisher information with respect to the location parameter (or simply Fisher information, heretoforth), defined [3] by

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

Indeed, contrary to the variance and the Rényi, Shannon and Tsallis entropies, the Fisher information has a locality property since its value mainly comes from the regions where the density is more oscillatory (i.e. when the density has more nodes per unit argument of x). In other terms, the Fisher information is very sensitive to the fluctuations of $\rho(x)$. Then, it provides an estimation of the oscillatory character of the density while the Rényi, Shannon and Tsallis entropies measure in different ways the total extent in which the density is distributed.

The five spreading measures previously defined, although interesting *per se*, cannot be mutually compared because either they are dimensionless or they do not have the same units. To overcome this problem, following Hall [4], we will use instead the so-called "direct spreading measures" to analyze the uncertainty of the random variable; namely, the standard deviation, $\Delta x = (V[\rho])^{\frac{1}{2}}$, and the information-theoretic lengths of Rényi, Shannon (also called entropy power) and Fisher defined by

$$L_{\alpha}^{R}[\rho] \equiv \exp(R_{\alpha}[\rho]),$$

$$L^{S}[\rho] \equiv \exp(S[\rho]),$$

and

$$\delta x \equiv L^F[\rho] \equiv \frac{1}{\sqrt{F[\rho]}},$$

respectively. All these quantities 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 approach to the Dirac delta. Moreover, all of them fulfil an uncertainty relation.

3 Calculation of the Dirichlet-like trigonometric functionals

In this section we give and prove Theorem 1, from which follows the main result of the paper.

Theorem 1 The integral $I_{n,k}$, defined in (2), has the value

$$I_{n,k} = (\pi n)^{-2k} \sum_{j=0}^{k-1} \binom{2j+2k-1}{2k-1} \frac{2\pi (\pi n)^{-2j} \left(-\frac{1}{4}\right)^j}{(2k-2j-1)!} \sum_{i=0}^{k-1} (-1)^i \binom{2k}{i} (k-i)^{2k-2j-1},$$

for n = 1, 2..., and k = 1, 2, ...

In particular for k = 1 and k = 2, one easily has the values

$$I_{n,1} = \frac{2}{\pi n^2}; \quad I_{n,2} = \frac{4}{3\pi^3 n^4} \left(1 + \frac{15}{2\pi^2 n^2} \right), \tag{6}$$

in agreement with the corresponding values already obtained in [13]. For completeness, let us also collect here that the asymptotical $(n \to \infty)$ values of $I_{n,k}$ are known [13] to be

$$I_{n,k} \simeq \frac{b_k}{\pi^{2k-1} n^{2k}},\tag{7}$$

where

$$b_k = 4k \sum_{i=0}^{k-1} \frac{(-1)^i (k-i)^{2k-1}}{i! (2k-i)!}; \quad k \ge 1.$$
(8)

It is worth pointing out that Eq. (7) can be obtained from Theorem 1 simply by taking the first term of the sum (i.e., j = 0).

To prove Theorem 1, we will use three Lemmas. In Lemma 1 we expand the reciprocal of the product $(t - \pi n/2)^{2k}(t + \pi n/2)^{2k}$ contained in the Dirichlet-like kernel [23] of the integral (3) as a sum of simple fractions. Putting this result into

Eq. (2), Lemma 2 shows that the calculation of $I_{n,k}$ reduces to the evaluation of the integral

$$K_{n,j} = \int_{-\infty}^{\infty} \frac{\sin^{2k} u}{u^{2(k-j)}} du.$$
⁽⁹⁾

Then, in Lemma 3 this integral is explicitly calculated, and consequently Theorem 1 follows in a straightforward manner.

Lemma 1 The following identity holds true:

$$\frac{1}{\left(t - \frac{\pi n}{2}\right)^{2k} \left(t + \frac{\pi n}{2}\right)^{2k}} = (\pi n)^{-2k} \sum_{j=0}^{2k-1} (\pi n)^{-j} \binom{j+2k-1}{2k-1} \times \left[\left(t + \frac{\pi n}{2}\right)^{j-2k} + (-1)^j \left(t - \frac{\pi n}{2}\right)^{j-2k} \right].$$
(10)

Proof of Lemma 1 We will expand $\frac{1}{(t-\frac{\pi n}{2})^{2k}(t+\frac{\pi n}{2})^{2k}} := A(t)$ into a sum of simple fractions; i.e. each term of this sum has one pole in variable *t* with certain multiplicity and the numerators (residues) of the terms do not depend on *t*. First, let us take

$$u := t - \frac{\pi n}{2} \Rightarrow A = \frac{(u + \pi n)^{-2k}}{u^{2k}} = (\pi n)^{-2k} \left[\sum_{j=0}^{2k-1} u^{j-2k} (\pi n)^{-j} {\binom{-2k}{j}} \right] + f(u),$$

where f(u) = O(1) when $u \to 0$. Now, let us use

$$u := t + \frac{\pi n}{2} \Rightarrow A = \frac{(u - \pi n)^{-2k}}{u^{2k}} = (\pi n)^{-2k} \left[\sum_{j=0}^{2k-1} (-1)^j u^{j-2k} (\pi n)^{-j} \binom{-2k}{j} \right] + \tilde{f}(u),$$

where $\tilde{f}(u) = O(1)$ when $u \to 0$. Here we used the notation

$$\binom{-2k}{j} = \frac{(-2k)(-2k-1)\cdots(-2k-j+1)}{j!}.$$

Then, coming back to variable t we have the following representation for A(t) as sum of simple fractions:

$$A(t) = (\pi n)^{-2k} \sum_{j=0}^{2k-1} (\pi n)^{-j} {\binom{-2k}{j}} \left[\left(t - \frac{\pi n}{2} \right)^{j-2k} + (-1)^j \left(t + \frac{\pi n}{2} \right)^{j-2k} \right] + \hat{f}(t),$$

🖄 Springer

where $\hat{f}(t) = f(t) + \tilde{f}(t)$. Since poles of A(t) with their multiplicities coincide with the poles of the sum from the right hand side, then function $\hat{f}(t)$ has no poles in the whole complex plain and therefore, by Liouville theorem, function $\hat{f}(t)$ must be a constant. Taking into account that $A(\infty) = 0$ and the sum from the right hand side also equal zero for $t \to \infty$ we get $\hat{f}(t) = 0$.

also equal zero for $t \to \infty$ we get $\hat{f}(t) = 0$. Finally, passing from $\binom{-2k}{j}$ to $\binom{j+2k-1}{2k-1}$ we arrive to validity of Lemma 1.

Lemma 2 The integrals $I_{n,k}$ defined by (2) simplify as

$$I_{n,k} = (\pi n)^{-2k} \sum_{j=0}^{k-1} 2(\pi n)^{-2j} \binom{2j+2k-1}{2k-1} \int_{-\infty}^{\infty} \frac{\sin^{2k} u}{u^{2(k-j)}} du.$$

Proof of Lemma 2 We substitute the sum from Lemma 1 in the expression (2) of $I_{n,k}$. Then, it is straightforward to see that

$$I_{n,k} = (\pi n)^{-2k} \sum_{j=0}^{2k-1} (\pi n)^{-j} {\binom{j+2k-1}{2k-1}} \left[\int_{-\infty}^{\infty} \sin^{2k} \left(t - \frac{\pi n}{2} \right) \left(t + \frac{\pi n}{2} \right)^{j-2k} dt + (-1)^{j} \int_{-\infty}^{\infty} \sin^{2k} \left(t - \frac{\pi n}{2} \right) \left(t - \frac{\pi n}{2} \right)^{j-2k} dt \right].$$
(11)

Due to the periodicity of the sine function, these two integrals have the same value:

$$\int_{-\infty}^{\infty} \sin^{2k} \left(t - \frac{\pi n}{2} \right) \left(t - \frac{\pi n}{2} \right)^{j-2k} dt = \int_{-\infty}^{\infty} \sin^{2k} \left(z + \frac{\pi n}{2} \right) \left(z + \frac{\pi n}{2} \right)^{j-2k} dz$$
$$= \int_{-\infty}^{\infty} \sin^{2k} \left(z - \frac{\pi n}{2} \right) \left(z + \frac{\pi n}{2} \right)^{j-2k} dz,$$

where the change of variable $t = z + \pi n$ has been used in the first equality.

Thus, the terms in (11) with odd *j* vanish, so we can express $I_{n,k}$ as

$$I_{n,k} = (\pi n)^{-2k} \sum_{j=0}^{k-1} (\pi n)^{-2j} \binom{2j+2k-1}{2k-1} 2 \int_{-\infty}^{\infty} \sin^{2k} \left(t - \frac{\pi n}{2}\right) \left(t - \frac{\pi n}{2}\right)^{2j-2k} dt.$$

Finally, the change of variable $u = t - \frac{\pi n}{2}$ yields the statement of the lemma. Lemma 3 The integrals $K_{n,j}$ defined by (9) are given by

$$\int_{-\infty}^{\infty} \frac{\sin^{2k} u}{u^{2(k-j)}} du = \frac{\pi \left(-\frac{1}{4}\right)^{j}}{(2k-2j-1)!} \sum_{i=0}^{k-1} (-1)^{i} \binom{2k}{i} (k-i)^{2k-2j-1}.$$

Proof of Lemma 3 We use the Fourier transform

$$\mathcal{F}[f](\omega) := \int_{-\infty}^{\infty} f(u)e^{-i\omega u}du,$$

to compute integral

$$\int_{-\infty}^{\infty} f(u)du = \mathcal{F}[f](0), \quad f(u) := \left(\frac{\sin u}{u}\right)^{2(k-j)} \sin u^{2j}.$$

We have

$$\mathcal{F}\left[\frac{\sin u}{u}\right](\omega) = \int_{-\infty}^{\infty} \frac{e^{iu} - e^{-iu}}{2iu} e^{-i\omega u} du = \int_{+i\infty}^{-i\infty} \frac{e^{-s} - e^s}{2s} e^{\omega s} \frac{ds}{i}$$
$$= \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} \left(\pi \frac{e^s - e^{-s}}{s}\right) e^{\omega s} ds,$$

where s = -iu. The last integral is computed using the table of inverse Laplace transforms (see [29], formulas 29.2.2 and 29.3.61):

$$\mathcal{F}\left[\frac{\sin u}{u}\right](\omega) = \pi \left(H(\omega+1) - H(\omega-1)\right),$$

where $H(\omega)$ is the Heaviside function

$$H(\omega - k) = \begin{cases} 1, \ \omega \ge k \\ 0, \ \omega < k \end{cases}.$$

Then we have

$$\mathcal{F}[\sin u](\omega) = \frac{1}{i} \frac{d}{d\omega} \mathcal{F}\left[\frac{\sin u}{u}\right](\omega) = \frac{\pi}{i} \left[\delta(\omega - 1) - \delta(\omega + 1)\right],$$

where $\delta(\omega)$ is a Dirac delta function, which is characterized by

$$F(\omega) * \delta(\omega - a) = \frac{1}{2\pi} F(\omega - a), \qquad (12)$$

where the convolution for Fourier transforms is defined as

$$F(\omega) * G(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\xi)G(\omega - \xi)d\xi,$$

and we have

$$\mathcal{F}[f](\omega) * \mathcal{F}[g](\omega) = \mathcal{F}[fg](\omega).$$

Therefore, since (12)

$$H(\omega+1) - H(\omega-1) = H(\omega) * [\delta(\omega+1) - \delta(\omega-1)],$$

we obtain

$$\mathcal{F}\left[\left(\frac{\sin u}{u}\right)^{2(k-j)}\sin^{2j}u\right](\omega) = (-1)^{j}\pi^{2k}\underbrace{H*H*\cdots*H}_{2(k-j)} \\ *\underbrace{\left[\delta(\omega+1)-\delta(\omega-1)\right]*\cdots*\left[\delta(\omega+1)-\delta(\omega-1)\right]}_{2k}.$$
 (13)

Computing

$$\underbrace{H * \dots * H}_{2(k-j)} = \frac{1}{(2\pi)^{2(k-j)-1}} \frac{|\omega_+|^{2(k-j)-1}}{(2(k-j)-1)!}, \quad |\omega_+| := \omega H(\omega),$$

we substitute the result in (13), and using (12) we can obtain an explicit form for $\mathcal{F}\left[\left(\frac{\sin u}{u}\right)^{2(k-j)}\sin^{2j}u\right](\omega)$. Finally, taking the obtained expression for $\omega = 0$, we arrive to assertion of the Lemma.

4 Rényi measures and Tsallis entropies in momentum space

In this Section we give the values of the entropic moments and the Rényi and Tsallis entropies as well as the associated Rényi lengths of the infinite-well potential in momentum space. Moreover, the uncertainty-like expressions which combines these momentum quantities with the corresponding ones in position space are also provided for integer orders.

According to Eqs. (1) and (3), one has that the momentum entropic moments are given by

$$W_{k}[\gamma_{n}] = \int_{-\infty}^{+\infty} \left[\gamma_{n}(p)\right]^{k} dp = \left(\frac{\pi n^{2}}{2}\right)^{k} a^{k-1} I_{n,k}, \quad k = 1, 2, \dots,$$
(14)

where the integral $I_{n,k}$ is given by Theorem 1. Notice that taken into account (6), one has the normalization $W_1[\gamma_n] = 1$ and the averaging momentum density

$$W_2[\gamma_n] = \langle \gamma_n \rangle = \frac{a}{3\pi} \left(1 + \frac{15}{2\pi^2 n^2} \right),$$

for k = 1 and 2, respectively. Moreover, taking into account (7) one has the asymptotical values

$$W_k[\gamma_n] \simeq rac{b_k}{2^k \pi^{k-1}} a^{k-1}; \quad k \ge 1, \ n \to +\infty.$$

Now, from Eqs. (1), (4) and (14) one finds the values for the momentum Rényi entropies and lengths

$$R_{k}[\gamma_{n}] = \frac{1}{1-k} \ln W_{k}[\gamma_{n}] = -\ln a + \frac{1}{1-k} \ln\left(\left(\frac{\pi n^{2}}{2}\right)^{k} I_{n,k}\right)$$
(15)

and

$$L_{k}^{R}[\gamma_{n}] = \exp\left(R_{k}[\gamma_{n}]\right) = \left[W_{k}[\gamma_{n}]\right]^{\frac{1}{1-k}} = \frac{1}{a}\left(\frac{\pi n^{2}}{2}\right)^{\frac{\kappa}{1-k}}\left(I_{n,k}\right)^{\frac{1}{1-k}}, \quad (16)$$

respectively. Moreover, from Eqs. (1), (5) and (14) one obtains the values for the momentum Tsallis entropies

$$T_k[\gamma_n] = \frac{1}{k-1} \left(1 - W_k[\gamma_n]\right) = \frac{1}{k-1} \left[1 - \left(\frac{\pi n^2}{2}\right)^k a^{k-1} I_{n,k}\right].$$
 (17)

The values of $I_{n,k}$ given by Theorem 1 together with Eqs. (15)–(17) provide the momentum Rényi and Tsallis quantities, respectively, in a straightforward manner. Moreover, since the Rényi and Tsallis entropies in position space are known [22, 13] to be

$$R_k[\rho_n] = \ln a + \frac{1}{1-k} \ln\left(\frac{2\Gamma\left(k+\frac{1}{2}\right)}{\sqrt{\pi}\Gamma(k+1)}\right)$$

and

$$T_k[\rho_n] = \frac{1}{k-1} \left[1 - \frac{2}{a^{k-1}\sqrt{\pi}} \frac{\Gamma\left(k+\frac{1}{2}\right)}{\Gamma(k+1)} \right],$$

respectively, with k = 1, 2, ..., it is possible to easily calculate the position-momentum Rényi uncertainty-like sum $R_k[\rho_n] + R_l[\gamma_n]$ and Tsallis uncertainty-like quotient $[1 + (1 - k)T_k[\rho_n]]^{\frac{1}{2k}} [1 + (1 - l)T_l[\gamma_n]]^{-\frac{1}{2l}}$.

Finally, let us examine the position-momentum product of the Rényi lengths, $L_k^R[\rho_n] \times L_k^R[\gamma_n]$. From (16) and the position Rényi length

$$L_{k}^{R}[\rho_{n}] = 2^{2 + \frac{1}{k-1}} a \binom{2k}{k}^{-\frac{1}{k-1}}$$

one has

$$L_{k}^{R}[\rho_{n}] \times L_{l}^{R}[\gamma_{n}] = 2^{2 + \frac{1}{k-1}} {\binom{2k}{k}}^{-\frac{1}{k-1}} \left[\left(\frac{\pi n^{2}}{2}\right)^{l} I_{n,l} \right]^{-\frac{1}{l-1}}$$

Now the use of Theorem 1 in this expression yields immediately the explicit value of this position-momentum uncertainty-like product. For further discussions on the uncertainty measures of the particle-in-a-box system, and its generalization to *D*-dimensions we refer to Ref. [13].

5 Conclusions and open problems

In this paper we have extended the information-theoretic analysis of the non-relativistic particle-in-a-box system (i.e., a particle moving in an infinite-well potential) [13, 19–22], by explicitly calculating the Rényi and Tsallis entropies of integer order for all ground and excited quantum states in momentum space. It has required the exact evaluation of the trigonometric functionals $I_{n,k}$ (see Eq. (2)) with the Dirichlet-like kernel $(\sin \theta_n/\theta_n)^{2k}$, so much useful in Fourier analysis. It is worth pointing out here that the calculation of these quantities for non-integer orders in both position and momentum spaces remains to be an open problem; they are needed to set up the corresponding uncertainty relations which link position and momentum Grant Shannon entropy is not yet known except for the lowest and highest excited states of the system. This is because this momentum functional has a trigonometric kernel of logarithmic form (see [13, Eqs. (13)–(14)]). Finally let us point out that the generalization to *D* dimensions and the inclusion of the relativistic effects to the entropies of the infinite-well potential are further interesting open problems.

Acknowledgments AIA is partially supported by the grants Chair Excellence program of Universidad Carlos III Madrid, Spain and Bank Santander, and grant RFBR 11-01-00245. DNT acknowledges support to the grant RFBR 10-01-000682. JSD and PSM are very grateful for partial support to Junta de Andalucía (under grants FQM-4643 and FQM-2445) and Ministerio de Ciencia e Innovación under project FIS2011-24540. JSD and PSM belong to the Andalusian research group FQM-0207. We appreciate C. Vignat's help in deriving the asymptotics (7)–(8).

References

- 1. M. Ohya, D. Petz, Quantum Entropy and Its Use (Springer, Berlin, 2004)
- J.B.M. Uffink, Measures of Uncertainty and the Uncertainty Principle. PhD Thesis, University of Utrecht, 1990. See also references herein
- 3. B.R. Frieden, Science from Fisher Information (Cambridge University Press, Cambridge, 2004)
- 4. M.J.W. Hall, Universal geometric approach to uncertainty, entropy and information. Phys. Rev. A **59**, 2602–2615 (1999)
- 5. A. Rényi, Probability Theory (North Holland, Amsterdam, 1970)
- C.E. Shannon, A mathematical theory of communication. Bell Syst. Tech. J. 27, 379–423, 623–656 (1948)
- 7. C. Tsallis, Possible generalization of Boltzmann-Gibbs statistics. J. Stat. Phys. 52, 479–487 (1988)

- R.G. Parr, W. Yang, *Density-Functional Theory of Atoms and Molecules* (Oxford University Press, New York, 1989)
- J.S. Dehesa, S. López-Rosa, A. Martínez-Finkelshtein, R.J. Yáñez, Information theory of *d*-dimensional hydrogenic systems: application to circular and Rydberg states. Int. J. Quantum Chem. 110, 1529–1548 (2010)
- J.S. Dehesa, W. Assche, R.J. Yáñez, Position and momentum information entropies of the D-dimensional harmonic oscillator and hydrogen atom. Phys. Rev. A 50, 3065–3079 (1994)
- I. Bialynicki-Birula, Formulations of uncertainty relations in terms of Rényi entropies. Phys. Rev. A 74, 052101 (2006)
- J.S. Dehesa, R.J. Yáñez, A.I. Aptekarev, V.S. Buyarov, Strong asymptotics of Laguerre polynomials and information entropies of two-dimensional harmonic oscillator and one-dimensional Coulomb potentials. J. Math. Phys. 39, 3050–3060 (1998)
- S. López-Rosa, J. Montero, P. Sánchez-Moreno, J. Venegas, J.S. Dehesa, Position and momentum information-theoretic measures of a *d*-dimensional particle-in-a-box. J. Math. Chem. 49, 971– 994 (2011)
- 14. A. Bohr, B.R. Mottelson, Nuclear Structure (World Scientific, Singapore, 1998)
- T.G. Pederson, P.M. Johansen, H.C. Pederson, Particle-in-a-box model of one-dimensional excitons in conjugated polymers. Phys. Rev. B 61, 10504–10510 (2000)
- A. Rubio, D. Sánchez-Portal, E. Artacho, P. Ordejón, J.M. Soler, Electronic states in a finite carbon nanotube: a one-dimensional quantum box. Phys. Rev. Lett. 82, 3520–3523 (1999)
- P. Harrison, Quantum Wells, Wires and Dots: Theoretical and Computational Physics of Semiconductor Nanostructures, 2nd edn. (Wiley, New York, 2005)
- B. Hu, B. Li, J. Liu, Y. Gu, Quantum chaos of a kicked particle in an infinite well potential. Phys. Rev. Lett. 82, 4224 (1999)
- V. Majernik, R. Charvot, E. Majernikova, The momentum entropy of the infinite potential well. J. Phys. A. Math. Gen. 32, 2207 (1999)
- V. Majernik, L. Richterek, Entropic uncertainty relations for the infinite well. J. Phys. A. Math. Gen. 30, L49–L54 (1997)
- J. Sánchez-Ruiz, Asymptotic formula for the quantum entropy of position in energy eigenstates. Phys. Lett. A 226, 7 (1997)
- J. Sánchez-Ruiz, Asymptotic formulae for the quantum Renyi entropies of position: application to the infinite well. J. Phys. A. Math. Gen. 32, 3419–3432 (1999)
- 23. H. Dym, H.P. McKean, Fourier Series and Integrals (Academic Press, New York, 1972)
- R.G. Catalan, J. Garay, R. López-Ruiz, Features of the extension of a statistical measure of complexity to continuous systems. Phys. Rev. E 66, 011102 (2002)
- E. Romera, A. Nagy, Fisher-Rényi entropy product and information plane. Phys. Lett. A 372, 6823– 6825 (2008)
- R. López-Ruiz, J. Sañudo, Complexity invariance by replication in the quantum square well. Open Syst. Inf. Dyn. 16, 423–427 (2009)
- A. Nagy, K.D. Sen, H.E. Montgomery Jr., LMC complexity for the ground state of different quantum systems. Phys. Lett. A 373, 2552–2555 (2009)
- 28. K.D. Sen, Statistical Measures: Applications to Electronic Structure (Springer, Berlin, 2011)
- M. Abramowitz, I.A. Stegun (eds.), Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables (National Bureau of Standars, U.S. Goverment Printing Office, Washington, D.C., 1964)
- 30. S. Zozor, M. Portesi, C. Vignat, Some extensions of the uncertainty principle. Phys. A 387, 19-20 (2008)
- H. Maassen, J.B.M. Uffink, Generalized entropic uncertainty relations. Phys. Rev. Lett. 60, 1103– 1106 (1988)
- A.K. Rajagopal, The Sobolev inequality and the Tsallis entropic uncertainty relation. Phys. Lett. A 205, 32–36 (1995)