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Standard and entropic uncertainty relations of the finite well

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Abstract

This paper deals with the standard and entropic uncertainty relations for the finite-potential well with different length and potential depth. We calculate the position and momentum dispersions and entropies that are dependent on the quantum states of the finite well and determine the corresponding standard and entropic uncertainty relations. Then we calculate the entropy of occurrence for the mass point inside and outside the well. We discuss the results and determine a class of probability distributions with a parameter for which the standard deviation becomes infinite, independent of the value of this parameter.

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1. Introduction

Recently, with the advent of ultraprecise measurement techniques being developed in experimental atomic physics [1] and quantum optics [2], renewed interest has arisen concerning the ultimate limitations of measurement imposed by quantum mechanics. An interesting problem is the limits placed on the joint measurability of non-commuting variables. In optics these might be, for example, the optical phase and the photon number, in atomic physics they might be the momentum and position of the free and bound particle. The fact that two non-commuting observables A and B cannot simultaneously obtain 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*. An uncertainty relation, as normally understood, provides an estimate of the minimum uncertainty expected in the outcome of a measurement of one observable, given the uncertainty in outcome of a measurement of another observable[4]. The limits of the measurability placed on the position and momentum of a particle depend on the concrete quantum system and are given by the standard and entropic uncertainty relations. Therefore, it is necessary to investigate these limits especially for the given quantum system and its quantum states.

This paper is devoted to the determination of position and momentum measurability limits of a finite-potential well both in the form of the momentum and position dispersions (standard deviations) and the Shannon entropies by means of which we construct the corresponding standard and entropic uncertainty relations. There are many authors (see e.g. [7, 11]) who generally demonstrated that the entropic uncertainty relation corresponds more to the uncertainty principle of quantum physics than to the Heisenberg one. We discuss this problem on the example of the finite well and show how the lower bounds of the product of position and momentum uncertainties as well as the sum of these uncertainties depend on its parameters and its quantum states.

The harmonic oscillator and potential well are perhaps the simplest systems that have been extensively studied both classically and quantum mechanically. The harmonic oscillator represents the main paradigm in quantum optics and the potential well serves as an important model in particle and condensed matter physics. In the latter, the overlapping of electron wavefunctions determines the probability of the tunnelling through barriers between neighbouring potential wells. These overlappings are mainly given by the spreading (measured by dispersions or entropies) of the electron wavefunctions in the array of the neighbouring wells. The dispersions and entropies of the position and momentum of the two-dimensional wells in periodic arrays of the two-dimensional quantum wells in a semiconductor film give important information about its transport properties [14].

While the position and momentum measurability limits of the harmonic oscillator and the hydrogen atom, in the form of their entropies and dispersions, have already been determined as a function of their quantum states (see [5, 8, 10] and references therein) the corresponding limits are only known for the infinite-potential well which represents the limiting case of the finite-potential well [6, 17]. In this paper we also determine these quantities for the shallow and the deep finite-potential well.

We recall that the entropic uncertainty relation for the position and momentum of a quantum system described by its normalized function $\psi(x)$ has the form [7]

$$S_x + S_p \geqslant S_{xp} \tag{1}$$

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

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

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 transfer of the wavefunction $\psi(x)$. Bialynicki-Birula and Mycielski and others [7] found that the lower non-trivial bound for the sum of position

[4] There is still active discussion on the joint measurement of two canonically conjugate observables and the physical interpretation of the uncertainty principle in quantum physics. Some authors believe these observables cannot be simultaneously measured at all, others believe that they can be measured simultaneously with unlimited accuracy, the standard view being that the measurement is possible but that the uncertainty relation limits its accuracy [15]. Another formulation of the uncertainty relation, based on the operational probability distributions of non-commuting observables, that explicitly takes into account the action of the measurement device, when determining their limits of measurability, have proposed Bužek *et al* [16]. The uncertainty relations, considered here, reflect the intrinsic properties of the quantum mechanical states, not taking into account the action of the measurement device.

and momentum entropies holds ($\hbar = 1$)

$$S_x + S_p \geqslant 1 + \ln \pi. \tag{4}$$

2. The finite-potential well

The finite-potential well is a quantum system with the potential [12]

$$U(x) = \begin{cases} -U & |x| \leqslant a \\ 0 & |x| > a. \end{cases}$$

For the sake of simplicity, next we only consider the symmetrical solutions of the corresponding Schrödinger equation (putting $2m/\hbar^2 = 1$)

$$\Psi(x) \equiv \begin{cases} \psi_I(x) = A\exp(\kappa x) & \text{for} \quad x < -a \quad \text{left-hand side of the well (area I)} \\ \psi_{III}(x) = A\exp(-\kappa x) & \text{for} \quad x > +a \quad \text{right-hand side of the well (area III)} \\ \psi_{II}(x) = B\cos(kx) & \text{for} \quad |x| < a \quad \text{in the well (area II)} \end{cases} \tag{5}$$

where $k = \sqrt{U - E}$, $\kappa = \sqrt{(-E)}$, κ and k are connected by the transcendent equation

$$\kappa a = (ka)\tan(ka) \tag{6a}$$

and the constants A and B are completely determined by the values of κ and k

$$A = B\frac{\kappa}{\sqrt{k^2+\kappa^2}}\exp(\kappa a) \qquad B = \left(\frac{\kappa}{1+\kappa a}\right)^{1/2}. \tag{6b}$$

In the following we calculate the position and momentum dispersions and entropies of the one-dimensional finite-potential well. The position probability density is $q(x) = |\Psi(x)|^2$ and the corresponding position dispersion and entropy are

$$(\Delta x)^2 = \int_{-\infty}^{\infty} q(x)x^2\,\mathrm{d}x$$

and

$$S_x = -\int_{-\infty}^{\infty} q(x)\log q(x)\,\mathrm{d}x.$$

Analytical evaluation of these integrals yields

$$(\Delta x)^2 = \frac{1}{2(k^2+\kappa^2)(1+\kappa a)}(2a^2\kappa^2 + 2a\kappa + 1) + \left(\frac{\kappa}{(1+a\kappa)12k^3}\right)[4a^3k^3 + 6a^2k^2\sin(2ak) + 6ak\cos(2ak) - 3\sin(2ak)]$$

and

$$S_x = \left(\frac{\kappa^2}{(1+a\kappa)(k^2+\kappa^2)}\right)\left[(2a\kappa+1) - \log\left(\frac{\kappa^3}{(1+\kappa a)(k^2+\kappa^2)}\right)\right] - I_1$$

where

$$\begin{aligned} I_1 &= \int_{-a}^{+a}\left(\frac{\kappa}{1+ka}\right)\cos^2 kx\log\left(\frac{\kappa}{1+\kappa a}\right)\cos^2 kx\,\mathrm{d}x \\ &= \left[\left(\frac{\kappa}{1+\kappa a}\right)\left(\frac{1}{2}x + \frac{1}{4k}\sin 2kx\right)\log\left(\frac{\kappa}{1+\kappa a}\right)\cos^2 kx\right]_{-a}^{+a} \\ &\quad + \frac{\kappa}{(1+\kappa a)k}\left[\frac{a}{2} - \frac{1}{4k}\sin 2ka\right]_{-a}^{a} + \left(\frac{\kappa}{1+\kappa a}\right)[I_t(ka) - I_t(-ka)] \end{aligned}$$

where

$$I_t(kx) = \frac{\mathrm{i}x^2}{2} - \frac{x\log[1-\exp(2\mathrm{i}kx)]}{k} + \frac{\mathrm{Li}_2(\mathrm{z})[2, -\exp(2\mathrm{i}kx)]}{2k^2}$$

and

$$\mathrm{Li}_2(\mathrm{z}) = \sum_{l=1}^{\infty} \frac{z^l}{l^2}.$$

The corresponding momentum wavefunction is given by the Fourier transform of the wavefunction (5)

$$\begin{aligned}\hat{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp\left(-\frac{\mathrm{i}px}{\hbar}\right) \mathrm{d}x \\ &= \frac{B}{\sqrt{2\pi}} \left[\frac{\sin(ak-ap)}{k-p} + \frac{\sin(ak+ap)}{k+p}\right] + 2R(p)\,[\kappa\cos(ap) - p\sin(ap)] \qquad (7)\end{aligned}$$

where

$$R(p) = \frac{A\exp(-\kappa a)}{\sqrt{2\pi}(\kappa^2+p^2)}.$$

Evaluation of the integral determining the momentum dispersion of the system under study yields

$$(\Delta p)^2 = \frac{\hbar^2}{2}\left(\frac{\kappa}{1+ka}\right)\left(2ak^2 + k\sin 2ak - \frac{\kappa^3}{k^2+\kappa^2}\right).$$

Inserting Δx and Δp into the Heisenberg uncertainty relation we obtain

$$\Delta x\,\Delta p = \frac{\hbar}{2} F_h(a, \kappa, k)$$

where $F_h(a, \kappa, k)$ represents a complicated function, of width a and depth U, of the potential well. Since the lower bound of the uncertainty product is $\hbar/2$ [12], $F_h(a, \kappa, k) \geqslant 1$. The analytical evaluation of the integral determining the momentum entropy $S_p(a, \kappa, k)$ is difficult due to the logarithms in its integrand, therefore we calculate them numerically. The sum of position and momentum entropies $S_x(a, \kappa, k)$ and $S_p(a, \kappa, k)$ represents the entropic uncertainty relation of the finite well.

We note that according to some authors, the measurement of the position of a particle in a quantum system does not yield its exact value, but only the interval (Partovi's 'bin' [13]) in which it occurs. One can calculate the probability that the particle in the considered quantum system occurs in one of these intervals, $P_1, P_2, \ldots, P_n$, and use the Shannon formula for the calculation of the measurement's entropy for the discrete probability distribution

$$I = -\sum_{i=1}^{n} P_i \log P_i.$$

If one denotes the probabilities of finding the particle inside and outside the well by P_1 P_2 and P_3 one obtains the corresponding Shannon entropy

$$I_0 = -\sum_{i=1}^{3} P_i \log P_i$$

where

$$P_1 = \int_{-\infty}^{-a} [\psi_I(x)]^2\,\mathrm{d}x = \frac{A^2\exp(-2a\kappa)}{2\kappa}$$

$$P_2 = \int_{-a}^{a} [\psi_{II}(x)]^2 \, dx = aB^2 + \frac{B^2 \sin(2ak)}{2k}$$

$$P_3 = \int_{a}^{\infty} [\psi_{III}(x)]^2 \, dx = \frac{A^2 \exp(-2a\kappa)}{2\kappa}.$$

The sum of the probabilities P_1, P_2, P_3 is

$$\sum_{1}^{3} P_i = aB^2 + \frac{B^2 \sin(2ka)}{2k} + \exp(-2a\kappa) = N. \tag{8}$$

Inserting equations (6*b*) into equation (8) and taking into account equation (6*a*), N becomes 1 as it should be. I_0 is called the entropy of occurrence and it obtains its maximum value for $P_1 = P_2 = P_3 = 1/3$. In figure 1 (top) the entropy of occurrence I_0 is plotted versus the depth and width of the shallow well. The probability of finding the particle inside the well increases as its depth increases. As $U \to 0$, $P_{II} \to 0$, i.e. the probability of finding the particle inside the well becomes zero and we have $I_0 = -2\log(1/2)$.

3. Results

We present the results of this study mainly in graphical form ($\hbar = 1$). In figure 1 (bottom) the dispersion of the position, Δx, for the shallow well is plotted against its depth and width. The product of the momentum and the position dispersions (the standard uncertainty relation) and the sum of the position and the momentum entropies (the entropic uncertainty relation) for the shallow well as a function of its depth are depicted in figure 2 (top) and (bottom), respectively.

The shallow well, with only one bound state, can generally be characterized as a quantum system with the large spread of its position probability density and relatively small spread of its momentum probability density.

The dispersion of the position and the position entropy as well as the dispersion of the momentum and the momentum entropy of the deep well, as a function of its quantum number n, are depicted in figure 3 (top) and (bottom), respectively. The position entropy for $n = 1$ and $a = 1$ has the value 0.43 which approaches the value of the position entropy of the infinite well $S_x = \ln(4) - 1$ [9]. The standard and entropic uncertainty relations of a deep well as a function of n are depicted in figure 4. As we see in figure 1, the probability of finding a particle in the central area of the well strongly depends on its width and depth. The deeper and the narrower the potential well, the larger the particle localization in its central area. Figure 1 (bottom) shows that the position dispersion also has a similar behaviour. The dependence of momentum dispersion and entropy, which generally increase with increasing the particle localization in the central area of the well exhibits just the opposite behaviour.

The remarkable property of the product of the position and momentum dispersions (the standard uncertainty relation) of a shallow well ($a = 1$) as a function of the well depth is that it possesses a minimum in the vicinity of depth $U = 4.5$, where the product of the dispersions of position and momentum gives the value of 0.506. This value is only slightly larger than the minimal uncertainty product given by Heisenberg uncertainty relation. The sum of entropies as a function of the depth of the shallow well also has its minimum in the vicinity of $U = 4.5$, where it gives the value 2.153. This value approaches to the minimal lower bound for the position–momentum entropic uncertainty relations, which is equal to $1 + \ln \pi$ [7].

The particle localization in the central area of a deep well is generally much larger than it is in a shallow well. The highest localization exhibits the ground state, the position entropy

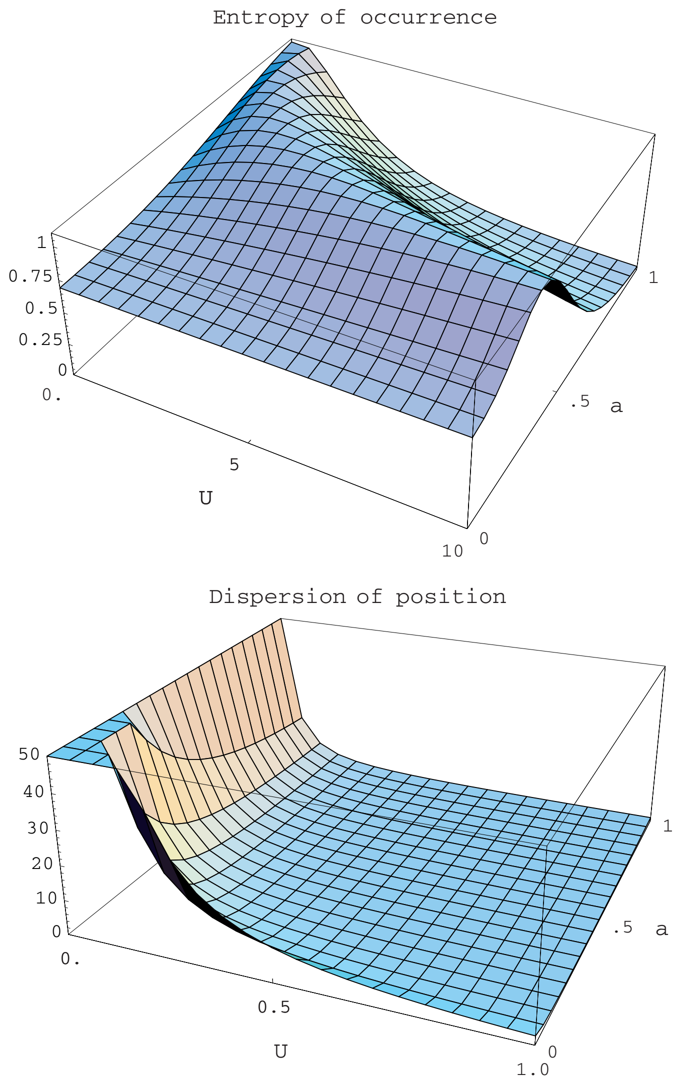

Figure 1. Top: the entropy of the occurrence plotted against the width and depth of the shallow well. Bottom: the dispersion of the position for the shallow well plotted against its depth and width.

of which, gives the value 0.43 which is slightly higher than the state-independent position entropy for the infinite well $\ln(4) - 1 = 0.3863$ [9]. An interesting feature of the deep finite-potential well is that its momentum dispersion and the entropy as a function of the quantum state n exhibits different behaviour. While the momentum entropy increases only slightly for $n > 2$, the momentum dispersion increases almost linearly, proportional to n. This is why the momentum probability distribution of the deep well has two distant peaks in the vicinity of which the momentum probability density is mainly concentrated. With increasing n the distance between both peaks also increases. The areas of the concentrated momentum probability are practically independent of n, therefore its entropy is almost independent of n while the momentum dispersion, in which the distance between these areas explicitly occurs,

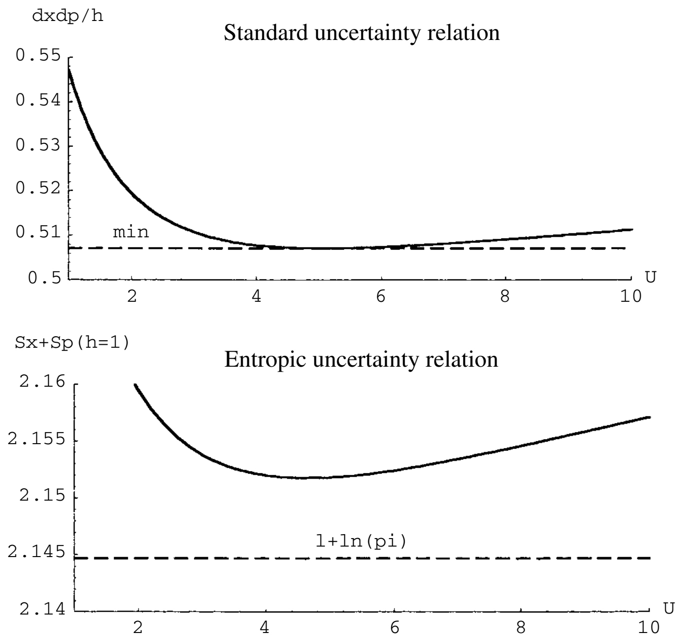

Figure 2. Top: the standard uncertainty relation of the shallow well plotted against its depth. Bottom: the entropic uncertainty relation for the shallow well plotted against its depth.

increases approximately linearly with n [6]. Due to this fact the standard and entropic uncertainty relations of the deep well differ considerably for $n > 2$, which can be seen in figure 4.

From what has been said so far the following points can be observed.

(a) The dependence of the Heisenberg uncertainty relation on the depth and the width of a shallow potential well is essentially similar to that of the entropic uncertainty relation. This means that for the quantum states of shallow wells both relations express the uncertainty principle equally well.
(b) For $A = 1$ and $U \approx 4$ both the entropic and the Heisenberg uncertainty relations have a minimum. In the vicinity of this depth the wavefunction of the wells are most similar to flat Gaussian functions. Therefore, here the position–momentum uncertainty product gives a value close to 0.5.
(c) There is a considerable difference between the dependences of the entropic and the Heisenberg uncertainty relations on quantum states for the deep potential well. Here the entropic uncertainty relation more adequately expresses the uncertainty principle than the Heisenberg one.
(d) The difference between both cases consists of the fact that the position and the momentum eigenfunctions of a shallow well are smooth and do not have sharp peaks, whereas the momentum eigenfunctions for the deep well exhibit two sharp distant peaks, causing a great difference between the momentum dispersion and the entropy.

Several authors have already pointed out the fact that standard deviation is not a good measure of uncertainty for probability distributions with several distant peaks, so that the Heisenberg inequality is not a proper uncertainty relation when position and/or momentum distributions are of this kind. See, e.g. [3, 4, 18]. However, these authors have also noted that

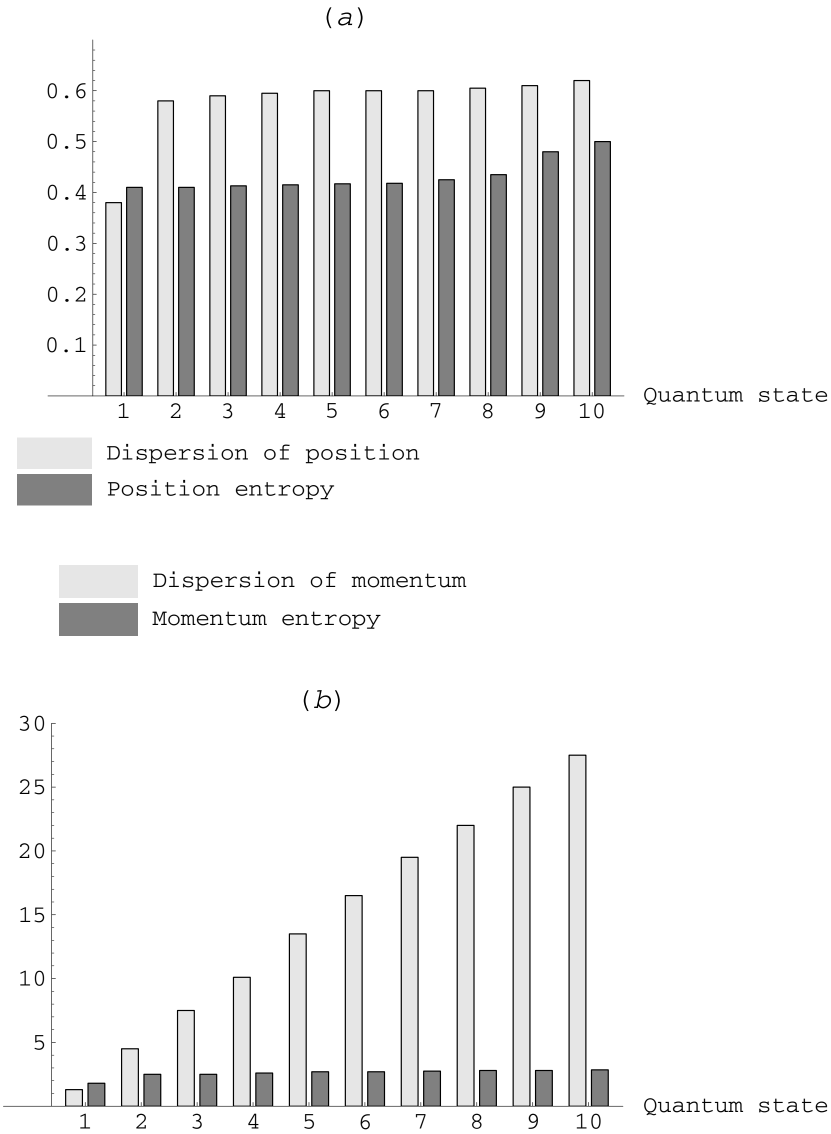

Figure 3. Top: the dispersion of position and position entropy for quantum states of the deep well. Bottom: the dispersion of momentum and momentum entropy for quantum states of the deep well.

Standard deviation can also fail to be a good measure of uncertainty for smooth one-hump curves. A well known instance is the Cauchy distribution,

$$p_c(x) = \frac{\gamma}{\pi}\frac{1}{(x-a)^2+\gamma^2} \qquad \gamma > 0$$

for which $\Delta x = \infty$ for any value of the parameter γ, although the probability distribution becomes increasingly narrow as γ decreases and tends to a Dirac delta distribution in the limit $\gamma \to 0$. On the other hand, the corresponding entropy $S_x = \log(4\pi\gamma)$, has a perfectly correct behaviour.

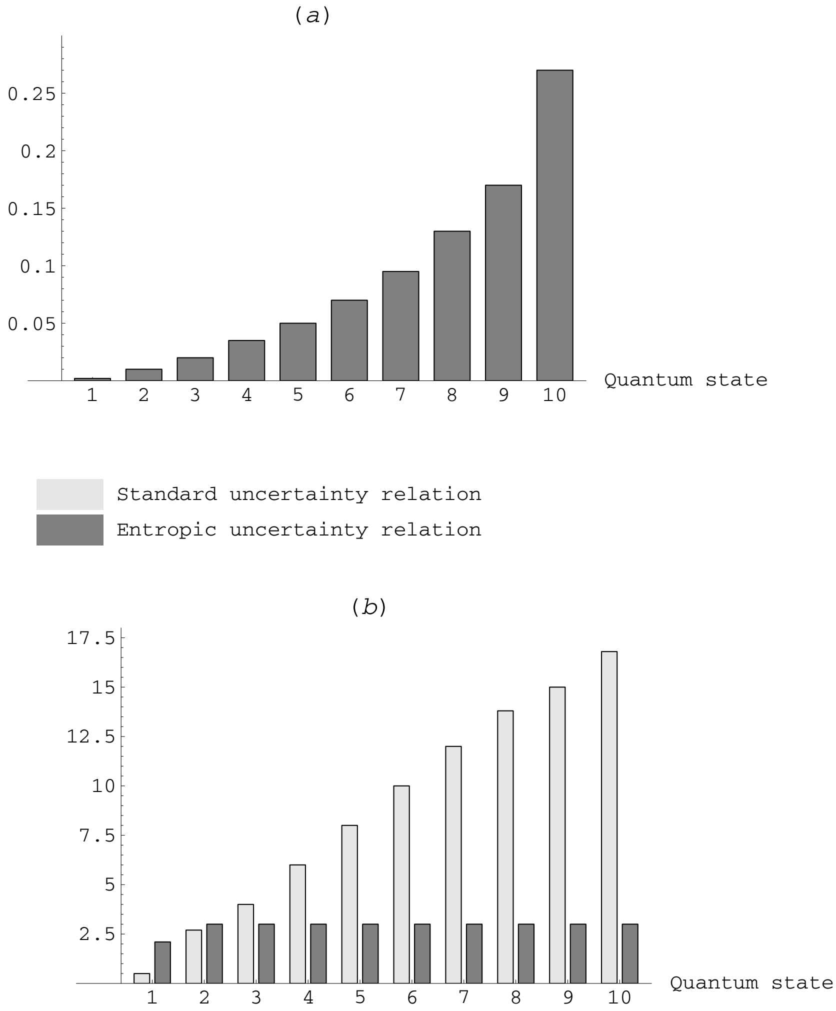

Figure 4. Top: the entropy of occurrence for quantum states of the deep well. Bottom: the standard and entropic uncertainty relations for quantum states of the deep well.

One can also find a class of probability distributions which exhibit similar properties. Let be a probability distribution with parameter a be written in the form

$$\frac{F(x,a)}{x^2}.$$

If for $F(x,a)$ holds

$$\int_{-\infty}^{\infty} F(x,a)\,\mathrm{d}x \to \infty$$

while

$$\int_{-\infty}^{\infty} \frac{F(x,a)}{x^2} = 1$$

then $\Delta x \to \infty$ for any value of parameter a. An instance of such a distribution (assign $\phi(x) = \sin(ax)/\sqrt{\pi a x}$ to the wavefunction) is

$$p(x) = \sin(ax)^2.$$

Here, the integral $\int_{-\infty}^{\infty} F(x,a)\,\mathrm{d}x$ tends to ∞, while

$$\int_{-\infty}^{\infty} \sin(ax)^2\,\mathrm{d}x = 1.$$

In this case, $\Delta x \to \infty$ is independent of the parameter a. On the other hand,

$$S_x = \int_{-\infty}^{\infty} (\sin(ax)^2)\log(\sin(ax)^2) = \log(\pi/a) + I/\pi$$

where [19]

$$I = -\int_{-\infty}^{\infty} \left(\frac{(\sin y^2)}{y^2}\right) \log\left(\frac{(\sin y)^2}{y^2}\right) \mathrm{d}y = 2\pi(1-\gamma) \approx 2.656$$

where γ is the Euler constant. Here, again S_x is finite and depends on a.

Another nice instance of a probability distribution with $\Delta x \to \infty$ is represented by the following function

$$p(x) = \frac{(\arctan ax)^2}{\pi \log(4) x^2}$$

for which

$$\int_{-\infty}^{\infty} \frac{(\arctan ax)^2}{\pi \log(4)}\,\mathrm{d}x \to \infty$$

while

$$\int_{-\infty}^{\infty} \frac{(\arctan ax)^2}{\pi \log(4) x^2}\,\mathrm{d}x = 1.$$

This probability distribution is represented by a smooth one-hump curve, which is symmetric about the y axis and for $a \to \infty$ it takes the form of a Dirac delta function.

In conclusion, we can state that standard deviation fails to be a good measure of uncertainty, and so the Heisenberg inequality $\Delta x \Delta p$ is not a proper uncertainty relation in quantum physics, neither for the probability distribution which possesses several distant peaks (as was demonstrated by the finite-potential well) nor if it belongs to the class of functions described above.

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