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A variation of the Heisenberg uncertainty relation involving an average

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Abstract
We derive a parameter-based position–momentum uncertainty relation involving the distance for a state to be displaced to become an orthogonal state and the average rather than the variance of the momentum. This may be useful when the variance of the momentum is infinite and thus the conventional uncertainty relations involving variances provide no useful information.

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How fast can a quantum state evolve to an orthogonal state under a unitary evolution governed by a Schrödinger equation? This problem is fundamental to studying the speed of dynamical evolution. It has been addressed by many authors, such as [1, 3, 5, 7, 8] among others. A standard result is

$$T_\psi \Delta_\psi H \geqslant \frac{\pi\hbar}{2}. \tag{1}$$

Here ψ is a pure state, H is the Hamiltonian, $\Delta_\psi H$ its standard deviation in the state ψ and T_ψ is the shortest time for ψ to evolve to an orthogonal state:

$$T_\psi := \inf\{t \geqslant 0 : \langle\psi|\mathrm{e}^{-\mathrm{i}tH/\hbar}|\psi\rangle = 0\}.$$

Inequality (1) is a kind of time–energy uncertainty relation. A shortcoming of this uncertainty relation is that if the variance of the Hamiltonian H does not exist, i.e. if $\Delta_\psi H = \infty$, then inequality (1) gives only the trivial estimate $T_\psi \geqslant 0$ and is useless. A surprising result of [4] is that inequality (1) still holds when the second moment (standard deviation) $\Delta_\psi H$ is replaced by the first moment (average) $\langle H\rangle_\psi$:

$$T_\psi \langle H\rangle_\psi \geqslant \frac{\pi\hbar}{2}. \tag{2}$$

Inequality (2) is a different kind of time–energy uncertainty relation. It is useful when $\Delta_\psi H$ is infinite while $\langle H\rangle_\psi$ is finite. Further, [6] have identified the intelligent states for this kind of uncertainty relation.

With the same theme, one may ask what the shortest distance is for a wavefunction to be displaced to become orthogonal. A position–momentum analogue of inequality (1) is

$$D_\psi \Delta_\psi P \geqslant \frac{\pi\hbar}{2}. \tag{3}$$

Here $\psi \in L^2(\mathbb{R}, \mathrm{d}x)$ is a Schrödinger wavefunction with unit norm, $P = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}$ is the momentum operator and

$$D_\psi := \inf\{\theta \geqslant 0 : \langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle = 0\}$$

is the smallest position displacement for ψ to become an orthogonal state (see [1, 2, 9] and references therein). This is the position–momentum counterpart of inequality (1).

However, when $\Delta_\psi P = \infty$, inequality (3) is useless. There are many ψ such that the first moment of P in ψ is finite while the second moment of P in ψ is infinite. Motivated by [4], we shall establish a position–momentum analogue of the time–energy inequality (2), or an uncertainty relation similar to (3), but with the variance $\Delta_\psi P$ being replaced by the average. The result (the subsequent inequality (4)) follows from an elementary inequality and a direct use of Fourier analysis.

Let $|P| = \sqrt{P^2}$ (positive root) be the absolute of the momentum observable. Mathematically, $|P|$ may be defined via the Fourier transform as

$$\widehat{|P|\psi}(\xi) := |\xi|\hat{\psi}(\xi).$$

Here the hat stands for the Fourier transform:

$$\hat{\psi}(\xi) := \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}x\xi/\hbar}\psi(x)\,\mathrm{d}x.$$

The average of $|P|$ in the state ψ is

$$\langle|P|\rangle_\psi = \langle\psi||P||\psi\rangle = \int_{\mathbb{R}} |\xi||\hat{\psi}(\xi)|^2\,\mathrm{d}\xi.$$

The reason for considering the average of $|P|$ rather than that of P is that the latter may be negative.

Our main result is

$$D_\psi\langle|P|\rangle_\psi \geqslant \frac{\pi\hbar}{2a} \tag{4}$$

where $a \approx 1.1383$.

To prove inequality (4), note that

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}x\xi/\hbar}\hat{\psi}(\xi)\,\mathrm{d}\xi$$

$$\mathrm{e}^{-\mathrm{i}\theta P/\hbar}\psi(x) = \psi(x-\theta) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}(x-\theta)\xi/\hbar}\hat{\psi}(\xi)\,\mathrm{d}\xi$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}x\xi/\hbar}\mathrm{e}^{-\mathrm{i}\theta\xi/\hbar}\hat{\psi}(\xi)\,\mathrm{d}\xi.$$

Consequently, by the Parseval identity,

$$\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle = \int_{\mathbb{R}} \hat{\psi}^*(\xi)\mathrm{e}^{-\mathrm{i}\theta\xi/\hbar}\hat{\psi}(\xi)\,\mathrm{d}\xi = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\theta\xi/\hbar}|\hat{\psi}(\xi)|^2\,\mathrm{d}\xi.$$

In the language of probability, $\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle$ as a function of θ is exactly the characteristic function (Fourier transform) of the probability density $|\hat{\psi}(\xi)|^2$. We want to evaluate the least positive zero point.

Let $a > 0$ be the smallest number such that

$$\cos x \geqslant 1 - \frac{2a}{\pi}|x| \qquad x \in \mathbb{R}. \tag{5}$$

This a is easily determined as $a = \frac{\pi}{2}\sin x^* \approx 1.1383$, while $x^* \approx 2.3311 \in [\frac{\pi}{2}, \pi]$ is the unique solution of $1 - x\sin x = \cos x$. Geometrically, $(x^*, \cos x^*) = (x^*, 1 - \frac{2a}{\pi}x^*)$ is the tangent point of the curve $y = \cos x$ and the line $y = 1 - \frac{2a}{\pi}x,\ x \geqslant 0$, in the interval $[\frac{\pi}{2}.\pi]$.

Thus we have

$$\begin{aligned}\mathrm{Re}\,\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle &= \int_{\mathbb{R}} \cos(-\theta\xi/\hbar)|\hat{\psi}(\xi)|^2\,\mathrm{d}\xi \\ &\geqslant \int_{\mathbb{R}} \Big(1 - \frac{2a}{\pi}(\theta|\xi|/\hbar)\Big)|\hat{\psi}(\xi)|^2\,\mathrm{d}\xi \quad \text{(by (5))} \\ &= 1 - \frac{2a}{\pi\hbar}\theta\langle|P|\rangle_\psi.\end{aligned}$$

When $\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle = 0$, we have $\mathrm{Re}\,\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle = 0$. Consequently,

$$0 \geqslant 1 - \frac{2a}{\pi\hbar}\theta\langle|P|\rangle_\psi.$$

In order for ψ to be displaced to an orthogonal state $\mathrm{e}^{-\mathrm{i}\theta P/\hbar}\psi$, θ should satisfy the above inequality. By the definition of D_ψ, we obtain inequality (4).

Note that in the derivation of inequality (4), we have not made full use of the condition $\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle = 0$; we have only used the condition $\mathrm{Re}\,\langle\psi|\mathrm{e}^{-\mathrm{i}\theta P/\hbar}|\psi\rangle = 0$. On the other hand, the right-hand side of inequality (4) differers from that of inequalities (1)–(3) by an inverse factor $a \approx 1.1383$.

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