Quantum states as vectors:

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}$$

vector

$|\psi\rangle = \sum_i \psi_i \hat{e}_i$ ← basis of the vector space

ψ_i = components of $|\psi\rangle$ in a certain basis $\hat{e}_i$.

finite vector space

$i \to \vec{r}, \vec{p}$ can be continuous

infinite vector state space.

$$\langle\psi| = (\psi_1^*, \psi_2^* \cdots \psi_N^*)$$

$$\langle\phi|\psi\rangle = \sum_i \phi_i^* \psi_i \Rightarrow \int d^3r\, \phi^*(\vec{r})\, \psi(\vec{r})$$

$$\Rightarrow \int \frac{d^3p}{(2\pi\hbar)^3} \phi^*(\vec{p})\, \psi(\vec{p})$$

The choice of basis:

$$|i\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \leftarrow i^{th} \text{ row} \quad \rightarrow \text{ unit vector}$$

$$\langle j | i \rangle = \delta_{ij}$$

$|\vec{r}\rangle$ = positional vector basis, zero except at $\vec{r}$.

$$\langle \vec{r}' | \vec{r} \rangle = \delta^3(\vec{r}' - \vec{r}) \longrightarrow \text{delta fct} \quad \int dx' f(x') \delta(x' - x) = f(x)$$

$$= \delta(x' - x)\,\delta(y' - y)\,\delta(z' - y)$$

continuum normalization

$\langle \vec{r} | \psi \rangle$ = component of ψ in the basis of $\vec{r}$.

$= \psi(\vec{r})$

representation

$$\int \frac{dk}{2\pi} e^{ik(x' - x)} = \delta(x' - x)$$

The outer product of basis

$$|i\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ 0 \end{pmatrix} \leftarrow i^{th} \text{ row} \qquad \langle j| = \underset{j^{th} \text{ column}}{(0, 0 \ldots\ 1, 0, 0\ )}$$

$$|i\rangle\langle j| = \begin{array}{cc} j^{th} \text{ column} & \\ \begin{pmatrix} 0 & \vdots & 0 \\ \cdots & 1 & \cdots \\ 0 & \vdots & 0 \end{pmatrix} & i^{th} \text{ row} \end{array} \qquad |i\rangle\langle i| = \begin{array}{cc} i^{th} & \\ \begin{pmatrix} \ddots & & 0 \\ & 1 & \\ 0 & & \ddots \end{pmatrix} & i^{th} \end{array}$$

$$\sum_i |i\rangle\langle i| = \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix} + \begin{pmatrix} 0 & & \\ & 1 & \\ & & 0 \; 0 \end{pmatrix} + \begin{pmatrix} 0 & & \\ & 0 & \\ & & 1 \end{pmatrix} + \cdots$$

$$= \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \; 1 \end{pmatrix} = \mathbb{1} \quad \text{unit matrix}$$

Similarly $\int d^3r \; |\vec{r}\rangle\langle\vec{r}| = \mathbb{1}$

Therefore: $|\psi\rangle = \mathbb{1}\,|\psi\rangle = \int d^3r\; |\vec{r}\rangle\langle r|\psi\rangle$

$$= \int d^3\vec{r}\; \psi(\vec{r})\, |\vec{r}\rangle$$

If $\psi(\vec{r}) = \delta(\vec{r}-\vec{r}_0)$

$$|\psi\rangle = |\vec{r}_0\rangle$$

$$\langle\vec{r}|\psi\rangle = \delta(\vec{r}-\vec{r}_0)$$

The distinction between the basis & the physical ψ

basis states are not necessary physical states.

Changing basis : The state vector formulation allows any basis to be used, not just the positional basis.

The most import other basis is momentum basis representation.

classical mechanics: we need both position + momentum

quantum mechanics: either the position or the momentum basis.

$$\psi(\vec{p}) = \langle \vec{p} | \psi \rangle = \int d^3r \, \langle \vec{p} | \vec{r} \rangle \langle \vec{r} | \psi \rangle$$

$$= \int d^3r \, \langle \vec{p} | \vec{r} \rangle \, \psi(\vec{r})$$

$$e^{-i \frac{\vec{p}}{\hbar} \cdot \vec{r}}$$

$$\psi(\vec{r}) = \langle r | \psi \rangle = \int \frac{d^3p}{(2\pi\hbar)^3} \langle r | p \rangle \langle p | \psi \rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} \langle \vec{r} | \vec{p} \rangle \, \psi(\vec{p})$$

(what is the operator $\vec{r}$, in the momentum representation?)

We know that

$\langle \vec{r} | \vec{p} \rangle =$ quantum state of momentum $\vec{p}$, in the coordinate basis

$$= e^{i \frac{\vec{p}}{\hbar} \cdot \vec{r}} \quad \text{because } \hat{p} = \frac{\hbar}{i} \vec{\nabla}$$

$$\psi(\vec{p}) = \int d^3r \, e^{-i \frac{\vec{p} \cdot \vec{r}}{\hbar}} \psi(r)$$

$$\psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{i \vec{p} \cdot \vec{r}/\hbar} \psi(p)$$

Also, we can deduce that

$$\langle \bar{r} | \psi \rangle = \psi(\bar{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \langle r | p \rangle \langle p | \psi \rangle$$

$$\int \frac{d^3p}{(2\pi\hbar)^3} |p\rangle\langle p| = \mathbb{1}$$

Since $\langle \psi | \psi \rangle = 1 \Rightarrow \int \frac{d^3p}{(2\pi\hbar)^3} \psi^*(\bar{p}) \psi(\bar{p}) = 1$

Observables as operators :

In contrast to classical mechanics, not all physical quantities are quantum mechanical observables.

Example: observables p_x^2, x^2, but $p_x x$ is not an observable.

$\Rightarrow$ observables as eigenvalues of some operators.

$$\vec{r}_{op} |\vec{r}\rangle = \vec{r} |\vec{r}\rangle \qquad \vec{r}_{op} = \hat{\vec{r}} \qquad \vec{p}_{op} |\vec{p}\rangle = \vec{p} |\vec{p}\rangle$$

$$\langle \vec{r}\,' | \vec{r}_{op} | \vec{r}\rangle = \vec{r} \langle \vec{r}\,' | \vec{r}\rangle = \vec{r}\, \delta(\vec{r}\,' - \vec{r})$$

$$\hookrightarrow \quad V_{op}(\vec{r}) |\vec{r}\rangle = V(\vec{r}) |\vec{r}\rangle$$

$$\hookrightarrow \quad \langle \vec{r}\,' | V_{op}(\vec{r}) | \vec{r}\rangle = V(\vec{r})\, \delta(\vec{r}\,' - \vec{r})$$

diagonal in their respective basis

Similarly
$$\vec{P}_{op} |\psi\rangle = \vec{P}_{op} \int \frac{d^3p}{(2\pi\hbar)^3} |\vec{p}\rangle\langle\vec{p}|\psi\rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} |\vec{p}\rangle \vec{p} \langle\vec{p}|\psi\rangle$$

therefore

$$\vec{P}_{op} = \int \frac{d^3p}{(2\pi\hbar)^3} |\vec{p}\rangle \vec{p} \langle\vec{p}| \qquad \vec{P}_{op} |\vec{p}\rangle = \vec{p} |\vec{p}\rangle$$

$$\boxed{\vec{F}(\vec{P}_{op}) = \int \frac{d^3p}{(2\pi\hbar)^3} |\vec{p}\rangle f(\vec{p}) \langle\vec{p}|} \qquad \vec{r}_{op} |\vec{r}\rangle = \vec{r} |\vec{r}\rangle$$

what is the representation of $\vec{P}_{op}$ in the $\vec{r}$-basis

$\hat{p} \equiv \vec{P}_{op}$

$$\langle \vec{r} | \hat{p} | \vec{p} \rangle = \vec{p} \langle \vec{r} | \vec{p} \rangle$$

$$= \vec{p}\, e^{i \vec{p}\cdot\vec{r}/\hbar}$$

$$= \frac{\hbar}{i} \vec{\nabla} \left(e^{i \vec{p}\cdot\vec{r}/\hbar} \right)$$

$$\langle \vec{r} | \hat{p} | \vec{p} \rangle = \frac{\hbar}{i} \vec{\nabla} \langle \vec{r} | \vec{p} \rangle$$

We derive the correct, usual representation that

$$\vec{P}_{op} = \frac{\hbar}{i} \vec{\nabla}$$

but remember $\langle \vec{p}' | \hat{p} | \vec{p} \rangle = \vec{p}\, \delta(\vec{p}' - \vec{p}) \frac{1}{(2\pi\hbar)^3}$

Thus the free-particle Schrödinger Eq.

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) = \frac{1}{2m}\left(\frac{\hbar\vec{\nabla}}{i}\right)^2 \psi(\vec{r},t)$$

$$i\hbar \frac{\partial}{\partial t} \langle r|\psi(t)\rangle = \frac{1}{2m}\langle r|\hat{p}^2|\psi(t)\rangle$$

This means that

operator

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \frac{1}{2m}\hat{p}^2|\psi(t)\rangle$$

with exact solution

$$|\psi(t)\rangle = e^{-i\frac{t}{\hbar}\frac{1}{2m}\hat{p}^2}|\psi(0)\rangle$$

and

$$\langle\vec{p}|\psi(t)\rangle = \langle\vec{p}|e^{-i\frac{t}{\hbar}\frac{1}{2m}\hat{p}^2}|\psi(0)\rangle$$

$$= \int\frac{d^3\vec{p}\,'}{(2\pi\hbar)^3}\langle\vec{p}|e^{-i\frac{t}{\hbar}\frac{1}{2m}\hat{p}^2}|\vec{p}\,'\rangle\langle p'|\psi(0)\rangle$$

$$\underbrace{\langle\vec{p}|\vec{p}\,'\rangle}_{(2\pi\hbar)^3\delta(\vec{p}-\vec{p}\,')} e^{-i\frac{t}{\hbar}\frac{1}{2m}\vec{p}\,'^2}\langle p'|\psi(0)\rangle$$

$$\boxed{\psi(\vec{p},t) = e^{-i\frac{t}{\hbar}\frac{1}{2m}\vec{p}^2}\psi(\vec{p},0)}$$

Similarly

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = V_{op}(\vec{r}) \, |\psi(t)\rangle$$

Solution

$$|\psi(t)\rangle = e^{-i\frac{t}{\hbar} V_{op}(\vec{r})} |\psi(t)\rangle$$

$$\boxed{\langle r|\psi(t)\rangle = e^{-i\frac{t}{\hbar} V(\vec{r})} \langle r|\psi(0)\rangle}$$

$$\boxed{\langle \hat{p}|\psi(t)\rangle = e^{-i\frac{t}{\hbar}\frac{\hat{p}^2}{2m}} \langle \hat{p}|\psi(0)\rangle}$$

For the full Schrödinger Eq.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \left[\frac{1}{2m}\hat{p}^2 + \underbrace{V(\hat{r})}_{\hat{V}}\right] |\psi(t)\rangle$$

$\Rightarrow$ exact solution

$\epsilon = -i\frac{t}{\hbar}$

$$|\psi(t)\rangle = e^{-i\frac{t}{\hbar}\left[\underbrace{\frac{1}{2m}\hat{p}^2}_{\hat{T}} + V(\hat{r})\right]} |\psi(0)\rangle$$

how to evaluate this?

$$H_{op} = \frac{1}{2m}\hat{p}^2 + V(\hat{r})$$

Quantum dynamics ⇒ Solution to the Schrödinger time-dependent Eq. .

$\epsilon = -i\frac{t}{\hbar}$

$$|\psi(t)\rangle = e^{\epsilon[\hat{T}+\hat{V}]}\,|\psi(0)\rangle \qquad \hat{T} = \frac{\hat{p}^2}{2m}$$

$$\hat{V} = V(\hat{r})$$

for ϵ (or t) small

$$e^{\epsilon(\hat{T}+\hat{V})} \approx e^{\epsilon\hat{T}}e^{\epsilon\hat{V}} + \mathcal{O}(\epsilon^2)$$

first-order algorithm

i.e. ϵ-order error in $H' = H + \epsilon \Delta H + \cdots$

Baker-Campbell-Hausdorff formula

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\cdots}$$

$$\approx e^{\frac{\epsilon}{2}\hat{V}}e^{\epsilon\hat{T}}e^{\frac{\epsilon}{2}\hat{V}}$$

second-order algorithm.

first order case: $\qquad \epsilon = -i\frac{\Delta t}{\hbar}$

$$\langle \vec{r}' | \psi(t+\Delta t)\rangle = \langle \vec{r}' | e^{\epsilon \hat{T}} e^{\epsilon \hat{V}} | \psi(0)\rangle \qquad \hat{T} = \frac{\hat{p}^2}{2m}$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} \langle \vec{r}' | e^{\epsilon \hat{T}} | p\rangle\langle p | e^{\epsilon \hat{V}} | \psi(0)\rangle$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} e^{\epsilon \frac{p^2}{2m}} \langle \vec{r}' | p\rangle\langle p | e^{\epsilon \hat{V}} | r\rangle\langle r | \psi(0)\rangle$$

$$= \underbrace{\int d^3\vec{r} \quad \langle p | r\rangle e^{\epsilon V(r)} \psi(r,0)}_{\psi_1(\vec{p},\Delta t) = FT(\psi_1(r,\Delta t))}$$

$$\langle p | r\rangle = e^{-i\frac{\vec{p}\cdot\vec{r}}{\hbar}} \qquad \underbrace{e^{\epsilon V(r)} \psi(r,0)}_{\psi_1(r,\Delta t)}$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} e^{i\frac{\vec{p}\cdot\vec{r}'}{\hbar}} e^{\epsilon\frac{p^2}{2m}} \psi_1(\vec{p},\Delta t)$$

$$\psi(\vec{r}',\Delta t) = FT^{-1}\left(e^{\epsilon\frac{p^2}{2m}} \psi_1(\vec{p},\Delta t)\right)$$

$$\begin{array}{lccc} \text{p-space} & \psi_2(\vec{p},\Delta t) = e^{\epsilon\frac{p^2}{2m}}\psi_1(\vec{p},\Delta t) & \xleftarrow{FT} & \\ & \big\downarrow FT^{-1} & & \underbrace{e^{\epsilon V(r)}\psi(r,0)}_{\psi_1(\vec{r},0)} \\ \text{r-space} & \psi(\vec{r},t+\Delta t) & & \end{array}$$

The second-order algorithm $e^{\frac{\epsilon}{2}V} e^{\epsilon T} e^{\frac{\epsilon}{2}V}$

$$\begin{array}{ccc} e^{\epsilon\frac{p^2}{2}} \psi_1(p,\Delta t) & \xleftarrow{FT} & \\ \big\downarrow FT^{-1} & & e^{\frac{\epsilon}{2}V(r)}\psi(r,0) = \psi_1(r,t) \\ \psi(r,t+\Delta t) = e^{\frac{1}{2}\epsilon V(\vec{r})}\psi_1(\vec{r},\Delta t) & & \end{array}$$

The free-particle

$$|\psi(t)\rangle = e^{-i\frac{t}{\hbar}\frac{\hat{p}^2}{2m}}|\psi(0)\rangle$$

$$\psi(r,t) = \langle r|\psi(t)\rangle = \langle r| e^{-i\frac{t}{\hbar}\frac{\hat{p}^2}{2m}}|\psi(0)\rangle$$

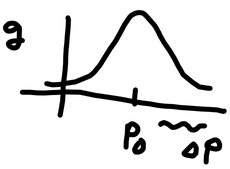
$$= \int\frac{d^3p}{(2\pi\hbar)^3}\langle r| e^{-i\frac{t}{\hbar}\frac{\hat{p}^2}{2m}}|p\rangle\langle p|\psi(0)\rangle$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3} e^{-i\frac{t}{\hbar}\overbrace{\frac{p^2}{2m}}^{E_p}}\langle r|p\rangle\,\psi(p,0)$$

$$\psi(p,0) = g(p)e^{-i\alpha(p)}$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3} e^{-i\frac{t}{\hbar}\frac{p^2}{2m}} e^{i\vec{p}\cdot\vec{r}/\hbar} g(p) e^{-i\alpha(p)}$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3} e^{i(\vec{p}\cdot\vec{r} - E_p t - \hbar\alpha)/\hbar} g(p)$$



↓ sum over interference term

∟ contribute only near phase stationary pt.

$$\phi = \vec{p}\cdot\vec{r} - E_p t - \hbar\alpha \qquad \vec{\nabla}_p\phi = 0$$

$$\vec{r} - \nabla_p E_p\, t - \underbrace{\hbar\nabla_p\alpha}_{\vec{r}_0} = 0$$

$$\nabla_p E_p = \nabla_p\frac{p^2}{2m} = \frac{\vec{p}}{m}$$

Group velocity

not the phase velocity

$$\frac{E_p}{p} = \frac{p}{2m}$$

1) $\vec{r} = \vec{v}t + \vec{r}_0$

the wave-packet moves with the group velocity $\vec{v} = \vec{\nabla}_p E_p$

2) uncertainty principle.

$$\psi(r) = \int \frac{d^3p}{(2\pi\hbar)^3}\, \psi(p)\, e^{i\bar{p}\cdot\bar{r}/\hbar}$$

$$\uparrow$$

$$\psi(p) = \int d^3r\, \psi(r)\, e^{-i\bar{p}\cdot\bar{r}/\hbar}$$