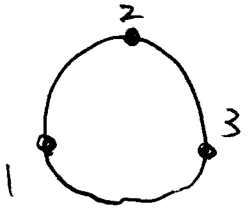
N-site ring

☆ Let's start with a simplest example: a 3-site ring.



The particle can only live on the sites

$|1\rangle, \quad |2\rangle, \quad |3\rangle$ (if you like, call it $|甲\rangle, |乙\rangle, |丙\rangle$)

The corresponding Hilbert space is 3-dimensional.
also $\langle m|n\rangle = \delta_{mn}$

☆ Let's define an operator: $\hat{哪}$

$$\hat{哪}\,|s\rangle = s\,|s\rangle \quad , \quad s = 1, 2, 3$$

eg. a state vector

$$|\psi\rangle = 3|1\rangle + 7|2\rangle + 5|3\rangle$$

$$\hat{哪}\,|\psi\rangle = (1\times 3)|1\rangle + (2\times 7)|2\rangle + (3\times 5)|3\rangle$$

☆ We can relate $\hat{哪}$ to the position operator $\hat{X}$ by

$$\hat{X} = \left(\frac{L}{3}\right) \times \hat{哪}$$ where L is the length of ring

and the representation of $\hat{X}$ in the Hilbert space is

$$\hat{X} \sim \left(\frac{L}{3}\right) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} = (\hat{X})^{\dagger}$$ (it is Hermitian!)

☆ Now, consider a 1-step translation which moves the particle from $|s\rangle \rightarrow |s+1\rangle$

Denote this displacement operator as $\hat{D}$, then

$$\hat{D}\,|s\rangle = |s+1\rangle ,$$ its representation $\sim \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

- Then for a state $|\psi\rangle = \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle)$

$\uparrow$ not necessary

$$\hat{D}|\psi\rangle = \frac{1}{\sqrt{3}}(|2\rangle + |3\rangle + |1\rangle) = |\psi\rangle. \quad \text{is the eigenstate of } \hat{D}.$$

- In fact, one can also construct a more complicate eigenstates of $\hat{D}$

$$|\psi_k\rangle \equiv \frac{1}{\sqrt{3}}(e^{i1k}|1\rangle + e^{i2k}|2\rangle + e^{i3k}|3\rangle)$$

then

$$\hat{D}|\psi_k\rangle = \frac{1}{\sqrt{3}}[e^{i1k}|2\rangle + e^{i2k}|3\rangle + e^{i3k}|1\rangle]$$

$$= e^{-ik}\frac{1}{\sqrt{3}}[e^{i2k}|2\rangle + e^{i3k}|3\rangle + e^{i4k}|1\rangle]$$

If we require that $|\psi_k\rangle$ is an eigenstate of $\hat{D}$ with eigenvalue $(e^{-ik\cdot 1})$ then $e^{i4k} = e^{i\cdot 1\cdot k}$

$$\Rightarrow \quad 3k = 2n\pi \quad \text{or} \quad k_n = \frac{2\pi n}{3}, \quad n: \text{integer}.$$

(Another way to see this is $(\hat{D})^3 = \hat{\mathbb{1}} = e^{-3ik}$)

- Now, let's write $|x_s\rangle \equiv |s\rangle$ which is the eigenstate of $\hat{X}$, and denote $|\psi_{k_n}\rangle \equiv |k_n\rangle$

$$|k_n\rangle = \sum_{s=1}^{3} \frac{1}{\sqrt{3}} e^{ik_n\cdot s}|s\rangle$$

since $x_s = (\frac{L}{3})\cdot s$, it can be expressed as

$$|k_n\rangle = \sum_{s=1}^{3} \frac{1}{\sqrt{3}} e^{ik_n(\frac{3x_s}{L})}|x_s\rangle = \sum_{s=1}^{3} \frac{1}{\sqrt{3}} e^{i\frac{2n\pi}{L}x_s}|x_s\rangle$$

where $n = 0, 1, 2$

Now we generalized the above disscussion from $3 \rightarrow N$,

$$K_n = \frac{2\pi n}{L}, \quad n = 0, 1, 2 \cdots (N-1) \qquad \hat{X} = \frac{L}{N}(\hat{\text{哪}})$$

$$\langle X_s | K_n \rangle = \underbrace{\frac{1}{\sqrt{N}}}_{\text{not necessary}} e^{i K_n X_s}$$

and $|K_n\rangle$ is the eigenstate of $\hat{D}$ with eigenvalue $e^{-i K_n \left(\frac{L}{N}\right)}$

☆ Now associate K_n to the momentum and define operator $\hat{P}$:

$$\underset{\left[\frac{ML}{T}\right]}{\hat{P}} \, |K_n\rangle = \underset{\left[\frac{ML^2}{T}\right]}{\hbar} \, \underset{\left[\frac{1}{L}\right]}{K_n} |K_n\rangle$$

which has eigenvalue $\hbar K_n$

☆ $\hat{D}|K_n\rangle = \exp\left[-i K_n \left(\frac{L}{N}\right)\right] |K_n\rangle = \exp\left[-i \frac{\hat{P}}{\hbar}\left(\frac{L}{N}\right)\right] |K_n\rangle$

so $\hat{D}$ can be viewed as

$$\hat{D} = \exp\left(-i \frac{\hat{P}}{\hbar}\left(\frac{L}{N}\right)\right]$$

☆ Note that we can define 2-step, 3step .. displacement operators as well,

$$\hat{D}_2 = (\hat{D})^2 = \exp\left(-i \frac{\hat{P}}{\hbar}\left(\frac{2L}{N}\right)\right]$$

$$\hat{D}_3 = (\hat{D})^3 = \exp\left(-i \frac{\hat{P}}{\hbar}\left(\frac{3L}{N}\right)\right]$$

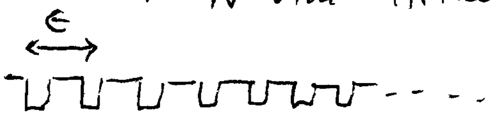
$$\vdots$$

$\Rightarrow \hat{P}$ is called the generator of translation

$\Rightarrow \hat{D}(\Delta x) = \exp\left(-\frac{i}{\hbar} \hat{P} \Delta x\right)$

Finally, let's go to the continuos limit with $N \to \infty$

$\to$ N-dim Hilbert space $\to$ ∞-dim Hilbert space



$$\epsilon = \frac{L}{N}$$

and $\quad X_s = s \times \epsilon$

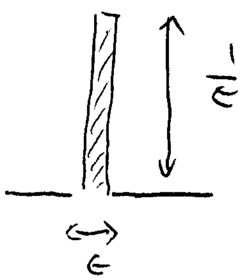
$$\sum_s \Rightarrow \sum_{X_s} \frac{1}{\epsilon} \underset{N\to\infty}{\Rightarrow} \int \frac{dx}{\epsilon}$$

$$\hat{X} | X_s \rangle = X_s | X_s \rangle$$

$$|\psi\rangle = \sum_s \underset{\substack{\uparrow \\ \text{coefficient}}}{\psi_s} |s\rangle = \sum_{X_s} \frac{1}{\epsilon} \psi_s(X_s) | X_s \rangle \Rightarrow \int dx \left(\frac{\psi_s(X_s)}{\sqrt{\epsilon}} \right) \frac{|X_s\rangle}{\sqrt{\epsilon}}$$

We may write $\quad \psi(x) \equiv \frac{1}{\sqrt{\epsilon}} \psi_s(X_s) \quad$ and $\quad |X\rangle \equiv \frac{1}{\sqrt{\epsilon}} |X_s\rangle \; \left(= \frac{1}{\sqrt{\epsilon}} |s\rangle \right)$

apparently, $\quad \langle x' | X \rangle = \frac{1}{\epsilon} \langle s' | s \rangle = \frac{1}{\epsilon} \delta_{s',s}$



$$\lim_{N\to\infty} \Rightarrow \delta(X' - x)$$

the Dirac delta function.

and $\quad \psi(x) = \frac{1}{\sqrt{\epsilon}} \langle X_s | \psi \rangle = \langle x | \psi \rangle \quad$ the Schrödinger W.F.

$$\langle \psi | \psi \rangle = \sum_s |\psi_s|^2 = \int \frac{dx}{\epsilon} |\sqrt{\epsilon}\, \psi(x)|^2 = \int dx\, |\psi(x)|^2$$

$$= \begin{cases} 1 & \text{if normalized} \\ \text{finite} & \text{if physical.} \end{cases}$$

$\Rightarrow$ Wave function is the coefficient the state projected onto a basis.

$$\psi(x) = \langle x | \psi \rangle, \quad \langle x | x' \rangle = \delta(x - x')$$

$$|\psi\rangle = \mathbb{1}_x |\psi\rangle = \int dx\, (|x\rangle\langle x|)\, |\psi\rangle = \int dx\, \psi(x)\, |x\rangle$$

Momentum eigenstates can also be used as a basis. (with undetermined normalization)

$$|k_n\rangle \propto \sum_s e^{ik_n x_s} |x_s\rangle$$

$$\langle k_m | k_n \rangle = \sum_{x_s} \langle k_m | x_s \rangle \langle x_s | k_n \rangle$$

$$\propto \sum_s e^{-ik_m x_s} e^{ik_n x_s}$$

If $k_n \neq k_m$, the phase oscillation makes the summation vanish. and the only nonzero inner products are those with $k_m = k_n$

$$\Rightarrow \langle k_m | k_n \rangle \propto \delta_{k_m, k_n} \Rightarrow \text{orthogonal.}$$

In the continuous limit

$$\phi_k(x) = \langle x | k \rangle = A e^{ikx}$$

(we already know that $\langle x | x' \rangle = \delta(x - x')$)

Then $\langle x | x' \rangle = \int dk \, \langle x | k \rangle \langle k | x' \rangle$

$$= |A|^2 \int dk \, e^{ikx} e^{-ikx'} = |A|^2 \, 2\pi \, \delta(x - x')$$

$$\Rightarrow A = \frac{1}{\sqrt{2\pi}}, \quad \phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

In the momentum basis

$$|\psi\rangle = \int dk \, |k\rangle \langle k | \psi \rangle$$

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

$$= \int dk \Big[\underbrace{\int dx \frac{1}{\sqrt{2\pi}} e^{-ikx} \psi(x)}_{\equiv \psi(k)} \Big] |k\rangle$$

$\equiv \psi(k)$ the Fourier transformation of $\psi(x)$

We see that the continuous basis satisfies

$$\langle \lambda | \lambda' \rangle = \delta(\lambda - \lambda') \qquad (\text{Dirac orthonormal})$$

If the spectrum of a hermitian operator is continuous, the eigenfunctions are <u>not</u> normalizable, they are <u>NOT</u> in Hilbert space and they donot represent possible physical state.

However, the eigenfunctions with real eigenvalues are Dirac orthonormalizable and complete.

$$\langle x | k \rangle \qquad \qquad \langle x | p \rangle$$

$$\phi_k(x) \longrightarrow \phi_p(x)$$

$$= \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ip}{\hbar}x}$$

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

$\boxed{\text{Momentum operator}}$ in the $|x\rangle$ basis ?

consider the 1-step infinitesimal translation $(N \to \infty)$

$$\hat{D}(\epsilon)|\psi\rangle \Rightarrow \sum_s \psi_s \hat{D}|s\rangle = \sum_{s'} \psi_{s'-1} |s'\rangle$$

$$\langle x_s | \hat{D}(\epsilon) | \psi \rangle = \psi_{s-1}$$

$$\hat{D}(\epsilon) = e^{-i\frac{\hat{p}}{\hbar}\epsilon} \simeq \mathbb{1} - \frac{i}{\hbar}\epsilon\hat{p}$$

$$\Rightarrow \langle x_s | \mathbb{1} - \frac{i\epsilon}{\hbar}\hat{p} | \psi \rangle = \psi_s - \frac{i\epsilon}{\hbar}\langle x_s | \hat{p} | \psi \rangle = \psi_{s-1}$$

$$\langle x_s | \hat{p} | \psi \rangle = -i\hbar \frac{\psi_s - \psi_{s-1}}{\epsilon}$$

$\Rightarrow \hat{p}$ in the x-basis $\Rightarrow \boxed{-i\hbar \frac{d}{dx}\psi(x)}$

$\boxed{\text{Q: How about time-evolution?}}$

$$T(0) = \mathbb{1}$$

$$T(a)T(b) = T(b)T(a) = T(a+b)$$

$$\Rightarrow T(\Delta t) = \lim_{N\to\infty} \left(T\left(\frac{\Delta t}{N}\right)\right)^N$$

$$= \lim_{N\to\infty} \left(\mathbb{1} - \frac{i}{\hbar}\left(\frac{\Delta t}{N}\right)\hat{H} \right)^N$$

$\frac{1}{[E][T]}$ $[T]$ $[E]$

$\frac{\Delta t}{N} \to 0$, T can be Taylor expanded around $\mathbb{1}$

the only relevant QM parameter is $\hbar$

$[\hbar] = [E][T]$

Introduce an operator $\hat{H}$ to do the expansion around $\mathbb{1}$.

$$\langle x | T(\epsilon) | \psi(t) \rangle = \langle x | \psi(t+\epsilon) \rangle = \psi(x, t+\epsilon)$$

or $= \langle x | \mathbb{1} - \frac{i}{\hbar}\epsilon \hat{H} | \psi(t) \rangle$

$$= \psi(x,t) - \frac{i}{\hbar}\epsilon \langle x | \hat{H} | \psi(t) \rangle$$

$$\Rightarrow \langle x | \hat{H} | \psi(t) \rangle = i\hbar \frac{\psi(x,t+\epsilon) - \psi(x,t)}{\epsilon} \xrightarrow[\epsilon \to 0]{} \boxed{i\hbar \frac{\partial}{\partial t}\psi(x,t)}$$

$$\Rightarrow \langle x | \hat{H} | \psi(t) \rangle = i\hbar \frac{\partial}{\partial t} \langle x | \psi(t) \rangle$$

or $\boxed{\hat{H}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)}$

Schrödinger Eq.

Actually, it's better to be written as

$$(\hat{H}\psi)(x) = i\hbar \frac{\partial}{\partial t}\psi(x)$$