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Heisenberg Uncertainty Principle:

Consider two Hermitian operators Ω, Λ with the following commutation relation:

$$[\Omega, \Lambda] = i\Gamma$$

Here Γ is a Hermitian operator too ($i\Gamma$ is therefore anti-Hermitian, as required from the commutator of two Hermitian operators).

Now:

$$(\Delta\Omega)^2(\Delta\Lambda)^2 = \langle\Psi|(\Omega - \langle\Omega\rangle)^2|\Psi\rangle\langle\Psi|(\Lambda - \langle\Lambda\rangle)^2|\Psi\rangle$$

Applying the Schwarz inequality, we find:

$$\langle\Psi|(\Omega - \langle\Omega\rangle)^2|\Psi\rangle\langle\Psi|(\Lambda - \langle\Lambda\rangle)^2|\Psi\rangle \geq \langle\hat{\Omega}\Psi|\hat{\Lambda}\Psi\rangle$$

where:

$$\hat{\Omega} = \Omega - \langle\Omega\rangle \quad , \quad \hat{\Lambda} \equiv \Lambda - \langle\Lambda\rangle$$

Thus:

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\Psi|\hat{\Omega}\hat{\Lambda}|\Psi\rangle|^2$$

But:

$$\hat{\Omega}\hat{\Lambda} = \frac{1}{2}[\hat{\Omega},\hat{\Lambda}] + \frac{1}{2}[\hat{\Omega},\hat{\Lambda}]_+$$

where $[\hat{\Omega},\hat{\Lambda}]_+ = \hat{\Omega}\hat{\Lambda} + \hat{\Lambda}\hat{\Omega}$ is the anti-commutator of $\hat{\Omega}$ and $\hat{\Lambda}$. This results in:

$$(\Delta\Omega)^2(\Delta\Lambda)^2 \geq |\langle\Psi|\frac{1}{2}[\hat{\Omega},\hat{\Lambda}] + \frac{1}{2}[\hat{\Omega},\hat{\Lambda}]_+|\Psi\rangle|^2$$

Note that $[\hat{\Omega},\hat{\Lambda}]$ is an anti-Hermitian operator, while $[\hat{\Omega},\hat{\Lambda}]_+$ is Hermitian. This implies that $\langle[\hat{\Omega},\hat{\Lambda}]\rangle$ is an imaginary number, while $\langle[\hat{\Omega},\hat{\Lambda}]_+\rangle$ is real. In consequence:

$$\left|\left\langle \frac{1}{2}[\hat{\Omega},\hat{\Lambda}] + \frac{1}{2}[\hat{\Omega},\hat{\Lambda}]_+ \right\rangle\right|^2 = \frac{1}{4}\langle\Psi|[\hat{\Omega},\hat{\Lambda}]_+|\Psi\rangle^2$$

$$+ \frac{1}{4}\langle\Psi|\Gamma|\Psi\rangle^2$$

$$[\Omega,\Lambda] = [\hat{\Omega},\hat{\Lambda}] = \Gamma$$

$$\Rightarrow (\Delta\Omega)^2(\Delta\Lambda)^2 \geq \frac{1}{4}\langle\Psi|\Gamma|\Psi\rangle^2 + \frac{1}{4}\langle\Psi|[\hat{\Omega},\hat{\Lambda}]_+|\Psi\rangle^2.$$

For example, consider the position and momentum operators X, P. In this case $\Gamma = I\hbar$, hence:

$$(\Delta X)^2 (\Delta P)^2 \geq \frac{\hbar^2}{4} + \frac{1}{4} \langle \psi | [X, P]_+ | \psi \rangle^2 \Rightarrow$$

$$(\Delta X)^2 (\Delta P)^2 \geq \frac{\hbar^2}{4} \Rightarrow \Delta X \, \Delta P \geq \frac{\hbar}{2}$$

This is the famous Heisenberg uncertainty principle.

In three dimensions, we have the additional relations:

$$\Delta Y \, \Delta P_y \geq \frac{\hbar}{2} \quad , \quad \Delta Z \, \Delta P_z \geq \frac{\hbar}{2}$$

The minimum uncertainty is obtained if $\langle [\hat{\Omega}, \hat{\Lambda}] \rangle = 0$.

In the case of X, P this requires that:

$$(P - \langle P \rangle)(X - \langle X \rangle) | \psi \rangle = -(X - \langle X \rangle)(P - \langle P \rangle) | \psi \rangle$$

This will be the case if:

$$(P - \langle P \rangle) | \psi \rangle = c \, (X - \langle X \rangle) | \psi \rangle$$

where c is a constant.

In the position eigenbasis this results in the following differential equation,

$$-i\hbar \frac{d}{dx} \psi_{(x)} = \left[c(x - x_0) + p_0\right] \psi_{(x)}$$

where $x_0 \equiv \langle X \rangle$ and $p_0 \equiv \langle P \rangle$. Thus:

$$\psi_{(x)} = \psi_{(0)}\, e^{\frac{i p_0 x}{\hbar}}\, e^{ic\frac{(x-x_0)^2}{2\hbar}}$$

Now, requiring that $\langle [(X - x_0), (P - p_0)]_+ \rangle = 0$, we find:

$$(c + c^*) \langle \psi | (X - x_0)^2 | \psi \rangle \Rightarrow c = i|c|$$

c an imaginary number

Finally, we have:

$$\psi_{(x)} = \psi_{(0)}\, e^{\frac{i p_0 x}{\hbar}}\, e^{-|c|\frac{(x-x_0)^2}{2\hbar}}$$

This is nothing but a Gaussian wavepacket. After defining $\Delta = \frac{\hbar}{|c|}$, we get:

$$\psi_{(x)} = \psi_{(0)}\, e^{\frac{i p_0 x}{\hbar}}\, e^{-\frac{(x-x_0)^2}{2\Delta^2}}$$

$$\Delta X = \Delta \quad , \quad \Delta P = \frac{\hbar}{2\Delta}$$

We conclude that minimum uncertainty is obtained for a

Gaussian wavepacket.

Applications:

In general one can apply the uncertainty principle to estimate energy eigenvalues of a system. As an example, consider particle in a box of length L. In this case:

$$\langle H \rangle = \frac{\langle p^2 \rangle}{2m} \quad , \quad \langle p \rangle = 0$$

Hence:

$$\Delta p^2 = \langle p^2 \rangle \Rightarrow \langle H \rangle = \frac{\Delta p^2}{2m}$$

Since the particle cannot be found outside the box, we have $\Delta x \leq \frac{L}{2}$. Then:

$$\Delta x \, \Delta p \geq \frac{\hbar}{2} \Rightarrow \Delta p \geq \frac{\hbar}{2\Delta x} \Rightarrow \Delta p \geq \frac{\hbar}{L}$$

$$\Rightarrow \Delta p^2 \geq \frac{\hbar^2}{L^2} \Rightarrow \langle H \rangle \geq \frac{\hbar^2}{2mL^2}$$

We recall that the energy eigenvalues in this case are given by:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \qquad n = 0, 1, 2, \ldots$$

Note that $E_n > \frac{\hbar^2}{2mL^2}$, as required by the uncertainty principle. Furthermore, $\frac{\hbar^2}{2mL^2}$ is a reasonable estimate of the ground state energy.

It is not surprising that we only find a lower bound because the eigenstates are not Gaussian wavepackets.