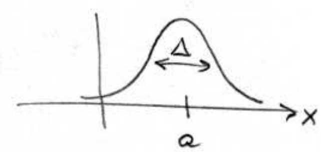
If the eigenvalues λ or ω are degenerate, measuring $\hat{\Lambda}$ and $\hat{\Omega}$ in different order will lead to different intermediate states, but the same probability $P(\lambda,\omega)$. If they are both degenerate, measuring both λ and ω does not uniquely define the state $|\omega,\lambda\rangle$ (there is still a manidimensional vector space spanned by all possible eigenstates $|\omega,\lambda\rangle$).

<u>Example:</u> Gaussian wave function

Consider $|\psi\rangle$ with $\psi(x) \equiv \langle x|\psi\rangle = A\, e^{-\frac{(x-a)^2}{2\Delta^2}}$



For $|\psi\rangle$ to be normalized, need

$$1 = \langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx\, \langle\psi|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = \int_{-\infty}^{\infty} |A|^2 e^{-\frac{(x-a)^2}{\Delta^2}} dx$$

$$= |A|^2 \sqrt{\pi\Delta^2} \quad \Rightarrow \quad \boxed{A = \frac{e^{i\alpha}}{(\pi\Delta^2)^{1/4}}}$$

The overall phase factor $e^{i\alpha}$ drops out from all probabilities, so we can set $\alpha = 0$ without loss of generality.

$$\Rightarrow \boxed{\psi(x) = \frac{e^{-\frac{(x-a)^2}{2\Delta^2}}}{(\pi\Delta^2)^{1/4}}}$$

<u>Expectation value of $\hat{X}$:</u>

$$\underline{\langle\hat{X}\rangle} = \langle\psi|\hat{X}|\psi\rangle = \int_{-\infty}^{\infty} dx\, \underbrace{\langle\psi|\hat{X}|x\rangle}_{x\,\langle\psi|x\rangle}\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\, x\, |\psi(x)|^2$$

$$\overset{y=x-a}{=} \int_{-\infty}^{\infty} dy\, \underset{\substack{\uparrow \\ \text{integrates to zero}}}{(y+a)}\, \frac{e^{-y^2/\Delta^2}}{\sqrt{\pi\Delta^2}} = a \int_{-\infty}^{\infty} \frac{e^{-y^2/\Delta^2}}{\sqrt{\pi\Delta^2}}\, dy = \underline{a} \checkmark$$

Uncertainty in $\hat{X}$:

$$(\Delta X)^2 = \langle\psi|(\hat{X} - \langle\hat{X}\rangle)^2|\psi\rangle = \langle\psi|\hat{X}^2 - \langle X\rangle^2|\psi\rangle$$

$$= \langle\psi|\hat{X}^2|\psi\rangle - a^2\langle\psi|\psi\rangle = \langle\hat{X}^2\rangle - a^2$$

$$\langle\hat{X}^2\rangle = \int_{-\infty}^{\infty} dx \langle\psi|\hat{X}^2|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\, x^2 \frac{e^{-\frac{(x-a)^2}{\Delta^2}}}{\sqrt{\pi\Delta^2}}$$

$$= \int_0^{\infty} dy\, \underbrace{(y+a)^2}_{y^2+2ay+a^2} \frac{e^{-y^2/\Delta^2}}{\sqrt{\pi\Delta^2}} = \int_0^{\infty} dy\, y^2 \frac{e^{-y^2/\Delta^2}}{\sqrt{\pi\Delta}} + 0 + a^2.1$$

$$= \frac{\Delta^2}{2} + a^2$$

$$\Rightarrow (\Delta X)^2 = \frac{\Delta^2}{2} \quad \Rightarrow \quad \boxed{\Delta X = \frac{\Delta}{\sqrt{2}}}$$

Expectation value of $\hat{P}$:

$$\langle\psi|\hat{P}|\psi\rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \langle\psi|x\rangle\underbrace{\langle x|\hat{P}|x'\rangle}_{-i\hbar\delta(x-x')\frac{d}{dx'}}\langle x'|\psi\rangle$$

$$= -i\hbar\int_{-\infty}^{\infty} dx\, \psi^*(x)\,\psi'(x) = -i\hbar\int_{-\infty}^{\infty} dx \frac{e^{-\frac{(x-a)^2}{2\Delta^2}}}{(\pi\Delta^2)^{1/4}}\left(-\frac{(x-a)}{\Delta^2}\right)\frac{e^{-\frac{(x-a)^2}{2\Delta^2}}}{(\pi\Delta^2)^{1/4}}$$

$$= -i\hbar\int_{-\infty}^{\infty} dy \frac{e^{-y^2/\Delta^2}}{\sqrt{\pi\Delta^2}}\frac{y}{\Delta^2} = 0$$

Or $\langle\psi|\hat{P}|\psi\rangle = \int_{-\infty}^{\infty} dp \langle\psi|\hat{P}|p\rangle\langle p|\psi\rangle = \int_{-\infty}^{\infty} dp\, p\, |\psi(p)|^2$

where

$$\psi(p) = \langle p | \psi \rangle = \int_{-\infty}^{\infty} dx \, \langle p | x \rangle \langle x | \psi \rangle$$

$$= \int_{-\infty}^{\infty} dx \, \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \psi(x) = \int_{-\infty}^{\infty} \frac{e^{-ipx/\hbar}}{(2\pi\hbar)^{1/2}} \frac{e^{-\frac{(x-a)^2}{2\Delta^2}}}{(\pi\Delta^2)^{1/4}} dx$$

$$= \left(\frac{\Delta^2}{\pi\hbar^2}\right)^{1/4} e^{-ipa/\hbar} \, e^{-p^2\Delta^2/2\hbar^2}$$

This is a Gaussian of width $\boxed{\Delta_p = \frac{\hbar}{\Delta}}$

multiplied by a phase factor $e^{-ipa/\hbar}$ of unit magnitude.

Hence $\int_{-\infty}^{\infty} dp \, p \, |\psi(p)|^2 = 0$ by symmetric integration

Uncertainty in $\hat{P}$:

Same calculation as for $\langle \hat{X}^2 \rangle$, except for Gaussian with different width $\Delta_p = \frac{\hbar}{\Delta}$:

$$\Rightarrow \boxed{\Delta P = \frac{\hbar}{\Delta} \frac{1}{\sqrt{2}}}$$

$$\Rightarrow \boxed{\Delta X \cdot \Delta P = \frac{\hbar}{2}}$$ a simple consequence of Fourier transforms!

This happens saturate the lower bound of the uncertainty relation (see Chapter 9)

$$\boxed{\Delta X \cdot \Delta P \geq \frac{\hbar}{2}}$$

Plane waves and other improper vectors in Hilbert space:

Look at the momentum eigenstates $|p\rangle$. Their x-basis representation is

$$\psi_p(x) = \langle x | p \rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}$$

They have uniform probability density for position x:

$$\rho(x) = |\psi_p(x)|^2 = \frac{1}{2\pi\hbar}$$

If we wanted to normalize this probability density over all x, the probability in any finite region of x-space would turn out to be zero. So, in a strict sense, a state of well-defined momentum p does not exist. To prepare it would require an apparatus that extends over all space. However, we can prepare a state that is arbitrarily close to $e^{ip_0x/\hbar}$ over a large finite region and tapers off to zero outside. Its Fourier transform $\psi(p)$ would be sharply peaked at p_0 and rapidly fall of at $p \neq p_0$. We never measure p with infinite resolution. So if it falls off to zero within our resolution, we can't tell the difference. The modified plane wave, that tapers off at infinity, is normalizable to unity and has $\rho(x) \approx \frac{1}{V}$ where V is the "volume" (in x) over which $\psi(x)$ is nonzero.

What saves us from the singularities of the δ-fct. $\langle p | p' \rangle = \delta(p-p')$ is that in a real experiment we always integrate over all momenta within our experimental resolution.

We work with exact plane waves since it is mathematically easier, but nothing is ever singular in experiment.

Generalization to more degrees of freedom

Modify postulate II:

Classical cartesian coordinates $x_1, x_2, \dots, x_N \longrightarrow \hat{X}_1, \hat{X}_2, \dots, \hat{X}_N$ (Hermitean) with $[\hat{X}_i, \hat{X}_j] = 0$. $\to$ simultaneous eigenbasis $|x_1, x_2, \dots, x_N\rangle$ ("coordinate basis"), normalized to

$$\langle x_1, x_2, \dots, x_N | x_1', x_2', \dots, x_N' \rangle = \delta(x_1 - x_1') \dots \delta(x_N - x_N')$$
$$\equiv \delta^{(N)}(\vec{x} - \vec{x}')$$

(this is not the N^{th} derivative of δ, but a δ-fct. in N dimensions.)

A system with N degrees of freedom is described by Hilbert space vectors in an $N \times \infty$ dimensional Hilbert space:

$$|\psi\rangle \underset{\substack{\text{coordinate}\\ \text{basis}}}{\longleftrightarrow} \langle x_1, x_2, \dots, x_N | \psi \rangle \equiv \psi(x_1, x_2, \dots, x_N)$$

$$\hat{X}_i|\psi\rangle \leftrightarrow \langle x_1, x_2, \dots, x_N|\hat{X}_i|\psi\rangle = x_i\,\psi(x_1, x_2, \dots, x_N)$$

$$\left(\hat{X}_i|x_1, x_2, \dots, x_N\rangle = x_i|x_1, x_2, \dots, x_N\rangle\right)$$

$$\hat{P}_i|\psi\rangle \leftrightarrow \langle x_1, x_2, \dots, x_N|\hat{P}_i|\psi\rangle = -i\hbar\frac{\partial}{\partial x_i}\psi(x_1, x_2, \dots, x_N)$$

Dependent variables $\omega(x_i, p_j) \longmapsto \hat{\Omega}(\hat{X}_i, \hat{P}_j)$

Probability for obtaining eigenvalues between x_1 and x_1+dx_1, x_2 and x_2+dx_2, ..., x_N and x_N+dx_N when measuring $\hat{X}_1, \hat{X}_2, \dots \hat{X}_N$:

$$\boxed{\frac{dP}{dx_1\dots dx_N}\,dx_1\dots dx_N = |\psi(x_1, x_2, \dots, x_N)|^2\,dx_1\,dx_2\dots dx_N}$$

Example

3-dimensional harmonic oscillator:

Classical Hamilton function $H(\vec{x}, \vec{p}) = \frac{p_x^2+p_y^2+p_z^2}{2m} + \frac{1}{2}m\omega^2(x^2+y^2+z^2)$

Quantum mechanical Hamilton operator:

$$\hat{H}(\hat{X}, \hat{Y}, \hat{Z}, \hat{P}_x, \hat{P}_y, \hat{P}_z) = \frac{\hat{P}_x^2+\hat{P}_y^2+\hat{P}_z^2}{2m} + \frac{1}{2}m\omega^2(\hat{X}^2+\hat{Y}^2+\hat{Z}^2)$$

(this is Hermitean)

To solve the eigenvalue equation

$$\hat{H}|E\rangle = E|E\rangle \qquad (E = \text{energy eigenvalue})$$

we can go to the coordinate representation, Where this turns into a differential equation:

$$\langle x,y,z|\hat{H}|E\rangle = E\langle x,y,z|E\rangle = E\,\psi_E(x,y,z)$$

$$\langle x,y,z|\underset{\substack{\uparrow\\ \hat{I}}}{\hat{H}}|E\rangle = \int_{-\infty}^{\infty}dx'\int_{-\infty}^{\infty}dy'\int_{-\infty}^{\infty}dz'\,\langle x,y,z|\frac{\hat{P}_x^2+\hat{P}_y^2+\hat{P}_z^2}{2m}+\frac{m\omega^2}{2}(\hat{X}^2+\hat{Y}^2+\hat{Z}^2)|x',y',z'\rangle$$

$$*\underbrace{\langle x',y',z'|E\rangle}_{\psi_E(x',y',z')}$$

$$\begin{aligned}\langle x,y,z|\hat{X}^2|x',y',z'\rangle &= x^2\,\delta(x-x')\,\delta(y-y')\,\delta(z-z')\\ &= xx'\,\delta(x-x')\,\delta(y-y')\,\delta(z-z')\\ &= x'^2\,\delta(x-x')\,\delta(y-y')\,\delta(z-z')\end{aligned}$$

etc.

$$\begin{aligned}\langle x,y,z|\hat{P}_y^2|x',y',z'\rangle &= \langle x,z|x',z'\rangle\langle y|\hat{P}_y^2|y'\rangle\\ &= \delta(x-x')\,\delta(z-z')\left(-\hbar^2\delta''(y-y')\right)\\ &= -\hbar^2\delta(x-x')\,\delta(z-z')\,\delta(y-y')\frac{\partial^2}{\partial y'^2}\end{aligned}$$

etc.

$$\Rightarrow \langle x,y,z|\hat{H}|E\rangle = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+\frac{m\omega^2}{2}(x^2+y^2+z^2)\right]\psi(x,y,z) \qquad (*)$$

$\Rightarrow$ Eigenvalue equation

$$\boxed{\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2+\frac{m\omega^2}{2}\vec{r}^{\,2}\right)\psi_E(\vec{r}) = E\,\psi_E(\vec{r})}$$

$(*)$ expresses this in Cartesian coordinates $\vec{r} = (x,y,z)$

What about other than Cartesian coordinates?

For example, spherical coordinates: $\psi_E(x,y,z) = \psi_E(r,\vartheta,\varphi)$:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi_E}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\,\frac{\partial\psi_E}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2\psi_E}{\partial\varphi^2}\right]$$

$$+\frac{m\omega^2 r^2}{2}\psi_E = E\,\psi_E(r,\vartheta,\varphi)$$

Can we get there directly from the classical expression

$$H(r,\vartheta,\varphi;\, p_r, p_\vartheta, p_\varphi) = \frac{1}{2m}\left(p_r^2 + \frac{p_\vartheta^2}{r^2} + \frac{p_\varphi^2}{r^2\sin^2\vartheta}\right) + \frac{m\omega^2}{2}r^2\ ?$$

<u>No</u>, at least not straightforwardly, by replacing

$$p_r \to -i\hbar\frac{\partial}{\partial r} \neq \hat{P}_r$$

There is a (much more complicated) prescription for "quantizing" in curvilinear coordinates (such as spherical coordinates), but we will postpone this.

Here we will use Cartesian coordinates to first work out the coordinate space matrix elements, then transform the result into curvilinear coordinates in a second step.