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Position-momentum uncertainty products

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Abstract
We point out two interesting features of position-momentum uncertainty product: $U = \Delta x \Delta p$. We show that two special (non-differentiable) eigenstates of the Schrödinger operator with the Dirac delta potential $[V(x) = -V_0 \delta(x)]$, $V_0 > 0$, also satisfy Heisenberg's uncertainty principle by yielding $U > \frac{\hbar}{2}$. One of these eigenstates is a zero-energy and zero-curvature bound state.

Keywords: uncertainty principle, Schrödinger equation, boundstates, position-momentum uncertainty product, Fourier transform, exactly solvable potentials, Dirac delta potential between two rigid walls

That the position (x) and momentum (p) of a particle, in the quantum world, cannot be measured precisely and simultaneously in the same direction is called Heisenberg's uncertainty principle. This is one of the most important features of the quantum world and in the realm of the Schrödinger equation it is precisely stated [1–3, 6–10] as

$$\Delta x \Delta p \geqslant \frac{\hbar}{2}, \tag{1}$$

as the commutator $[x, p] = \mathrm{i}\hbar$. The uncertainty ΔA in an observable corresponding to an operator A for an energy eigenstate $\psi(x)$ is defined as

$$\Delta A = \sqrt{\langle \psi | A^2 | \psi \rangle - \langle \psi | A | \psi \rangle^2}. \tag{2}$$

The equality sign in (1) is well known to occur for the ground state, $\psi_0(x) = A\mathrm{e}^{-\alpha x^2}$, of a one-dimensional harmonic oscillator. For the ground state, $\psi_0(x) = A \sin(\pi x/a)$, of the well-known infinitely deep well (IDW) potential, this product turns out to be $\frac{\hbar}{2}\sqrt{\frac{\pi^2-6}{3}}$ [3], which is (approximately $0.5678\hbar$) a little more than $\hbar/2$ and does not depend on the value of the width of the well. In textbooks, these two potentials are usually discussed for the uncertainty product. We shall be denoting the uncertainty product (1) as $U_{\psi(x)}$ as it is a property of the eigenstate.

In this work, we point out two interesting features of U. Firstly, for potentials which possess a finite number of discrete bound states, U admits the minimum value of $\frac{\hbar}{2}$ when their

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depth tends to infinity. Secondly, $U_{\psi(x)} = U_{\phi(x)}$, where $\phi(p)$ is the Fourier transform of $\psi(x)$. Then we obtain U for two eigenstates of a Schrödinger operator with Dirac delta potential. Both of these eigenstates are non-differentiable at $x = 0$ and finding U for them becomes tricky, as acknowledged in [6]. More interestingly, one of them is a novel zero-energy and zero-curvature bound state [11, 12]. One may wonder whether these eigenstates would satisfy the uncertainty principle by yielding $U > \frac{\hbar}{2}$.

Using special higher-order functions, beautiful expressions of the uncertainty products for the exactly solvable symmetric Rosen–Morse potential, $V_{\mathrm{SRM}}(x) = s(s+1)\tanh^2(x)$ [2], and the Morse oscillator, $V_M(x) = \lambda^2(1-\mathrm{e}^{-x})^2$ [2], have been obtained [4] in terms of polygamma function, $\Psi'(z)$ [5] (not to be confused with the wave function, $\psi(x)$). For the ground state of V_{SRM}, we have [4]

$$\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{s^2\Psi'(s)}{s+1/2}}, \quad s > 0. \tag{3}$$

For the Morse oscillator we have [4]

$$\Delta x \Delta p = \frac{\hbar}{2}\sqrt{(2\lambda-1)\Psi'(2\lambda-1)}, \quad \lambda > 1/2. \tag{4}$$

For large values of z, $\Psi'(z) \sim \frac{1}{z} + \frac{1}{2z^2}$. Also we have a recurrence relation $\Psi'(z+1) = \Psi'(z) - 1/z^2$, with $\Psi'(1/2) = \frac{\pi^2}{2}$, $\Psi'(1) = \frac{\pi^2}{6}$. When s or λ increases, the number of bound states possessed by these two potentials increases and the ground state lies deeper and deeper. Interestingly, in the limit when $s, \lambda \to \infty$, both the uncertainty products (3,4) can be readily checked to tend to the minimal value of $\hbar/2$ for ground states. Perhaps, this could be a common feature of one-dimensional potentials possessing a finite number of discrete eigenvalues.

Let $\phi(p)$ be the momentum space representation of the eigenfunction which is the Fourier transform of the eigenstate $\psi(x)$; then physical quantities like $\langle x\rangle$, Δx, $\langle p\rangle$, Δp and U are known [1–3, 6–10] to be independent of the representation (use $\phi(p)$ or $\psi(x)$). The proof of this is often left as an exercise. In principle, one can do all calculations in momentum space just as well (though not always as easily) as in position space.

Now if we are given $\psi(x)$ and $\phi(x)$ (notice that it is x and not p which is the argument of ϕ), here, we point out that the well-known equivalence of results using $\psi(x)$ or its momentum representation, $\phi(p)$, manifests in

$$(\Delta x)_{\psi(x)} = (\Delta p)_{\phi(x)}, \quad (\Delta p)_{\psi(x)} = (\Delta x)_{\phi(x)}, \Rightarrow U_{\psi(x)} = U_{\phi(x)}. \tag{5}$$

Therefore, if one finds $U_{\psi(x)}$, one has found $U_{\phi(x)}$ as well. However, it may turn out that one may not be attainable as easily as the other one. In table 1, we display several pairs of ground states, $\psi_0(x)$ and $\phi_0(x)$, which may look similar (see rows 2 and 3) or dissimilar (see rows 1, 4-7) but they essentially give rise to the same value for U. For the proof of the equivalence in (5) see the appendix. Next, in the following, we present the determination of the uncertainty product for two special eigenstates: *Case*(I) and *Case*(II).

Case (I)—Dirac delta well

This potential $V(x) = -V_0\delta(x)$, $V_0 > 0$ is well known to have a single bound state at $E = -\frac{mV_0^2}{2\hbar^2}$ and its normalized eigenfunction is given as [6–9]

$$\psi_0(x) = \sqrt{\alpha}\,\mathrm{e}^{-\alpha|x|}, \quad \alpha = \frac{mV_0}{\hbar^2}. \tag{6}$$

The expectation value of x for this state vanishes as it is an even parity state. The expectation value of x^2 for this state is given as

$$\langle\psi_0|x^2|\psi_0\rangle = \alpha\int_{-\infty}^{\infty} x^2\,\mathrm{e}^{-2\alpha|x|}\,\mathrm{d}x = \frac{1}{2\alpha^2}. \tag{7}$$

Table 1. The ground states, $\psi_0(x)$, of various potentials, $V(x)$, the corresponding $\phi_0(x)$ and the position momentum uncertainty products, U. $\phi_0(p)$ is the Fourier transform of $\psi_0(x)$. Here IDW is the infinitely deep well potential of width a, HO is the harmonic oscillator, $V(x) = x^2/4$, $V_{\rm SRM}(x)$ and $V_M(x)$ are given above equation (3). The pairs of wave functions $\psi_0(x)$ and $\phi_0(x)$, which are Fourier transforms of each other, may look incidentally similar (see rows 2 and 3) or generally dissimilar (see rows 1,4–7) they would however give rise to the same value for U.

SN	$V(x)$	$\psi_0(x)$	$\phi_0(x)$	U	Reference
1	IDW	$\sqrt{\frac{2}{a}}\sin\pi x/a,\ 0\leqslant x\leqslant a;$ 0, otherwise	$2\sqrt{a\pi}\,\frac{1+e^{iax}}{(\pi^2-a^2x^2)}$	$\frac{\hbar}{2}\sqrt{\frac{\pi^2-6}{3}}$	[3]
2	HO	$\frac{e^{-x^2/2}}{\pi^{1/4}}$	$\frac{e^{-x^2/2}}{\pi^{1/4}}$	$\frac{\hbar}{2}$	[1–3, 6–10]
3	$V_{\rm SRM}(s=1)$	$\frac{1}{\sqrt{2}}\mathrm{sech}\,x$	$\frac{\sqrt{\pi}}{2}\mathrm{sech}\,\frac{x\pi}{2}$	$\frac{\hbar\pi}{6}$	Equation (3) [4]
4	$V_{\rm SRM}(s=2)$	$\frac{\sqrt{3}}{2}\mathrm{sech}^2 x$	$\sqrt{\frac{3\pi}{8}}x\,\mathrm{cosech}\,\frac{x\pi}{2}$	$\hbar\sqrt{\frac{\pi^2-6}{15}}$	Equation (3) [4]
5	$V_M(\lambda=1)$	$\sqrt{2}e^{-(e^x-x/2)}$	$\frac{1}{\sqrt{\pi}}\Gamma(\frac{1}{2}+ix)$	$\frac{\hbar\pi}{2\sqrt{6}}$	Equation (4) [4]
6	$-V_0\delta(x)$	$\frac{1}{\sqrt{a}}e^{-\lvert x\rvert/a}$	$\sqrt{\frac{2a}{\pi}}\,\frac{1}{1+a^2x^2}$	$\frac{\hbar}{\sqrt{2}}$	Equation (12)
7	Equation (19)	$\sqrt{\frac{3}{2a}}(1-\lvert x\rvert/a),\ \lvert x\rvert\leqslant a$; $0,\ \lvert x\rvert>a$	$\sqrt{\frac{3a}{\pi}}\left(\frac{\sin ax/2}{ax/2}\right)^2$	$\sqrt{\frac{3}{10}}\hbar$	Equation (25)

When the momentum operator $p = -i\hbar\frac{d}{dx}$ operates over ψ_0, we have

$$p\psi_0(x) = i\hbar\alpha\sqrt{\alpha}\,e^{-\alpha|x|}\frac{d|x|}{dx} = i\hbar\alpha\sqrt{\alpha}\,e^{-\alpha|x|}\mathrm{sgn}(x), \tag{8}$$

where $\mathrm{sgn}(x)$ is called the signum function and is defined as

$$\mathrm{sgn}(x) = \begin{cases} -1, & x<0, \\ 0, & x=0, \\ +1, & x>0. \end{cases} \tag{9}$$

So it follows that

$$\langle\psi_0|p|\psi_0\rangle = \langle\psi_0(x)|p\psi_0(x)\rangle = i\alpha^2\hbar\int_{-\infty}^{\infty} e^{-2\alpha|x|}\,\mathrm{sgn}(x)\,dx \tag{10}$$

vanishes as $\mathrm{sgn}(x)$ is an odd function. This conforms to the fact that, for a bound state, the expectation value of momentum is zero. Next we find

$$\langle p\psi_0|p\psi_0\rangle = \alpha^3\hbar^2\int_{-\infty}^{\infty} e^{-2\alpha|x|}(\mathrm{sgn}(x))^2\,dx = \alpha^2\hbar^2, \tag{11}$$

as $(\mathrm{sgn}(x))^2 = 1$, except at $x = 0$. The momentum being a Hermitian operator, equation (11) gives nothing but $\langle\psi_0|p^2|\psi_0\rangle$, giving us, from equations (2), (7) and (11)

$$U_{\psi_0} = \Delta x\Delta p = \frac{\hbar}{\sqrt{2}}. \tag{12}$$

We can also write

$$\mathrm{sgn}(x) = 2\theta(x) - 1, \tag{13}$$

where $\theta(x)$ is called the Heaviside step function, which is defined as [1, 2, 6, 7]

$$\theta(x) = \begin{cases} 1, & x>0 \\ 0, & x<0 \end{cases} \tag{14}$$

and the Dirac Delta function, $\delta(x)$, is defined as [1, 2, 6, 7]

$$\delta(x) = \frac{\mathrm{d}\theta(x)}{\mathrm{d}x}. \tag{15}$$

Differentiating equation (8) with respect to x and multiplying it by $-\mathrm{i}\hbar$, we can write

$$p^2\psi_0 = -\hbar^2\sqrt{\alpha}[\alpha^2\,\mathrm{e}^{-\alpha|x|}(\mathrm{sgn}(x))^2 - 2\alpha\delta(x)\,\mathrm{e}^{-\alpha|x|}]. \tag{16}$$

We can get $\langle\psi_0|p^2|\psi_0\rangle$ alternatively as

$$\langle\psi_0|p^2|\psi_0\rangle = -\hbar^2\alpha\left[\alpha^2\int_{-\infty}^{\infty}\mathrm{e}^{-2\alpha|x|}\,\mathrm{d}x - 2\alpha\int_{-\infty}^{\infty}\mathrm{e}^{-2\alpha|x|}\delta(x)\,\mathrm{d}x\right] = \hbar^2\alpha^2. \tag{17}$$

The second integral in (17) is 1 using the property that [1, 2, 6, 7]

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,\mathrm{d}x = f(0) = \int_{-a}^{b} f(x)\delta(x)\,\mathrm{d}x, \quad ab > 0. \tag{18}$$

We would like to mention that Ex-4 on p 47 in [8] and Ex 1.1 on p 16 in [9], finding the uncertainty product for a hypothetical Lorentzian eigenstate $\psi_0(x) = A[x^2+\alpha^2]^{-1}$, lead to the same result as (12). This is only a verification of the equivalence (5). It may be verified (see row 6 in table 1) that for the Lorentzian state $\psi_0(x)$, $\phi_0(x)$ is nothing but the symmetric exponential function appearing in equation (6).

Case (II)—Dirac delta between two rigid walls

This potential

$$V(x) = \begin{cases}\infty, & |x| \geqslant a \\ -V_0\delta(x), & |x| < a\end{cases} \quad V_0 > 0 \tag{19}$$

possesses [11, 12] an interesting zero-energy, zero-curvature bound state conditionally when $\frac{maV_0}{\hbar^2} = 1$. The normalized ground state can be written as

$$\psi_0(x) = \sqrt{\frac{3}{2a}}\left(1 - \frac{|x|}{a}\right), \quad -a \leqslant x \leqslant a. \tag{20}$$

Notice that $\psi_0(x)$ vanishes at $x = \pm a$ due to the presence of rigid walls. Due to the symmetry of this state, $\langle x\rangle = 0$ and $\langle x^2\rangle$ can be found as

$$\langle\psi_0|x^2|\psi_0\rangle = \frac{3}{2a}\int_{-a}^{a} x^2\left(1-\frac{|x|}{a}\right)^2\mathrm{d}x = \frac{a^2}{10}. \tag{21}$$

The action of p over $\psi_0(x)$ is

$$p\psi_0(x) = \mathrm{i}\hbar\sqrt{\frac{3}{2a^3}}\,\mathrm{sgn}(x), \tag{22}$$

which being an odd function gives the expectation value of p as

$$\langle\psi_0|p\psi_0\rangle = \mathrm{i}\hbar\frac{3}{2a^3}\int_{-a}^{a}\left(1-\frac{|x|}{a}\right)\mathrm{sgn}(x)\,\mathrm{d}x = 0. \tag{23}$$

However, we have

$$\langle p\psi_0|p\psi_0\rangle = \hbar^2\frac{3}{2a^3}\int_{-a}^{a}(\mathrm{sgn}(x))^2\,\mathrm{d}x = \frac{3\hbar^2}{a^2}, \tag{24}$$

which is nothing but $\langle\psi_0|p^2\psi_0\rangle$, then from equations (2), (21) and (24) we have the uncertainty product for the zero-energy and zero curvature eigenstate [11, 12] as

$$U_{\psi_0} = \Delta x\Delta p = \sqrt{\frac{3}{10}}\hbar, \tag{25}$$

which is approximately $0.5477\hbar$ greater than $\hbar/2$ and rightly so. Alternatively, if we differentiate equation (22) with respect to x and multiply it by $-\mathrm{i}\hbar$, then we can write

$$p^2\psi_0 = 2\hbar^2\sqrt{\frac{3}{2a^3}}\,\delta(x). \tag{26}$$

We recover the result (24) as

$$\langle\psi_0|p^2\psi_0\rangle = 2\hbar^2\frac{3}{2a^2}\int_{-a}^{a}\left(1-\frac{|x|}{a}\right)\delta(x)\,\mathrm{d}x = \frac{3\hbar^2}{a^2}, \tag{27}$$

by using (18). In table 1, see that the Fourier transform of the eigenstate, $\psi_0(x)$, given by equation (20) is $\phi_0(p) = \sqrt{\frac{3a}{\pi}}\left(\frac{\sin ap/2}{ap/2}\right)^2$, $-\infty < p < \infty$. By using $\phi_0(p)$, the result (25) can be recovered again but by carrying out apparently different integrations, which may not be easier to do.

Lastly, we would like to remark that these two special eigenstates of two potentials could be a new addition to the exercises of finding the uncertainty products and confirming that in one dimension these are greater than $\hbar/2$. Our exposition that the ground state attains the minimum uncertainty product ($\frac{\hbar}{2}$) when the depth of the potential tends to infinity requires further confirmation. Students may find the equivalence of the uncertainty product revealed here interesting and enriching. The handling of the notional functions such as $\mathrm{sgn}(x)$, $\theta(x)$ and $\delta(x)$ here is also instructive.

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Appendix

The basic definition of the Dirac delta function is

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}(a_1-a_2)b}\,\mathrm{d}b = \delta(a_1-a_2). \tag{A.1}$$

We can differentiate (A.1) with respect to a_1, n times, to get the definition of derivatives of the Dirac delta function as

$$\frac{(i)^n}{2\pi}\int_{-\infty}^{\infty}b^n\,\mathrm{e}^{\mathrm{i}(a_1-a_2)b}\,\mathrm{d}b = \left(\frac{\partial}{\partial a_1}\right)^n\delta(a_1-a_2) = \delta^{(n)}(a_1-a_2) \tag{A.2}$$

Using integration by parts, we can write

$$\int_{-\infty}^{\infty} f(a_1)\delta^{(1)}(a_1-a_2)\,\mathrm{d}a_1 = f(a_1)\delta(a_1-a_2)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f^{(1)}(a_1)\delta(a_1-a_2)\,\mathrm{d}a_1 = -f^{(1)}(a_2). \tag{A.3}$$

Similarly repeated integrations by parts lead to

$$\int_{-\infty}^{\infty} f(a_1)\delta^{(n)}(a_1-a_2)\,\mathrm{d}a_1 = -\int_{-\infty}^{\infty} f^{(n)}(a_1)\delta(a_1-a_2)\,\mathrm{d}a_1 = (-1)^n f^{(n)}(a_2). \tag{A.4}$$

Now let $\psi(x)$ be an eigenstate whose Fourier transform or momentum representation is $\phi(p)$. So we can write

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}px/\hbar}\psi(x)\,\mathrm{d}x, \quad \text{or,} \quad \psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}px/\hbar}\phi(p)\,\mathrm{d}p. \tag{A.5}$$

We find $\langle\psi(x)|x|\psi(x)\rangle$ denoting it as

$$\langle x\rangle_{\psi(x)} = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi^*(p_1)\, x\, \mathrm{e}^{-\mathrm{i}(p_1-p_2)x/\hbar}\phi(p_2)\,\mathrm{d}x\,\mathrm{d}p_1\,\mathrm{d}p_2. \quad \text{(A.6)}$$

Carrying out the $x-$integration using (A.2) and then carrying out p_1-integration using (A.3), we get $\langle\psi|x|\psi\rangle$, which we denote as

$$\langle x\rangle_{\psi(x)} = \int_{-\infty}^{\infty} \phi^*(p_2)(-\mathrm{i}\hbar)\frac{\partial}{\partial p_2}\phi(p_2)\,\mathrm{d}p_2 = \int_{-\infty}^{\infty} \phi^*(x)(-\mathrm{i}\hbar)\frac{\partial}{\partial x}\phi(x)\,\mathrm{d}x = \langle p\rangle_{\phi(x)}. \quad \text{(A.7)}$$

Normally, one would like to term the second part in the above equations as $\langle\phi(p)|x|\phi(p)\rangle$, namely the expectation value of x in momentum space, which is the same as $\langle\psi(x)|x|\psi(x)\rangle$. Here we depart from this and instruct that the third part in the above equations is merely due to the fact that in a definite integral the name of the variable is only a dummy one so p_2 could be changed to x. Then follows the last part wherein we identify $-\mathrm{i}\hbar\frac{\partial}{\partial x}$ as momentum operator p. Similarly, we can prove that $\langle x^2\rangle_{\psi(x)} = \langle p^2\rangle_{\phi(x)}$, $\langle p\rangle_{\psi(x)} = \langle x\rangle_{\phi(x)}$, $\langle x^2\rangle_{\phi(x)} = \langle p^2\rangle_{\psi(x)}$. Hence the claim in (5) is proved.

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