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1999 J. Phys. A: Math. Gen. 32 2207

(http://iopscience.iop.org/0305-4470/32/11/013)

J. Phys. A: Math. Gen. **32** (1999) 2207–2216. Printed in the UK PII: S0305-4470(99)91292-1

The momentum entropy of the infinite potential well

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Received 7 April 1998, in final form 2 November 1998

Abstract. This paper deals with the determination of the momentum information entropy for the infinite potential well in dependence on its quantum states and presents an asymptotical formula for the information entropy in its momentum space. The upper bound of the sum of the position and momentum information entropies for the stationary states of the potential well is also estimated.

1. Introduction

With the advent of new and precise measurement techniques [1], renewed interest has arisen concerning the ultimate limitations of measurement imposed by quantum mechanics. An interesting problem represents the limits placed on the joint measurability of noncommuting variables bounded by the uncertainty relations. The fact that two noncommuting observables A and B cannot simultaneously have sharp eigenvalues represents the cornerstone of the *principle* of uncertainty in quantum mechanics and can be quantitatively expressed in different forms, commonly called uncertainty *relations*. A clear distinction has to be made between the uncertainty principle and its possible expressions in the form of uncertainty relations (see, e.g. [2]).

In accordance with present understanding the quantum system is described by a complex function $\Psi(x, t)$, which is linked with the function of the probability density of finding a particle at position x at time t by the equation $\rho_x(x, t) = |\Psi(x, t)|^2$. The corresponding Fourier transform $\Phi(x, t)$ is connected with the probability of finding a particle with momentum p at time t by the equation $\rho_p(p, t) = |\Phi(p, t)|^2$. According to experimental arrangements the particle can be described by various wavefunctions and therefore with various position and momentum density functions. It holds that the sharper the density function is for the particle position $\rho_x(x, t)$ the steeper the density function is for its momentum $\rho_p(p, t)$. This is to express it in the form of a relation between the 'widths' of position and momentum probability distributions. Such a relation is usually called as the position–momentum uncertainty relation. Generally, an uncertainty relation of two noncommuting observables provides an estimate of the minimum uncertainty (imprecision) expected in the outcome of a measurement of an observable, given the uncertainty in outcome of a measurement of another one. The uncertainty in a measurement of a classical as well as quantum mechanical quantity is commonly expressed by the standard deviation about its mean. The standard deviation is a measure of the scatter of measured values of a physical quantity. From the mathematical point of view, a measured quantity represents a random variable $\tilde{x}$, i.e., a mathematical quantity capable of assuming the

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set of values $x_1, x_2, \ldots, x_n$ with probabilities $P(x_i), P(x_2), \ldots, P(x_n)$ [11]. Since in classical physics this probability distribution is assumed to be Gaussian, representing (for $n \to \infty$) a one-hump symmetrical function, this measure of the scatter appears to be appropriate here. The mean value of measured classical quantity is generally also the most probable one. Another situation arises if the probability distribution function consists of two (or more) distant peaks. Then, although the probability to find the value of the measured quantity is concentrated in the vicinity of the peaks, the standard deviation depends on the *distance* between these peaks. Here, the mean value may not be the most probable value in the measurement and in some cases it may even be equal to zero. This often holds for probability distributions of the noncommuting observables. A typical example is the momentum probability density of particle in an infinite potential well which has for $n > 2$ two distant peaks (see figure 2). Here it is not appropriate to express the scatter of the measured values in the form of standard deviation but to use other measures for it which are *independent* of the distance between the peaks. Therefore, the essential problem, when constructing uncertainty relations, is how to express quantitatively the uncertainties (imprecisions) of the measured noncommuting observables with general probability distributions.

2. Entropic uncertainty relations

The standard deviations of two noncommuting observables A and B were used in the Heisenberg uncertainty relation (see, e.g. [29, 30]) usually written in the form [29]

$$\Delta A \Delta B \geqslant \tfrac{1}{2} |\langle \Psi | [\hat{A}, \hat{B}] | \Psi \rangle| \tag{1}$$

where ΔA and ΔB represent the square root of the second central moment (standard deviation or variance) of A and B, respectively, and $[\hat{A}, \hat{B}]$ is their commutator. We remark that principally one may use instead of the second central statistical moments higher statistical moments of noncommuting observables when formulating a Heisenberg-like uncertainty relation [26].

The vast literature on the Heisenberg uncertainty relation continues to grow and contains criticisms, notable in the following points [5, 14, 23].

(i) If one of two noncommuting observables A or B is in its eigenstate then $\Delta A = 0$ or $\Delta B = 0$ and so the left-hand side of (1) is also equal to zero although the right-hand side for these observables is by definition, different from zero.
(ii) If X and P are two noncommuting observables with continuous probability densities, then their standard deviations may not represent the appropriate measure for the uncertainty of these observables, especially if their probability densities exhibit several sharp distant peaks [9].
(iii) For some quantum systems the standard deviations of the noncommuting observables lead to an uncertainty relation in which the standard deviation of one of the observables is *independent* of the standard deviation of the complementary observable [5, 14]. Such an uncertainty relation does not fulfil the demand put on any form of uncertainty relation.

The standard deviations of the position and momentum were used by Heisenberg in 1927 in his famous uncertainty relation (*Unschärferelation*) [25]. At that time the standard deviation represented the generally accepted measure of the imprecision of a measurement. Since its appearance, the Heisenberg uncertainty relation has been the subject of hundreds of papers in which the standard deviations and the corresponding uncertainty relations of various noncommuting observables were determined. Meanwhile, however, new scientific disciplines have arisen which give new possibilities to express the uncertainty of a measured classical as well as quantum mechanical quantity. Inspired by the Boltzmann–Gibbs entropy Shannon has published fundamental work on the communication theory [27] in which he introduced the most important entropic measure of uncertainty of a random variable, namely the information entropy. In the last few decades, many authors have shown that the uncertainty relations, in which the entropic measures of uncertainty are used instead of the moment, do not suffer from the shortcomings mentioned above [5, 23, 26]. The uncertainty relations where the information entropies for the uncertainty of noncommuting observables are employed are called the *entropic uncertainty relations*. Principally, other entropic measures may be used when formulating 'entropic' uncertainty relations of the noncommuting observables. The simplest one appears to be the so-called information 'energy' defined as [12, 26]

$$H^{(e)}(\tilde{x}) = \sum_{i=1}^{n} P_i^2.$$

This entropic measure of uncertainty, similar to information entropy, also gives the degree of the spreading of the probability distribution of observables. However, the information entropy has an exceptional position between the entropic measures of uncertainty. Aside from its meaning as an uncertainty measure of an observable, the information entropy enables one to determine the amount of information obtained from a certain measurement. One only needs to know the information entropy of an observable before and after its measurement. The difference of these two information entropies yields the amount of information gained in the measurement [31].

In the mathematical formulation of the entropic uncertainty relation, we consider the state vector $|\Psi\rangle$ in N-dimensional Hilbert space and two noncommuting observables A and B having nondegenerate spectra of their eigenvectors $|a_i\rangle$ and $|b_j\rangle$. The entropic uncertainty relation is an inequality of the form [17]

$$S^{(A)} + S^{(B)} \geqslant S_{AB}$$

where

$$S^{(A)} = -\sum_i |\langle\psi|a_i\rangle|^2 \ln |\langle\psi|a_i\rangle|^2$$

and

$$S^{(B)} = -\sum_j |\langle\psi|b_j\rangle|^2 \ln |\langle\psi|b_j\rangle|^2$$

is the information entropy of the observable A and B, respectively. S_{AB} is a positive constant which represents the lower bound of the sum of information entropies S_A and S_B [23]. For the continuous observables X_c and P_c, described by the wavefunctions $\psi(x)$ and $\varphi(p)$, the entropic uncertainty relation reads [5, 17]

$$S^{(X_c)} + S^{(P_c)} \geqslant S_{XP}$$

where

$$S^{(X_c)} = -\int_{-\infty}^{\infty} |\psi(q)|^2 \ln |\psi(q)|^2 \,\mathrm{d}q$$

and

$$S^{(P_c)} = -\int_{-\infty}^{\infty} |\varphi(p)|^2 \ln |\varphi(p)|^2 \,\mathrm{d}p.$$

represents the differential entropy of X_c and P_c, respectively. S_{XP} is the lower bound of the sum of these information entropies. Białynicki-Birula and Mycielski [17], Maassen and

Uffink [22], Sánchez-Ruiz [23] have shown that nontrivial lower bounds for S_{AB} and S_{XP} exist for any two observables with no common eigenstates.

Accordingly, the entropic uncertainty relation for the position and momentum of a quantum system described by its normalized function $\psi(x)$ has the form [17]

$$S_x + S_p \geqslant S_{xp}$$

where S_x and S_p are the information entropies of its position and momentum

$$S_x = -\int_{-\infty}^{\infty} |\psi(x)|^2 \log|\psi(x)|^2 \, \mathrm{d}x \tag{2}$$

and

$$S_p = -\int_{-\infty}^{\infty} |\hat{\varphi}(p)|^2 \log|\hat{\varphi}(p)|^2 \, \mathrm{d}p \tag{3}$$

respectively, where $\hat{\varphi}(p)$ is the Fourier transform of the wavefunction $\psi(x)$. S_{px} represent the lower bound of the sum of position and momentum information entropies. Białynicki-Birula and Mycielski [17] and Maassen and Uffink [22] found that the lower nontrivial bound for the sum of position and momentum entropies exists and is given as ($\hbar = 1$)

$$S_x + S_p \geqslant 1 + \ln \pi.$$

Recently, there has been considerable interest in finding the dependencies of $S_x(n)$, $S_p(n)$ and $S_{xp}(n)$ on the quantum states of a quantum system [4,18–21]. Since the limits of measurability placed on the position and momentum of a particle depends on the concrete quantum system it is necessary to further investigate these limits for each system and its quantum states. We address the question: what are the values $S_p(n)$ and $S_{xp}(n)$ for the set of stationary states of an infinite potential well? There is a specific motivation for the study of this system since a one-dimensional box of length a and infinitely high potential walls often served as a model system for the analysis of different types of uncertainty relation [24]. Whereas the position and momentum measurability limits of the harmonic oscillator, in the form of their entropies and standard deviations, have been already determined as a function of its quantum states (see, e.g. [4] and references therein) the corresponding limits for the infinite potential well [5,8] are only partly known. The aim of this paper is the determination of the momentum information entropy and the corresponding entropic uncertainty relation of an infinite potential well as a function of its quantum states. We succeed in determining the asymptotical value of momentum information entropy of the infinite well for $n \to \infty$ and found the *upper* bound of information entropy in its momentum space.

3. The infinite potential well

We recall that the infinite potential well is a quantum system defined as ($\hbar = 1$) [6]:

$$U(x) = \begin{cases} 0 & \text{for} \quad |x| \leqslant a \\ +\infty & \text{for} \quad |x| > a \end{cases} \tag{4}$$

where $U(x)$ is the potential. Its wavefunctions, the energy eigenvalues and the momentum wavefunctions are

$$\psi_n(x) = \begin{cases} \dfrac{1}{\sqrt{a}} \sin\left[\dfrac{\pi n}{2a}(x-a)\right] & \text{for} \quad |x| \leqslant a \\ 0 & \text{for} \quad |x| > a \end{cases} \tag{5}$$

$$E_n = \frac{n^2\pi^2}{8ma^2} \qquad n = 1, 2, 3, \ldots \tag{6}$$

$$u_n(p) = \sqrt{\frac{\pi n^2}{2a^3}} \frac{\sin(ap - \frac{\pi}{2}n)}{\left(p^2 - \frac{\pi^2 n^2}{4a^2}\right)} \exp(\mathrm{i}\alpha_n) \tag{7}$$

respectively.

The position and momentum standard deviations, Δx and Δp, and the Heisenberg relations of uncertainty for this quantum system as functions of its width a and quantum number n were determined by Peslak [7]:

$$\Delta x(a, n) = \frac{a}{\sqrt{3}} \sqrt{1 - \frac{6}{\pi^2 n^2}} \tag{8}$$

and

$$\triangle p(a, n) = \frac{\pi n}{2a}. \tag{9}$$

The position momentum uncertainty product is

$$\triangle x(n, a) \triangle p(n, a) = \frac{1}{2\sqrt{3}} \sqrt{\pi^2 n^2 - 6}. \tag{10}$$

A striking property of this uncertainty relation is that its right-hand side *does not depend* on width a. The lower and upper bound of the uncertainty product, $\Delta x \Delta p$, of the infinite potential well ranges between a value of 0.5678 and infinity. Equation (9) shows that the momentum standard deviation increases linearly with n. This is why there are two sharp peaks in the momentum probability density function, $|u_n(p)|^2$, for $n > 2$, whose distance increases with the quantum number n. Since momentum standard deviation strongly depends on the distance between both peaks, its standard deviation increases linearly with n, although the probability density of finding the momentum of a particle in the well is concentrated mainly in the vicinity of these peaks.

4. The asymptotical behaviour of $S_p(a, n)$ and $S_{px}(a, n)$

In order to determine the position–momentum entropic uncertainty relations for the infinite potential well we need to evaluate the corresponding integrals (2) and (3). Inserting the position wavefunctions ψ_n into equation (2) we get the dependence of the position information entropy of the infinite potential well on its width a and quantum number n. These integrals were analytically calculated for the whole range of a and n by Sánchez-Ruiz [8] who obtained the following simple result:

$$S_x(n, a) = \ln(4a) - 1. \tag{11}$$

It is remarkable that $S_x(a, n)$ *does not depend* on the quantum number n. Inserting the momentum wavefunctions $u_n(p)$ into (3) we obtain the corresponding momentum information entropy

$$S_p(a, n) = -\int_{-\infty}^{\infty} \frac{\pi n^2}{2a^3} \frac{\sin^2(ap - \frac{\pi}{2}n)}{\left(p^2 - \frac{\pi^2 n^2}{4a^2}\right)^2} \ln\left[\frac{\pi n^2}{2a^3} \frac{\sin^2(ap - \frac{\pi}{2}n)}{\left(p^2 - \frac{\pi^2 n^2}{4a^2}\right)^2}\right] \mathrm{d}p. \tag{12}$$

The analytical calculation of the momentum information entropy represents a considerably more difficult problem than that of the position information entropy. Therefore, we shall next try to estimate it using certain mathematical properties of $S_p(n, a)$ and making some plausible assumptions on $S_p(a, n)$ which we then verify by means of numerical calculations [3].

Using the substitution $ap = t$, the integral (12) turns out to be

$$S_p(n) = -\ln(4a) - \ln\left(\frac{\pi}{8}\right) - \frac{\pi}{2}\int_{-\infty}^{\infty} n^2 \frac{\sin^2(t - \frac{\pi}{2}n)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2} \ln\left[n^2 \frac{\sin^2(t - \frac{\pi}{2}n)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2}\right] \mathrm{d}t. \tag{13}$$

Taking into account equation (11), we have

$$S_p(n) = -\ln 4a + 1 + f(n) - 1 = -S_x(n, a) + f(n) - 1 \tag{14}$$

where

$$f(n) = \ln\left(\frac{8}{\pi}\right) - \frac{\pi}{2}\int_{-\infty}^{\infty} n^2 \frac{\sin^2(t - \frac{\pi}{2}n)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2} \ln\left[n^2 \frac{\sin^2(t - \frac{\pi}{2}n)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2}\right] \mathrm{d}t. \tag{15}$$

Substitution of (15) into (14) gives

$$\begin{aligned}[S_x(a, n) + S_p(a, n)] &= f(n) - 1 \\ &= \ln\left(\frac{8}{\pi}\right) - \frac{\pi}{2}\int_{-\infty}^{\infty} n^2 \frac{\sin^2(t - \frac{\pi}{2}n)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2} \ln\left[n^2 \frac{\sin^2(t - \frac{\pi}{2}n)}{\left(t^2 - \frac{\pi^2 n^2}{4}\right)^2}\right] \mathrm{d}t - 1. \end{aligned} \tag{16}$$

Since the integrand in equation (16) is an even function, the integral in it, after the substitution $t - \pi n/2 = r$, obtains the following form

$$f(n) = \ln\left(\frac{8}{\pi}\right) - \pi\int_{-\pi n/2}^{\infty} n^2 \frac{\sin^2 r}{(r^2 + \pi n r)^2} \ln\left[n^2 \frac{\sin^2 r}{(r^2 + \pi n r)^2}\right] \mathrm{d}r. \tag{17}$$

In order to find the asymptotical value of $f(n)$ we implicitly assume that the $n \to \infty$ limit of integral in equation (17) coincides with the integral of the $n \to \infty$ limit of the integrand. The validity of this procedure is then confirmed by the numerical calculations. We realize that the interchange of the order of the operations 'limit' and 'integration' needs a rigorous mathematical proof. However, to bring this proof, which is also interesting for determining asymptotical values of other information entropies, we require further study which would exceed the scope of this paper. It will be the subject of a subsequent paper.

Let us consider an arbitrary *finite* real number r for which it holds

$$\lim_{n\to\infty} n^2 \frac{\sin^2 r}{(r^2 + \pi n r)^2} = \frac{\sin^2 r}{\pi^2 r^2} \qquad \lim_{n\to\infty} -\pi n/2 = -\infty < r.$$

If $n \to \infty$, the integrand in equation (19) becomes the following function:

$$\frac{\sin^2 r}{\pi^2 r^2} \ln \frac{\sin^2 r}{\pi^2 r^2}.$$

Therefore,

$$\lim_{n\to\infty} f(n) = \ln\left(\frac{8}{\pi}\right) - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin^2 r}{r^2} \ln \frac{\sin^2 r}{\pi^2 r^2}\, \mathrm{d}r.$$

Taking into account that

$$\int_{-\infty}^{\infty} \frac{\sin^2 r}{r^2}\, \mathrm{d}r = \pi$$

we find

$$\lim_{n\to\infty} f(n) = \ln(8\pi) - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin^2 r}{r^2} \ln \frac{\sin^2 r}{r^2}\, \mathrm{d}r$$

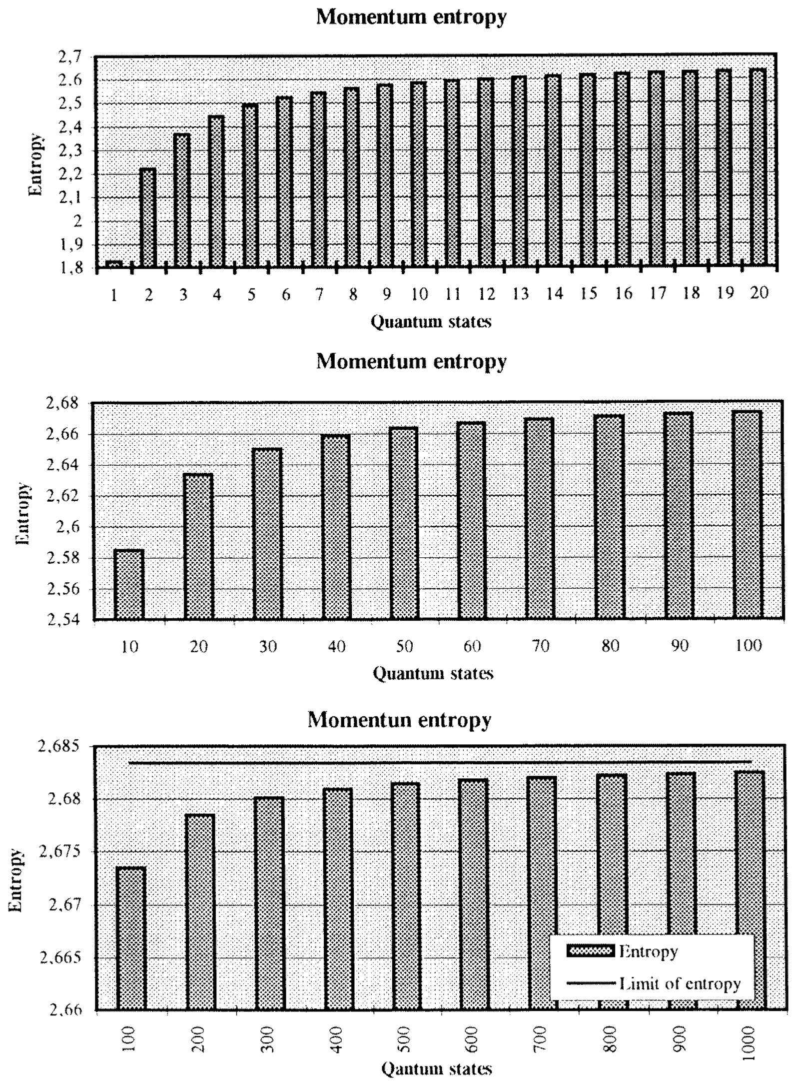

Figure 1. The momentum information entropy of the infinite potential well as a function of its quantum states. The horizontal line in the bottom figure represents the estimated upper bound.

and

$$\lim_{n\to\infty} S_p(n) = -\ln 4a + \ln 8\pi - \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin^2 r}{r^2} \ln \frac{\sin^2 r}{r^2}\,\mathrm{d}r. \tag{18}$$

The exact analytical value of the integral in (18) has been found in a very recent work by Sánchez-Ruiz [10], who was able to prove that

$$\int_0^{\infty} \frac{\sin^2 r}{r^2} \ln \frac{\sin^2 r}{r^2}\,\mathrm{d}r = -\pi(1-\gamma) \tag{19}$$

where γ is Euler's constant. The value of the integral in (18) is

$$\varrho = -\int_{-\infty}^{\infty} \frac{\sin^2 r}{r^2} \ln \frac{\sin^2 r}{r^2}\,\mathrm{d}r = 2\pi(1-\gamma) \approx 2.6564.$$

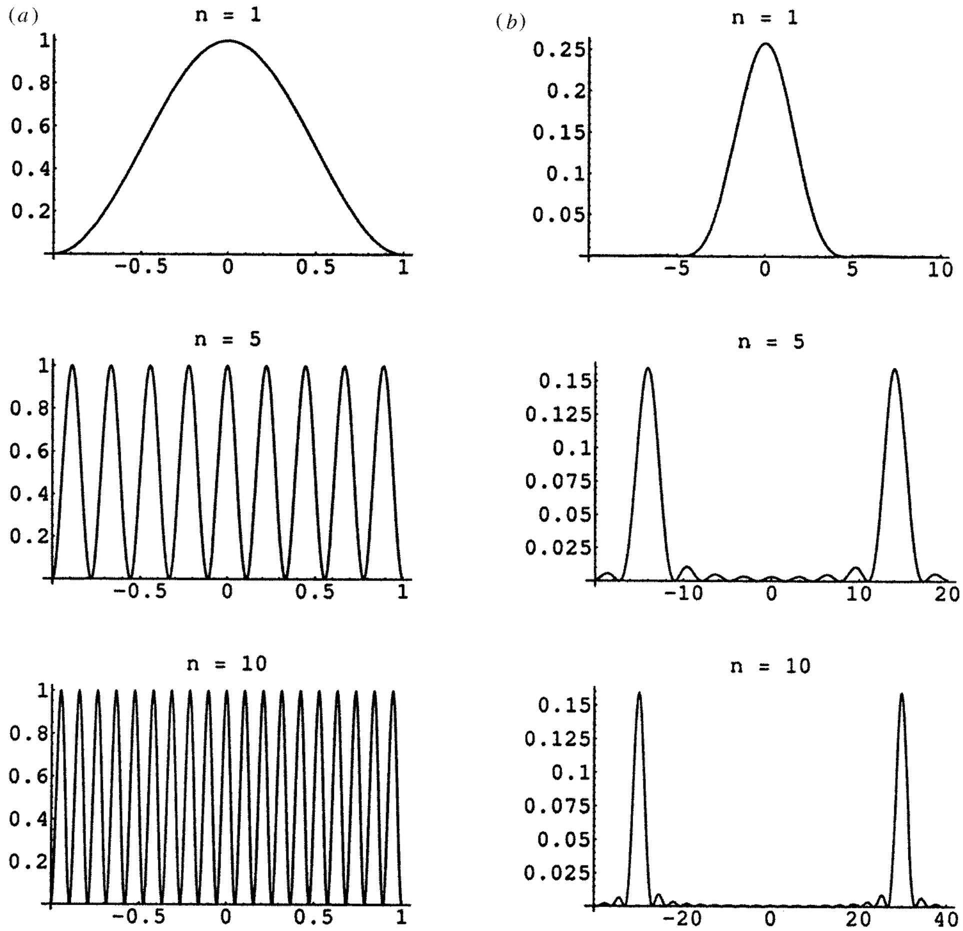

Figure 2. The position probability density (*a*) and momentum probability density (*b*) for the symmetric wavefunctions of the infinite potential well corresponding to $n = 1, 5, 10$.

Accordingly, we obtain for the asymptotical value of $S_p(a, n)$

$$\lim_{n\to\infty} S_p(a, n) = -\ln 4a + \ln 8\pi + \frac{\varrho}{\pi} = -\ln 4a + \lim_{n\to\infty} f(n).$$

Hence, the asymptotical value of the sum of position and momentum entropies S_{xp} is

$$\lim_{n\to\infty} [S_x(n) + S_p(n)] = \lim_{n\to\infty} f(n) - 1 = \ln 8\pi + \frac{\varrho}{\pi} - 1 \approx 3.0697.$$

This value represents the estimated upper bound of $S_{xp}(a, n)$. The value of $S_{xp}(a, n)$ ranges between a value of 2.212 and a value of 3.0697. How close the momentum information entropy as a function of the increasing quantum number n approaches to the estimated upper bound is shown in figure 1 (bottom).

In contrast to the corresponding Heisenberg uncertainty relation the upper bound of momentum information entropy for $n \to \infty$ is a finite number. If one takes for the uncertainties of position and momentum their standard deviations, one has, for $n \to \infty$, $\Delta x \approx a/\sqrt{3}$ and $\Delta p \approx \infty$ which means that in this case the momentum is completely uncertain, *independent* of a. This indicates that it is not possible to derive from the Heisenberg uncertainty relation the central claim of uncertainty principle, namely, the impossibility of an arbitrarily sharp specification of both position and momentum. In contrast to this $S_p(a, n)$ is for $n \to \infty$ finite and depends on the width of well a.

5. Concluding remarks

There is still active discussion of joint measurement of two canonically conjugate observables and the physical interpretation of the uncertainty principle in quantum physics [28]. Whilst some authors believe these observables cannot be measured simultaneously, others believe that they can be measured simultaneously with unlimited accuracy. The standard view is that the measurement is possible but that the uncertainty relation limits its accuracy [15,16]. Recently, a new formulation of uncertainty relation, based on the operational probability distributions of noncommuting observables have been proposed by Bužek *et al* [13]. This operational uncertainty relation explicitly takes into account the action of a measurement device, which due to internal classical or quantum noise, may enlarge the total uncertainty of a measured observable.

An interesting feature of the infinite potential well is that its standard deviation and information entropy in the momentum space of its quantum states exhibit considerably different behaviour. Whereas the momentum information entropy only slightly increases for $n > 2$, the momentum standard deviation increases almost linearly proportional to n. This is why the momentum probability distribution of the infinite well has two distant peaks in the vicinity of which the momentum probability density is mainly concentrated (see figure 2). The areas of the concentrated momentum probability density are practically independent of n, therefore its information entropy is almost independent on n whereas the standard deviation, in which the distance between these areas explicitly occurs, increases approximately linearly with n [9]. Due to this fact the standard and entropic uncertainty relations of the infinite well also considerably differ for $n > 2$. This shows that the use of momentum information entropy here corresponds more to the demands put on the measure for uncertainty of an observable than the standard deviation.

Acknowledgments

The support by the Grant Agency of the Czech Republic (GAČR) No 202/97/0166 and also partly by grant No 2/4109 of VEGA is greatly acknowledged.

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