Postulates of Quantum Mechanics

P1: Representation of states

The state at any time *t* is represented by

Classical	Quantum
$x(t)$: position $p(t)$: momentum	$\vert\psi\rangle$: a vector in a Hilbert space ('ket' ψ)

For quantum states,

Principle of superposition
If $|\psi_1\rangle$ & $|\psi_2\rangle$ are possible states, $\alpha|\psi_1\rangle + \beta|\psi_2\rangle$ is also a possible state.

('bra' ψ) ('dagger': Adjoint or Hermitian conjugate)
$\langle\psi| = (|\psi\rangle)^\dagger$: co-vector corresponding to $|\psi\rangle$

$\langle\psi_2|\psi_1\rangle$: a number called inner product of $|\psi_1\rangle$ & $|\psi_2\rangle$

$\sqrt{\langle\psi|\psi\rangle}$: norm of $|\psi\rangle$

(Note)
In this course, I will use only normalized vectors ($\langle\psi|\psi\rangle = 1$).
Please get familiar with the rules of vectors & inner products!

P2: Representation of observables

Observables (Dynamical variables) are represented by

Classical	Quantum
x & p are independent variables. $\omega = \omega(x, p)$: function of x & p	$\hat{X}$ and $\hat{P}$ are Hermitian operators. $\left[\hat{X}, \hat{P}\right] = i\hbar$ (Canonical commutation rule) $\hat{\Omega}\left(\hat{X}, \hat{P}\right) = \omega\left(x \to \hat{X}, p \to \hat{P}\right)$

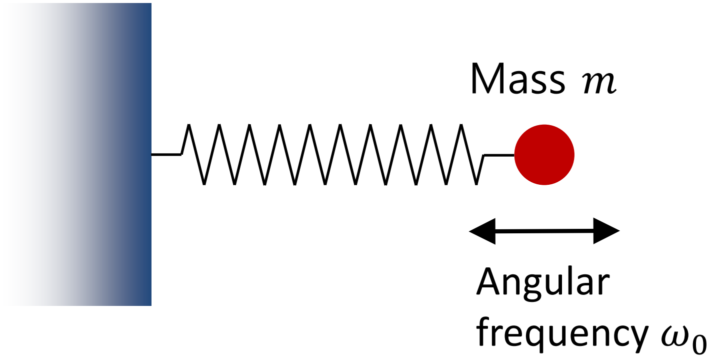
(Ex) Harmonic oscillator

Hamiltonian

$$H(x, p) = \frac{p^2}{2m} + \frac{1}{2} m {\omega_0}^2 x^2$$

Hamiltonian operator

$$\hat{H}\left(\hat{X}, \hat{P}\right) = \frac{\hat{P}^2}{2m} + \frac{1}{2} m {\omega_0}^2 \hat{X}^2$$



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$\hat{\Omega}|\omega_i\rangle = \omega_i|\omega_i\rangle$ You get eigenvectors & eigenvalues of $\hat{\Omega}$

$\hat{X}$, $\hat{P}$ and $\hat{\Omega}$ are Hermitian operators. ($\hat{\Omega}^\dagger = \hat{\Omega}$)

(1) Eigenvalues are real.

(2) There exists a complete basis of orthonormal eigenvectors ($|\omega_1\rangle, |\omega_2\rangle, \ldots, |\omega_n\rangle$)

	(Orthonormality)	(Completeness relation)
Discrete variables	$\langle \omega_i \| \omega_j \rangle = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$ (Kronecker delta)	$\sum_i \|\omega_i\rangle\langle\omega_i\| = I$
Continuous variables	$\langle x \| x' \rangle = \delta(x - x') = \begin{cases} \infty, & x = x' \\ 0, & x \neq x' \end{cases}$ (Dirac delta function)	$\int \|x\rangle\langle x\| \, dx = I$

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Representation of $\hat{X}$ and $\hat{P}$ in the X-basis ($\hat{X}|x\rangle = x|x\rangle$)

$$\langle x|\hat{X}|x'\rangle = x'\langle x|x'\rangle = x'\delta(x - x')$$

$$\langle x|\hat{P}|x'\rangle = -i\hbar\delta'(x - x')$$

Can you then derive the following?

$$\langle x|\hat{X}|\psi\rangle = x\psi(x)$$

$$\langle x|\hat{P}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x)$$

$$\langle x|[\hat{X}, \hat{P}]|\psi\rangle = i\hbar\psi(x)$$

(Don't use the canonical commutation rule.)

(Note on the Dirac delta function)

$$\langle x|x'\rangle = \delta(x - x') = \begin{cases} \infty, & x = x' \\ 0, & x \neq x' \end{cases}$$

$$\int \delta(x - x')dx' = 1$$

$$\int f(x')\delta(x - x')dx' = f(x)$$

$$\int f(x')\delta'(x - x')dx' = f'(x)$$

P3: Measurement of observables

Measurement of an observable on a state

Classical	Quantum
Measurement of ω on a state (x, p) (1) A value $\omega(x,p)$ is obtained (2) The state remains unaffected	Measurement of Ω on a state $\|\psi\rangle$ (1) One of the eigenvalues ω_i of $\hat{\Omega}$ is obtained with probability $P(\omega_i) = \|\langle\omega_i\|\psi\rangle\|^2$ (2) $\|\psi\rangle \rightarrow \|\omega_i\rangle$ (collapse of the state)

Discrete variables

$$|\psi\rangle = |\psi\rangle \sum_i |\omega_i\rangle\langle\omega_i| = \sum_i |\omega_i\rangle \langle\omega_i|\psi\rangle$$

$$= \sum_i a_i |\omega_i\rangle$$

$P(\omega_i) = |a_i|^2$: Probability of obtaining ω_i

Continuous variables

$$|\psi\rangle = |\psi\rangle \int |x\rangle\langle x|\, dx = \int |x\rangle\langle x|\psi\rangle\, dx$$

$$= \int |x\rangle \underline{\psi(x)}\, dx$$

Wavefunction in the X basis

$P(x) = |\psi(x)|^2$: probability density

$P(x)dx$: probability of finding the particle in between $(x, x + dx)$

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In terms of a projection operator $\widehat{\mathbb{P}}_\omega = |\omega\rangle\langle\omega|$,

$$|\psi\rangle \to |\omega\rangle = \frac{\widehat{\mathbb{P}}_\omega|\psi\rangle}{\sqrt{\langle\widehat{\mathbb{P}}_\omega\psi|\widehat{\mathbb{P}}_\omega\psi\rangle}}$$

with probability $P(\omega) = \langle\psi|\widehat{\mathbb{P}}_\omega|\psi\rangle = \langle\widehat{\mathbb{P}}_\omega\psi|\widehat{\mathbb{P}}_\omega\psi\rangle$

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(Example) Consider a normalized state $|\psi\rangle = \frac{1}{2}|\omega_1\rangle + \frac{i}{2}|\omega_2\rangle - \frac{1}{\sqrt{2}}|\omega_3\rangle$

($\{|\omega_i\rangle\}$: complete orthonormal basis of $\widehat{\Omega}$)

Measurement of Ω on the state yields

ω_1, with probability $P(\omega_1) = |\langle\omega_1|\psi\rangle|^2 = \frac{1}{4}$, the state being changed $|\psi\rangle \rightarrow |\omega_1\rangle$,

or ω_2, with probability $P(\omega_2) = |\langle\omega_2|\psi\rangle|^2 = \frac{1}{4}$, the state being changed $|\psi\rangle \rightarrow |\omega_2\rangle$,

or ω_3, with probability $P(\omega_3) = |\langle\omega_3|\psi\rangle|^2 = \frac{1}{2}$, the state being changed $|\psi\rangle \rightarrow |\omega_3\rangle$.

Other ω_i's are not obtained.

We can make not an exact prediction but a statistical prediction on the measurement prior to the measurement.

Ensemble

How to test a state $|\psi\rangle = \sum_i a_i |\omega_i\rangle$ by measurement of Ω

(Example) $|\psi\rangle = \sqrt{\frac{1}{3}}|\omega_1\rangle + \sqrt{\frac{2}{3}}|\omega_2\rangle$

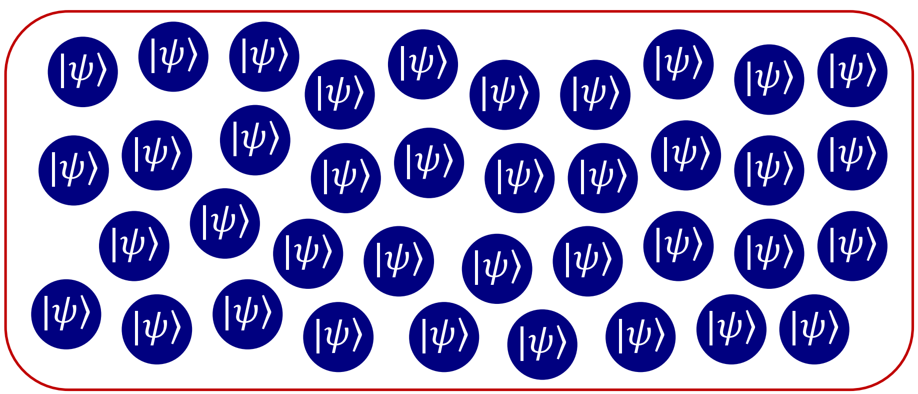
Measurement of Ω will yield either ω_1 or ω_2, the state being collapsed to $|\omega_1\rangle$ or $|\omega_2\rangle$.

If you have only one particle, you can not determine the coefficients.

In order to determine the coefficients precisely,
you need a set of a large # of particles all in the same state $|\psi\rangle$ and repeat the measurement.

Ensemble

Pure ensemble ($\leftrightarrow$ Mixed ensemble)



Pure ensemble of particles
in the state $|\psi\rangle$

Ensemble

Statistical quantities for an ensemble regarding the measurement of Ω

Expectation value (ensemble average) (corresponding to 'mean' in statistics)

$$\langle \Omega \rangle = \sum_i |\langle \omega_i | \psi \rangle|^2 \omega_i = \langle \psi | \hat{\Omega} | \psi \rangle$$

Uncertainty (corresponding to 'standard deviation' in statistics)

$$\Delta\Omega = \left[\sum_i |\langle \omega_i | \psi \rangle|^2 (\omega_i - \langle \Omega \rangle)^2 \right]^{1/2} = \left[\langle \psi | (\hat{\Omega} - \langle \Omega \rangle)^2 | \psi \rangle \right]^{1/2}$$

Ensemble

N particles of

$$|\psi\rangle = \sqrt{\frac{1}{2}}(|\omega_1\rangle + |\omega_2\rangle)$$

Pure ensemble

N/2 particles of $|\omega_1\rangle$

N/2 particles of $|\omega_2\rangle$

Mixed ensemble

Can you distinguish between the two ensembles by measurement of Ω?

It may fail if you are unlucky. What is the case? What is the probability that it happens?

Measurement of two observables

$$|\psi\rangle \xrightarrow{\text{Measurement of } \Omega} |\omega\rangle$$

$P(\omega) = |\langle\omega|\psi\rangle|^2$

The state is changed in general.

$$|\omega\rangle \xrightarrow{\text{Measurement of } \Omega} |\omega\rangle$$

$P(\omega) = |\langle\omega|\omega\rangle|^2 = 1$

The eigenstate is unaffected (as in classical mechanics)

$$|\psi\rangle \xrightarrow{\text{Measurement of } \Omega} |\omega\rangle \xrightarrow{\text{Measurement of } \Lambda} |\lambda\rangle \xrightarrow{\text{Measurement of } \Omega} |\omega\rangle \quad ???$$

No, in general.

Yes, only for the simultaneous eigenstate $|\omega, \lambda\rangle$ of $\hat{\Omega}$ & $\hat{\Lambda}$.

$$\begin{aligned} \hat{\Omega}|\omega, \lambda\rangle &= \omega|\omega, \lambda\rangle \\ \hat{\Lambda}|\omega, \lambda\rangle &= \lambda|\omega, \lambda\rangle \end{aligned} \longrightarrow [\hat{\Omega}, \hat{\Lambda}]|\omega, \lambda\rangle = 0$$

(1) $\hat{\Omega}$ and $\hat{\Lambda}$ are compatible: $[\hat{\Omega}, \hat{\Lambda}] = 0$ (Two operators commute.)

Complete basis of simultaneous eigenvectors $|\omega, \lambda\rangle$

$$\sum |\omega, \lambda\rangle\langle\omega, \lambda| = I$$

$$P(\omega, \lambda) = |\langle\omega, \lambda|\psi\rangle|^2 = P(\lambda, \omega)$$

(2) $\hat{\Omega}$ and $\hat{\Lambda}$ are incompatible: $[\hat{\Omega}, \hat{\Lambda}] =$ something having no zero eigenvalue

$P(\omega, \lambda) \neq P(\lambda, \omega)$

$[\hat{X}, \hat{P}] = i\hbar$ X and P cannot be well defined simultaneously for any state (Heisenberg uncertainty principle)

Measurement of two observables

For a momentum eigenstate $\hat{P}|p\rangle = p|p\rangle$,
what is $\psi_p(x) = \langle x|p\rangle$?

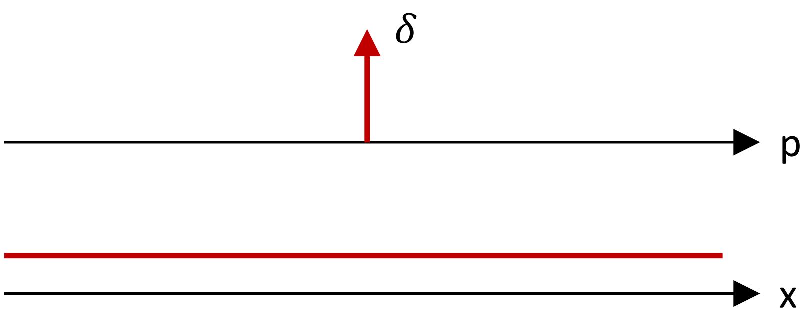
$$\langle x|\hat{P}|p\rangle = p\langle x|p\rangle$$

$$-i\hbar\frac{d\psi_p(x)}{dx} = p\psi_p(x)$$

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

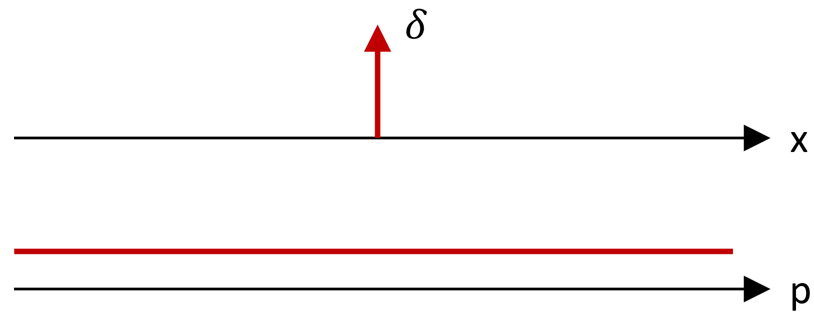
Normalized so that $\langle p|p'\rangle = \delta(p - p')$

Plane wave (constant amplitude over entire x)



For a position eigenstate $\hat{X}|x\rangle = x|x\rangle$,
what is $\psi_x(p) = \langle p|x\rangle$?

$$\psi_x(p) = \psi_p^*(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}$$



If we know $\psi(x) = \langle x|\psi\rangle$,
how can we get $\psi(p) = \langle p|\psi\rangle$?

$$\langle p|\psi\rangle = \int \langle p|x\rangle\langle x|\psi\rangle dx = \int \psi_x(p)\psi(x)dx$$

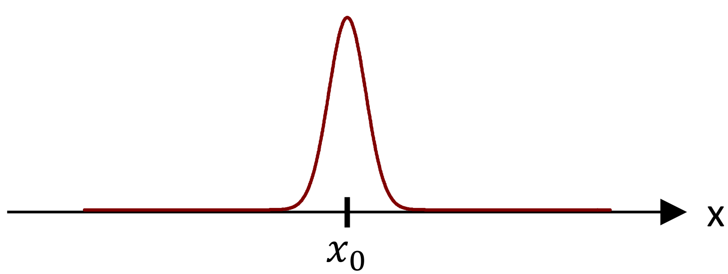
Measurement of two observables

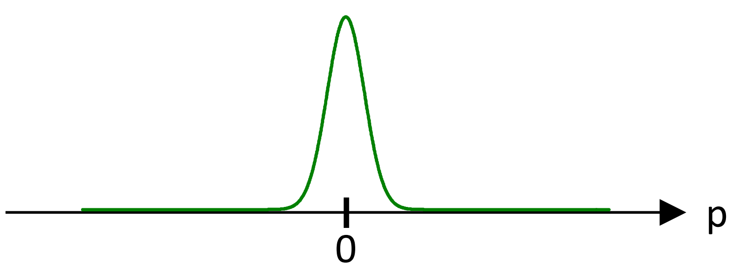
If $\psi(x) = \langle x|\psi\rangle$ is known,

$$\psi(p) = \langle p|\psi\rangle = \int \psi_x(p)\psi(x)dx \qquad \psi_x(p) = \psi_p^*(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

(like Fourier transform)

For a Gaussian wavefunction (wavepacket)





$$\psi(x) = \frac{1}{(\pi\Delta)^{1/4}} e^{-(x-x_0)^2/2\Delta^2} \qquad \psi(p) = \left(\frac{\Delta^2}{\pi\hbar^2}\right)^{1/4} e^{-ipx_0/\hbar} e^{-p^2\Delta^2/2\hbar^2}$$

$$\langle X\rangle = \langle\psi|\hat{X}|\psi\rangle = \int x|\psi(x)|^2 dx = x_0 \qquad \langle P\rangle = \langle\psi|\hat{P}|\psi\rangle = \int p|\psi(p)|^2 dp = 0$$

$$\Delta X = \left[\langle\psi|(\hat{X} - \langle X\rangle)^2|\psi\rangle\right]^{1/2} = \Delta/\sqrt{2} \qquad \Delta P = \left[\langle\psi|(\hat{P} - \langle P\rangle)^2|\psi\rangle\right]^{1/2} = \hbar/\sqrt{2}\Delta$$

$\Delta X \Delta P = \hbar/2$ for Gaussian wavefunctions

$\Delta X \Delta P \geq \hbar/2$ (Heisenberg uncertainty relation), in general.