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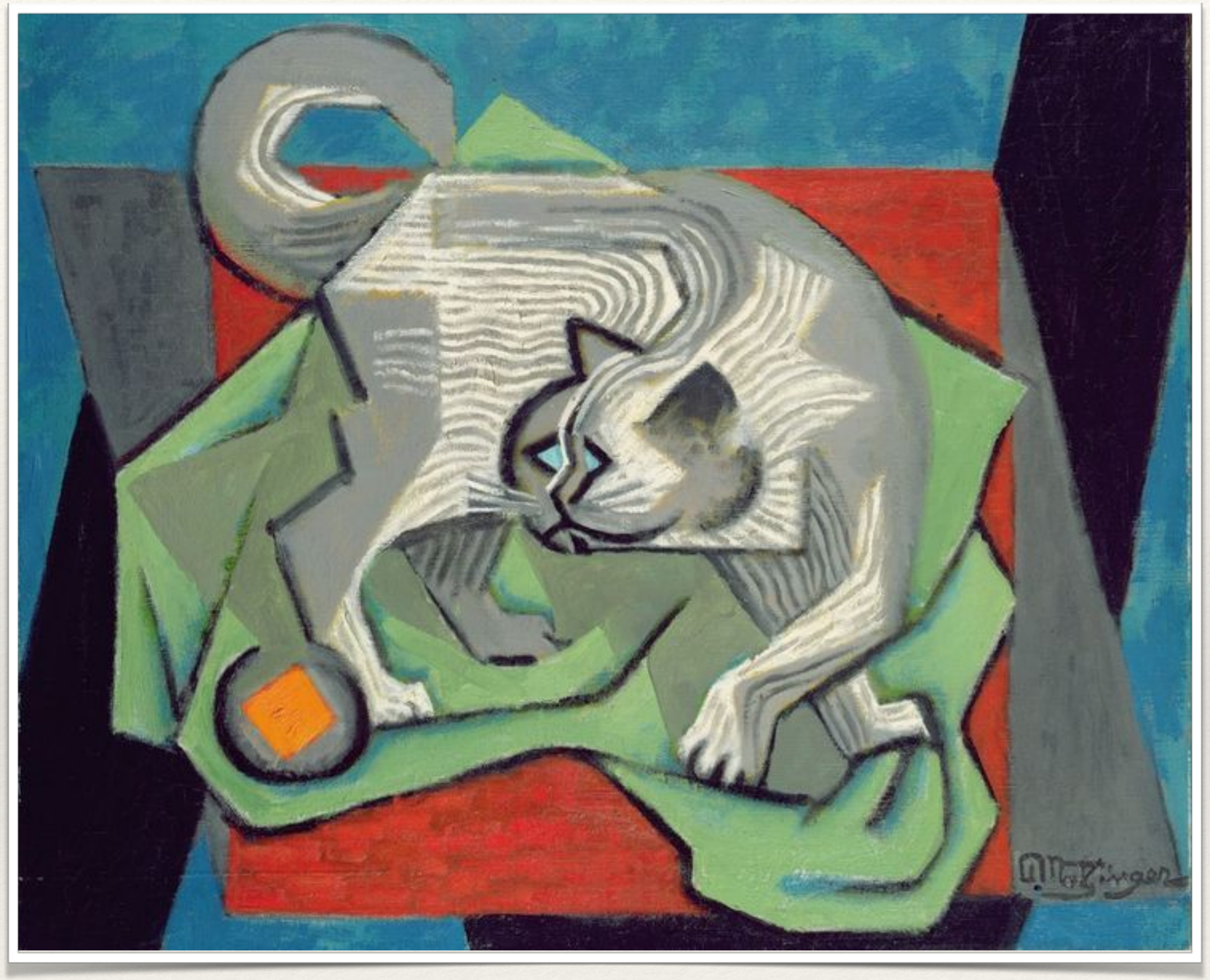
Quantum Mechanics

Lecture 3

Translation and momentum operators;
Time-independent Schrödinger equation;
Uncertainty relations;
Canonical commutation relations.



A quick recap

Time dynamics is unitary and generated by H, the Hamiltonian:

$$U(\mathrm{d}t) = 1 - \frac{i}{\hbar} H \mathrm{d}t \qquad U(t)^\dagger U(t) = 1 \qquad H = H^\dagger \qquad U(t)\,|\,\psi(0)\rangle = |\,\psi(t)\rangle$$

When H is independent of time, Schrödinger equation is solved by:

$$U(t) = \mathrm{e}^{-iHt/\hbar} \qquad U(t)U(s) = U(t+s) \qquad [H, U(t)] = 0 \qquad \langle H \rangle = \langle E \rangle = \text{const.}$$

Wave functions in the position basis and relation between position eigenstates:

$$|\,\psi\rangle = \int_{-\infty}^{\infty} \langle x\,|\,\psi\rangle\,|\,x\rangle \mathrm{d}x \;\Rightarrow\; \psi(x) := \langle x\,|\,\psi\rangle \qquad \Pr(a < x < b) = \int_a^b |\,\langle x\,|\,\psi\rangle\,|^2 \mathrm{d}x$$

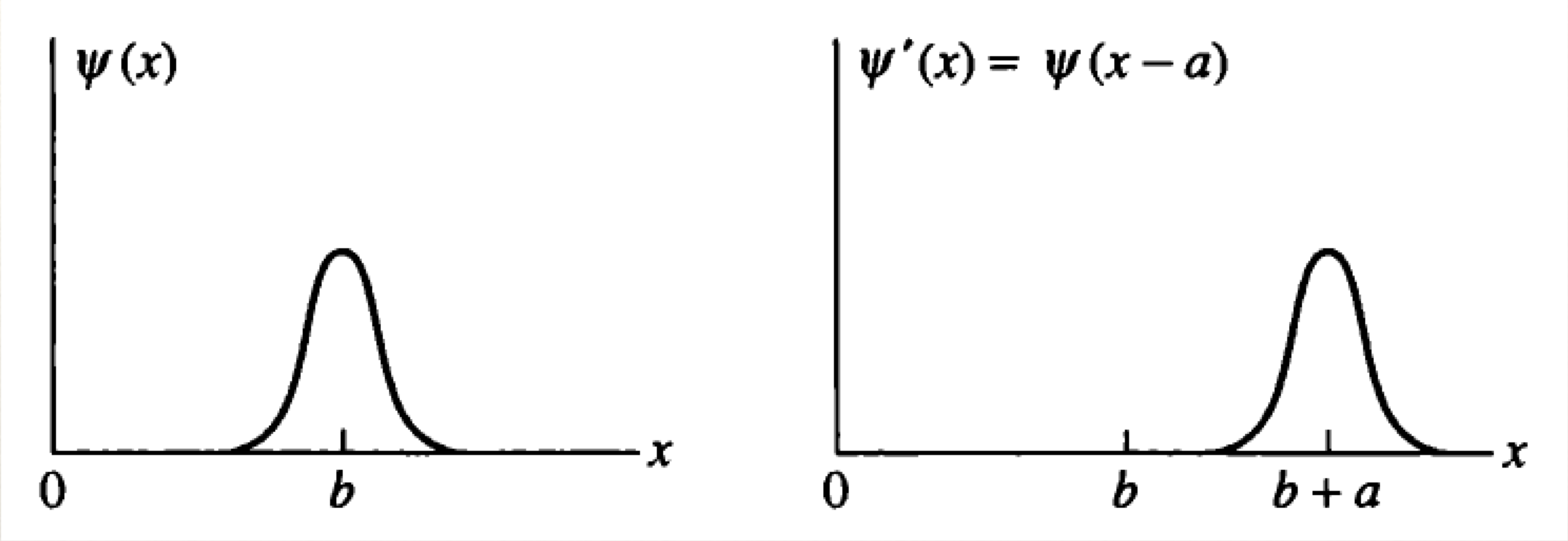
$$\langle x\,|\,x'\rangle = \delta(x - x')$$ Dirac delta function

Translation operator

A natural operation on the line is to translate a wave function.

Define:

$$T(a)\,|\,x\rangle = |\,x + a\rangle$$



This acts by pushing the wave function to the right by a.

This is invertible and unitary: $|\psi'\rangle = T(a)\,|\,\psi\rangle \;\Rightarrow\; \langle\psi'\,|\,\psi'\rangle = \langle\psi\,|\,T(a)^\dagger T(a)\,|\,\psi\rangle = 1$

$$\Rightarrow\; T(a)^\dagger T(a) = 1 \qquad T(-a)T(a) = 1 \qquad \Rightarrow\; T(-a) = T^\dagger(a)$$

The wave function in the position basis transforms as:

$$\langle x\,|\,\psi'\rangle = \langle x\,|\,T(a)\,|\,\psi\rangle = \left[\langle x\,|\,T^\dagger(-a)\right]|\,\psi\rangle = \langle x - a\,|\,\psi\rangle = \psi(x - a)$$

Generator of translation

As we did with time translation, let us look at the generator of space translation.

$$T(\mathrm{d}x) = 1 - \frac{i}{\hbar}\hat{p}\,\mathrm{d}x \qquad\qquad T(\mathrm{d}x)\,|\,x\rangle = |\,x + \mathrm{d}x\rangle$$

And as before, unitarity demands that

$$T(\mathrm{d}x)^\dagger T(\mathrm{d}x) = 1 + \frac{i}{\hbar}(\hat{p}^\dagger - \hat{p})\mathrm{d}x \;\Rightarrow\; \hat{p} = \hat{p}^\dagger$$

Exponentiation gives finite-size translations:

$$T(a) = \mathrm{e}^{-i\hat{p}a/\hbar} \qquad\qquad T(a)^\dagger T(a) = \mathrm{e}^{+i\hat{p}^\dagger a/\hbar}\mathrm{e}^{-i\hat{p}a/\hbar} = \mathrm{e}^{+i(\hat{p}^\dagger - \hat{p})a/\hbar} = 1$$

(since they commute)

Commutator with position

The generator of translation **does not** commute with the position operator.

$$\hat{x}T(\delta x) - T(\delta x)\hat{x} = \hat{x}\left(1 - \frac{i}{\hbar}\hat{p}\delta x\right) - \left(1 - \frac{i}{\hbar}\hat{p}\delta x\right)\hat{x} = \left(-\frac{i\delta x}{\hbar}\right)(\hat{x}\hat{p} - \hat{p}\hat{x}) = \left(-\frac{i\delta x}{\hbar}\right)[\hat{x}, \hat{p}]$$

This is an operator, so we can act both sides on any state.
For a position eigenstate:

$$\begin{aligned}(\hat{x}T(\delta x) - T(\delta x)\hat{x})\,|x\rangle &= \hat{x}T(\delta x)\,|x\rangle - T(\delta x)\hat{x}\,|x\rangle \\ &= \hat{x}\,|x + \delta x\rangle - xT(\delta x)\,|x\rangle \\ &= (x + \delta x)\,|x + \delta x\rangle - x\,|x + \delta x\rangle \\ &= \delta x\,|x + \delta x\rangle\end{aligned}$$

Therefore in the limit:

$$\delta x\left(\frac{-i}{\hbar}\right)[\hat{x}, \hat{p}]\,|x\rangle = \delta x\,|x + \delta x\rangle$$

$$\left(\frac{-i}{\hbar}\right)[\hat{x}, \hat{p}]\,|x\rangle = |x\rangle$$

True for all $|x\rangle$, therefore: $$[\hat{x}, \hat{p}] = i\hbar$$

Momentum operator

We can identify the generator of translation with the *linear momentum* operator.

Why? First, the units are correct:

$$[\hat{p}] = \frac{[\hbar]}{[\mathrm{d}x]} = \frac{[M][L]^2}{[T]}\frac{1}{[L]} = \frac{[M][L]}{[T]}$$

Second, it reproduces classical "p=mv" in expectation:

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

Assume the total energy is a kinetic energy term plus a general potential function V.

$$\frac{\mathrm{d}\langle\hat{x}\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\langle\psi|[H,\hat{x}]|\psi\rangle = \frac{i}{2m\hbar}\langle\psi|[\hat{p}^2,\hat{x}]|\psi\rangle = \frac{i}{2m\hbar}\langle\psi|\hat{p}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{p}|\psi\rangle = \frac{\langle\hat{p}\rangle}{m}$$

Make essential use of $[\hat{x},\hat{p}] = i\hbar$

Momentum operator in the position basis

How is the momentum operator represented in the position basis?

$$T(\delta x)\,|\psi\rangle = |\phi\rangle$$

Taylor expand position basis wave function to first order:

$$\phi(x) = \psi(x - \delta x) = \psi(x) - \delta x \frac{\partial}{\partial x}\psi(x)$$

But we also have: $T(\delta x)\,|\psi\rangle = \left(1 - \frac{i\delta x}{\hbar}\hat{p}\right)|\psi\rangle$

$$\langle x\,|\,T(\delta x)\,|\,\psi\rangle = \langle x\,|\left(1 - \frac{i\delta x}{\hbar}\hat{p}\right)|\,\psi\rangle = \langle x\,|\,\psi\rangle - \left(\frac{i\delta x}{\hbar}\right)\langle \psi\,|\,\hat{p}\,|\,\psi\rangle = \psi(x) - \left(\frac{i\delta x}{\hbar}\right)\langle x\,|\,\hat{p}\,|\,\psi\rangle$$

$$-\delta x \frac{\partial}{\partial x}\psi(x) = -\left(\frac{i\delta x}{\hbar}\right)\langle x\,|\,\hat{p}\,|\,\psi\rangle \;\Rightarrow\; \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) = \langle x\,|\,\hat{p}\,|\,\psi\rangle$$

Holds for all states, therefore the position basis representation is:

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

Schrödinger equation in 1D

In the position basis, we can write the Schrödinger equation for a 1D system as:

$$i\hbar\langle x|\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \langle x|H|\psi(t)\rangle$$

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \langle x|\frac{\hat{p}^2}{2m} + V(\hat{x})|\psi(t)\rangle = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\langle x|\psi(t)\rangle = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t)$$

Therefore:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t)$$

Time-independent Schrödinger equation in 1D

Starting with an energy eigenstate leads to the time-independent equation:

$$U(t)\,|\,E\rangle = \mathrm{e}^{-iEt/\hbar}\,|\,E\rangle \;\Rightarrow\; \psi_E(x,t) = \mathrm{e}^{-iEt/\hbar}\langle x\,|\,E\rangle = \mathrm{e}^{-iEt/\hbar}\psi_E(x)$$

$$i\hbar\frac{\partial}{\partial t}\psi_E(x,t) = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi_E(x,t) \qquad \Rightarrow\; i\hbar\frac{\partial}{\partial t}\mathrm{e}^{-iEt/\hbar}\psi_E(x) = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\mathrm{e}^{-iEt/\hbar}\psi_E(x)$$

$$\Rightarrow\; E\,\psi_E(x) = \left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi_E(x) \qquad \Rightarrow\; \boxed{-\frac{2m\big(E - V(x)\big)}{\hbar^2}\psi_E(x) = \frac{\partial^2}{\partial x^2}\psi_E(x)}$$

Build general solutions using superpositions of solutions for each E.

Uncertainty relations and canonical commutation relations

Using the Cauchy-Schwarz inequality, it is easy to show the Heisenberg uncertainty relation:

$$\Delta\hat{x}\Delta\hat{p} \geq \frac{\hbar}{2} \qquad \Delta\hat{x} = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2} \qquad \Delta\hat{p} = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2}$$

In more than one dimension, we have independent linear momenta that have pairwise commutation relations:

$$[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}$$

Each component of linear momentum commutes with the position operators in the **transverse** directions, but satisfies the canonical commutation relation in the direction where it generates translation.

$$[\hat{x}_j, \hat{x}_k] = [\hat{p}_j, \hat{p}_k] = 0$$