Quantum Mechanics

Mathematical Interlude

Fourier transform of a delta function

Plancherel's theorem

$$\delta(x) = \frac{1}{2\pi}\int e^{ikx}dx$$

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} F(k)e^{ikx}\,dk \iff F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)e^{-ikx}\,dx$$

When the **spectrum** of a hermitian operator is continuous, the individual solutions are not-normalisable. Nevertheless, there is a sense of orthonormality and completeness among the eigenvectors.

Let $f_p(x)$ be the eigenfunction and p the eigenvalue of the momentum operator.

$$\frac{\hbar}{i}\frac{d}{dx}f_p(x) = pf_p(x). \quad f_p(x) = Ae^{ipx/\hbar}$$

$$\int_{-\infty}^{\infty} f_{p'}^*(x)\,f_p(x)\,dx = |A|^2\int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\,dx = |A|^2 2\pi\hbar\,\delta(p-p')$$

If we pick $A = 1/\sqrt{2\pi\hbar}$, so that $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$.

$$\langle f_{p'}|f_p\rangle = \delta(p-p').$$

$$\Updownarrow$$

$$\langle f_m|f_n\rangle = \delta_{mn}$$

Any (square-integrable) function $f(x)$ can be written in the form

$$f(x) = \int_{-\infty}^{\infty} c(p)\,f_p(x)\,dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} c(p)e^{ipx/\hbar}\,dp.$$

Generalised Statistical Interpretation

If you measure an observable $Q(x, p)$, you would get one of the eigenvalue of $\hat{Q}\left(\hat{x}, \hat{p}\right)$

If the spectrum of $\hat{Q}$ is discrete, the probability of getting a particular e.value q_n associated with e.vector $f_n(x)$ is

$$\boxed{|c_n|^2. \quad \text{where} \quad c_n = \langle f_n | \Psi \rangle.}$$

Ortho-normalised

If the spectrum of $\hat{Q}$ is continuous with e.values $q(z)$ associated with e.vectors $f_z(x)$, the probability of getting a result in the range dz is

$$\boxed{|c(z)|^2 \, dz \quad \text{where} \quad c(z) = \langle f_z | \Psi \rangle}$$

$$\boxed{\langle Q \rangle = \sum_n q_n |c_n|^2.}$$

Upon measurement, the wave function collapses to f_n or a narrow range about f_z depending on the precision of the measurement.

Completeness $\longrightarrow$ $\Psi(x, t) = \sum_n c_n f_n(x)$

$$1 = \langle \Psi | \Psi \rangle = \left\langle \left(\sum_{n'} c_{n'} f_{n'} \right) \middle| \left(\sum_n c_n f_n \right) \right\rangle = \sum_{n'} \sum_n c_{n'}^* c_n \langle f_{n'} | f_n \rangle$$

$$= \sum_{n'} \sum_n c_{n'}^* c_n \delta_{n'n} = \sum_n c_n^* c_n = \sum_n |c_n|^2.$$

$$\boxed{\begin{aligned} \Phi(p, t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x, t) \, dx; \\ \Psi(x, t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \Phi(p, t) \, dp. \end{aligned}}$$

Generalised Uncertainty Principle

For any observable A, we have

$$\sigma_A^2 = \langle(\hat{A} - \langle A\rangle)\Psi|(\hat{A} - \langle A\rangle)\Psi\rangle = \langle f|f\rangle,$$

where $f \equiv (\hat{A} - \langle A\rangle)\Psi$. Likewise, for any *other* observable, B,

$$\sigma_B^2 = \langle g|g\rangle, \quad \text{where } g \equiv (\hat{B} - \langle B\rangle)\Psi.$$

Therefore

$$\sigma_A^2\sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2.$$

Now, for any complex number z,

$$|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 \geq [\mathrm{Im}(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2.$$

Therefore, letting $z = \langle f|g\rangle$,

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}[\langle f|g\rangle - \langle g|f\rangle]\right)^2.$$

But

$$\begin{aligned}
\langle f|g\rangle &= \langle(\hat{A} - \langle A\rangle)\Psi|(\hat{B} - \langle B\rangle)\Psi\rangle = \langle\Psi|(\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)\Psi\rangle \\
&= \langle\Psi|(\hat{A}\hat{B} - \hat{A}\langle B\rangle - \hat{B}\langle A\rangle + \langle A\rangle\langle B\rangle)\Psi\rangle \\
&= \langle\Psi|\hat{A}\hat{B}\Psi\rangle - \langle B\rangle\langle\Psi|\hat{A}\Psi\rangle - \langle A\rangle\langle\Psi|\hat{B}\Psi\rangle + \langle A\rangle\langle B\rangle\langle\Psi|\Psi\rangle \\
&= \langle\hat{A}\hat{B}\rangle - \langle B\rangle\langle A\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle \\
&= \langle\hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle.
\end{aligned}$$

Similarly,

$$\langle g|f\rangle = \langle\hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle,$$

so

$$\langle f|g\rangle - \langle g|f\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle = \langle[\hat{A}, \hat{B}]\rangle,$$

where

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

is the commutator of the two operators

$$\boxed{\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A}, \hat{B}]\rangle\right)^2.}$$

Energy Time Relation

As a measure of how fast the system is changing, let us compute the time derivative of the expectation value of some observable, $Q(x, p, t)$:

$$\frac{d}{dt}\langle Q\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle = \left\langle\frac{\partial\Psi}{\partial t}\middle|\hat{Q}\Psi\right\rangle + \left\langle\Psi\middle|\frac{\partial\hat{Q}}{\partial t}\Psi\right\rangle + \left\langle\Psi\middle|\hat{Q}\frac{\partial\Psi}{\partial t}\right\rangle.$$

Now, the Schrödinger equation says

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$$

(where $H = p^2/2m + V$ is the Hamiltonian). So

$$\frac{d}{dt}\langle Q\rangle = -\frac{1}{i\hbar}\langle\hat{H}\Psi|\hat{Q}\Psi\rangle + \frac{1}{i\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle.$$

But $\hat{H}$ is hermitian, so $\langle\hat{H}\Psi|\hat{Q}\Psi\rangle = \langle\Psi|\hat{H}\hat{Q}\Psi\rangle$, and hence

$$\boxed{\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{Q}]\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle.}$$

Now, suppose we pick $A = H$ and $B = Q$, in the generalized uncertainty principle, and assume that Q does not depend explicitly on t:

$$\sigma_H^2\sigma_Q^2 \geq \left(\frac{1}{2i}\langle[\hat{H}, \hat{Q}]\rangle\right)^2 = \left(\frac{1}{2i}\frac{\hbar}{i}\frac{d\langle Q\rangle}{dt}\right)^2 = \left(\frac{\hbar}{2}\right)^2\left(\frac{d\langle Q\rangle}{dt}\right)^2.$$

Or, more simply,

$$\sigma_H\sigma_Q \geq \frac{\hbar}{2}\left|\frac{d\langle Q\rangle}{dt}\right|.$$

Let's define $\Delta E \equiv \sigma_H$, and

$$\Delta t \equiv \frac{\sigma_Q}{|d\langle Q\rangle/dt|}.$$

Then

$$\Delta E\,\Delta t \geq \frac{\hbar}{2},$$

and that's the energy-time uncertainty principle. But notice what is meant by Δt, here: Since

$$\sigma_Q = \left|\frac{d\langle Q\rangle}{dt}\right|\Delta t,$$

Δt represents the *amount of time it takes the expectation value of Q to change by one standard deviation.* In particular, Δt depends entirely on what observable (Q) you care to look at—the change might be rapid for one observable and slow for another. But if ΔE is small, then the rate of change of *all* observables must be very gradual; or, to put it the other way around, if *any* observable changes rapidly, the "uncertainty" in the energy must be large.