20190319, Ch2 Quantum Dynamics

Monday, March 18, 2019 2:56 PM

Reminder: short Quiz in-class next week.
60 min. A4 formula sheet double sided.
Homework level difficulty. Chapter 1 covered.

$\boxed{\text{Mr. Zhang HW Q+A : Sunday 3PM}}$

Homework:

① a particle in a one dimensional infinite deep well

$$V(x) = \begin{cases} 0, & -\frac{a}{2} < x < \frac{a}{2} \\ \infty, & \text{other} \end{cases}$$

suppose at $t=0$, $\psi(x, t=0) = \frac{4}{\sqrt{a}} \cos\frac{\pi}{a}x \sin^2\frac{\pi}{a}x$, $-\frac{a}{2} < x < \frac{a}{2}$

try to find $\psi(x,t)$.

sketch $|\psi(x,t)|^2$, at $t = 0, t = \frac{ma^2}{8\pi^2\hbar}, t = \frac{ma^2}{4\pi^2\hbar}, t = \frac{3ma^2}{8\pi^2\hbar}, t = \frac{ma^2}{2\pi^2\hbar}$ discuss its evolution over time

② with $|\alpha\rangle$ a Gaussian wavepacket,

$\langle x|\alpha\rangle = \frac{1}{\pi^{1/4}\sqrt{d}} \exp\left[ikx - \frac{x^2}{2d^2}\right]$, we have

proved $\langle p|\alpha\rangle = \sqrt{\frac{d}{\hbar\sqrt{\pi}}} \exp\left(\frac{-(p-\hbar k)^2 d^2}{2\hbar^2}\right)$.

with $H = \frac{p^2}{2m}$ a free particle with wavefunction

$\psi(x, t=0) = \langle x|\alpha\rangle$,

(2.1) find $\psi(p,t)$

(2.2) find $\psi(x,t)$

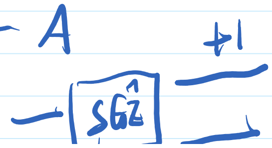
(2.3) sketch $|\psi(x,t)|^2$, at $t = 0, t = \frac{\hbar k^2}{2m}$ discuss its evolution over time

Postulates of Quantum Mechanics

基本假設

post. #1. At any time t, the state of a physical system is defined by a ket $|\psi(t)\rangle$ or "state" in a relevant Hilbert space H.

post #2. The only possible result of measuring observable A is one of the eigenvalues of A



$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

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asides ① if A = Hermitian, then meas. gives a real number

② if A's spectrum is discrete, then we only see quantized result.

post. #3. every measurable physical quantity A is described by a Hermitian operator.

post #4 if $A|u_\alpha\rangle = a_\alpha|u_\alpha\rangle$

then for a system in $|\psi\rangle$

when we measure A, then the probability of getting a_α

is $P(a_\alpha) = |\langle u_\alpha|\psi\rangle|^2$

aside: if we have degenerate a_α's

$|u_{\alpha,1}\rangle, |u_{\alpha,2}\rangle \cdots$ share the same eigen value, then $P(a_\alpha)$

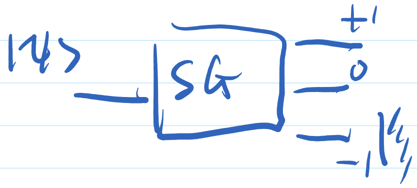
$P(a_\alpha) = \sum_i |\langle u_{\alpha,i}|\psi\rangle|^2$

example: $\hat{A} = \mathbb{1}$, all a_α's $= 1$

Post. #5. if a measurement projects $|\psi\rangle$ into a new state $|u_\alpha\rangle$

then a physical new state should be

$$|u_\alpha'\rangle = \frac{|u_\alpha\rangle}{\sqrt{\langle u_\alpha|u_\alpha\rangle}} \quad \text{so that } \langle u_\alpha'|u_\alpha'\rangle = 1$$



→ if we see click at "-1" we know state $|-1\rangle$

→ otherwise, in possible superposition

$$|\psi\rangle \to |+1\rangle\langle +1|\psi\rangle + |0\rangle\langle 0|\psi\rangle$$

post. #6. Between measurement the state vector $|\psi(t)\rangle$ evolves in time with time dependent Schrödinger's equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle$$

here $\hat{H}$ is a Hamiltonian.

Ch 2. Quantum Dynamics.

- non-relativistic.
- we think about time as a parameter

we don't have $\hat{T}$ time operator

position representation $\langle x|\psi\rangle = \psi(x)$

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

§1 time evolution operator and Hamiltonian.

(displacement)

$$\mathcal{U}(dt')|\psi(t)\rangle = |\psi(t+dt')\rangle$$

$\hookrightarrow \underline{U(dt')|\psi(t)\rangle = |\psi(t+dt')\rangle}$

$UU^\dagger = \mathbb{1}$, $U^\dagger = U^{-1}$

displacement op.

$\hat{\mathcal{T}}(dx') = \mathbb{1} - i\frac{\hat{P}}{\hbar}dx'$

$\pm ?$

$\Rightarrow$ similar to momentum,

we have $\begin{cases} U(dt') = \mathbb{1} - i\frac{\hat{H}}{\hbar}dt' \\ \hat{H} \text{ is Hermitian, Hamiltonian.} \end{cases}$

$\text{left} = \left(\mathbb{1} - i\frac{\hat{H}}{\hbar}dt'\right)\psi(x,t) = \underline{\psi(x,t)} - i\frac{\hat{H}}{\hbar}dt'\,\psi(x,t)$

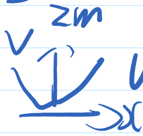
$\text{right} = \psi(x,t+dt') = \underline{\psi(x,t)} + \left(\frac{\partial}{\partial t}\psi(x,t)\right)\cdot dt'$

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

Schrödinger's equation. in position repr.

$\boxed{i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle}$

H : Hamiltonian in analog to classical mechanics $\begin{cases} H = T + V \\ T \text{ kinetic energy } T = \frac{P^2}{2m} \\ V \text{ potential energy} \end{cases}$



$V = U(x)$

$\hat{H} = \hat{T} + \hat{V}$

$= \frac{\hat{P}^2}{2m} + \hat{V}(x)$

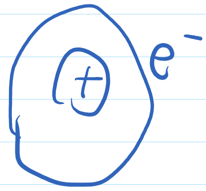
examples:

① a free particle $V = 0$

$\hat{H} = \frac{\hat{P}^2}{2m}$

② Hydrogen atom

(2) Hydrogen atom



$$\hat{H} = \frac{\hat{P}_e^2}{2m_e} + \frac{\hat{P}_n^2}{2m_n} - \frac{e^2}{4\pi\varepsilon_0 |\vec{r}_e - \vec{r}_n|}$$

(3) a partile magnetic moment $\vec{\mu}$, in external magnetic field $\vec{B}$

$$\hat{H} = -\vec{\mu}\cdot\vec{B}$$

(1) $\hat{H} = \frac{\hat{P}^2}{2m}$, $H(\hat{p})$, convenient to work in momentum representation.

$\{|p\rangle\}$ as our basis.

$\rightarrow H|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$ apply $\langle p|$ on left

$$\text{left} = \langle p|\frac{\hat{P}^2}{2m}|\psi(t)\rangle = \frac{p^2}{2m}\langle p|\psi(t)\rangle = \frac{p^2}{2m}\psi(p,t)$$

$$\text{right} = i\hbar\langle p|\frac{\partial}{\partial t}|\psi(t)\rangle \xlongequal{\frac{\partial}{\partial t}\langle p| = 0} i\hbar\frac{\partial}{\partial t}\langle p|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\psi(p,t)$$

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

$$\psi(p,t) = \psi(p,0)\underbrace{e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}}_{e^{-i\phi}}$$

if we let $\psi(p,0) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{px}{\hbar}} \sim \langle x|p\rangle$

in this case

$$\psi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{px}{\hbar}}\, e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{p}{\hbar}(x + \underline{\frac{pt}{m}})}$$

$\psi(p,0) = \langle p | x \rangle$ momentum repres. of $|x\rangle$

$\psi(p,t) = \langle p | x + \frac{pt}{m} \rangle$ if we set $v = \frac{p}{m}$

$x + \frac{pt}{m} = x + vt$

comment: we should observe structure of H, and choose the right repres.

if we have $\psi(x, t=0) \xrightarrow{\text{Fourier transform}} \psi(p, t=0)$

rewriting it in p-repres.

$$\psi(p,t) = \psi(p, t=0)\, e^{-i\frac{p^2}{2m}\frac{t}{\hbar}}, \quad \text{if } H = \frac{p^2}{2m}$$

if we need $\psi(x,t)$, we can get it from another Fourier transformation from $\psi(p,t)$.

§2. Static Schrödinger's equation

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

in position repres.

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

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

$$H = \frac{p^2}{2m} + V(x), \quad \hat{p} \longleftrightarrow -i\hbar\frac{\partial}{\partial x}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)+V(x)\,\psi(x,t)=i\hbar\frac{\partial}{\partial t}\psi(x,t)}$$

$$\langle x|p^2|\psi\rangle \neq -\hbar^2\left(\frac{\partial\psi(x)}{\partial x}\right)^2$$

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle = -i\hbar\frac{\partial}{\partial x}\psi(x)$$

$$\langle x|\hat{p}^2|\psi\rangle \xlongequal{|\phi\rangle=\hat{p}|\psi\rangle} \langle x|\hat{p}|\phi\rangle = -i\hbar\frac{\partial}{\partial x}\langle x|\phi\rangle$$

$$= (-i\hbar)\frac{\partial}{\partial x}\left(\langle x|p|\psi\rangle\right)$$

$$= (-i\hbar)\frac{\partial}{\partial x}\left((-i\hbar)\frac{\partial}{\partial x}\langle x|\psi\rangle\right)$$

$$= -\hbar^2\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\psi(x)\right) = -\hbar\frac{\partial^2}{\partial x^2}\psi(x)$$

it's best to separct the variables

分离变量.

$$\psi(x,t) = \Psi(x)\,\phi(t)$$

$\hat{H}$ is Hermitian.

$$H|\psi_E\rangle = E|\psi_E\rangle$$

eigen value eigen state

eigen energy

if we assume $|\psi(t=0)\rangle = |\psi_E\rangle$

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

$t\to 0$: $$\langle\psi_E|H|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\langle\psi_E|\psi(t)\rangle$$

$$E\langle\psi_E|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\langle\psi_E|\psi(t)\rangle$$

using the energy representation.

using the energy representation.

$\langle \psi_E | \psi(t) \rangle = g(t)$

$E g(t) = i\hbar \frac{\partial}{\partial t} g(t) \Rightarrow g(t) = e^{-i\frac{Et}{\hbar}} g(t=0)$

$\Rightarrow$ $\boxed{\text{we know the inner product of a state } |\psi(t)\rangle \text{ with eigenstate } |\psi_E\rangle \text{ is getting a phase } e^{-i\frac{Et}{\hbar}} \text{ over time}}$ ☆

probability of measuring with H after time t of evolution. is the same as any other time.

$P_E(t) = |\underline{\langle \psi_E | \psi(t) \rangle}|^2$

$= |\underline{e^{-i\frac{Et}{\hbar}}} \langle \psi_E | \psi(t=0) \rangle|^2$

$= |\langle \psi_E | \psi(t=0) \rangle|^2$

$= P_E(t=0)$

☆

推论 theorem.

$|\psi(t=0)\rangle \xlongequal{\text{discrete}} \sum_i c_i |\psi_E^i\rangle$ in the basis of energy $\{|\psi_E^i\rangle\}$ of eigenstates of $|\psi$

$|\psi(t)\rangle \xlongequal{H \neq H(t)} \sum_j c_j e^{-i\frac{E_j t}{\hbar}} |\psi_E^j\rangle$

- separation of variable

$\psi(x,t) \xlongequal{\text{work in energy basis}} \underline{\phi(x)\, e^{-i\frac{Et}{\hbar}}}$

$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$

$(\,,\ \boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + V(x)\,\phi(x) = E\phi(x)}$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + V(x)\,\phi(x) = E\phi(x)}$$

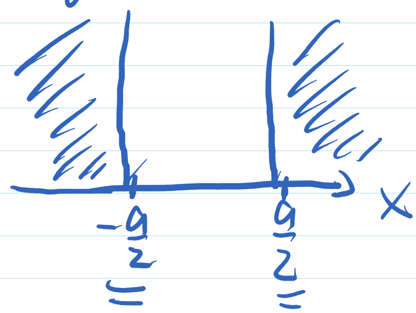
t-independent Schrödinger's equation
in a static form.

$$\frac{\partial^2}{\partial x^2}\phi(x) + \frac{2m}{\hbar^2}(E - V(x))\,\phi(x) = 0$$

energy

example #1. infinitely deep square potential

$$V(x) = \begin{cases} 0, & -\frac{a}{2} < x < \frac{a}{2} \\ +\infty, & \text{otherwise} \end{cases}$$



at $x > \frac{a}{2}$ or $x < -\frac{a}{2}$, $V \to +\infty$

$$\frac{\partial^2}{\partial x^2}\phi(x) + \frac{2m}{\hbar^2}(E - \underset{+\infty}{V})\,\phi(x) = 0$$

$\phi(x)$ needs to be finite, continous, single value
$|\phi(x)|^2$ need integratable

$\frac{\partial^2}{\partial x^2}\phi(x) \nrightarrow \infty$, $E\phi(x) \nrightarrow \infty$, need $V\phi(x) = 0$

$\Rightarrow$ only choice is $\phi(x) = 0$, at $x > \frac{a}{2}$ or $x < -\frac{a}{2}$

in $-\frac{a}{2} < x < \frac{a}{2}$ $V=0$: $\frac{\partial^2\phi}{\partial x^2} + \frac{2m}{\hbar^2}E\,\phi = 0$

$$\Rightarrow \begin{cases} \phi(x) = A\sin(kx + \varphi) \\ k = \sqrt{\frac{2mE}{\hbar^2}} \end{cases}$$

$$\phi(x) = \begin{cases} 0 & x < -\frac{a}{2},\ x > \frac{a}{2} \\ A\sin(kx+\varphi) & -\frac{a}{2} < x < \frac{a}{2} \end{cases} \xrightarrow{\text{continous}} \begin{cases} A\sin(\frac{ka}{2}+\varphi) = 0 \\ A\sin(-\frac{ka}{2}+\varphi) = 0 \end{cases}$$

$A \neq 0$

$A\sin(kx+\varphi)$ $\quad -\frac{a}{2}<x<\frac{a}{2}$ $\quad \left\{ A\sin(-\frac{ka}{2}+\varphi)=0 \right.$

$A\neq 0$

$\pm k\frac{a}{2}+\varphi = n\pi$, $n=0,\pm1,\pm2,\dots$ $n\in\mathbb{Z}$

$\Rightarrow \boxed{ka = l\pi}$ $\quad k\frac{a}{2}+\varphi = n\pi$, $-\frac{ka}{2}+\varphi = n'\pi$

$\ominus$ ↳ $ka = (n-n')\pi = l\pi$

$k = \sqrt{\frac{2mE}{\hbar}} = \frac{l\pi}{a}$, $l\in\mathbb{Z}$

$\Rightarrow \boxed{E = \frac{l^2\pi^2\hbar^2}{2ma^2}}$, $l^2 = 1, 2, \dots$

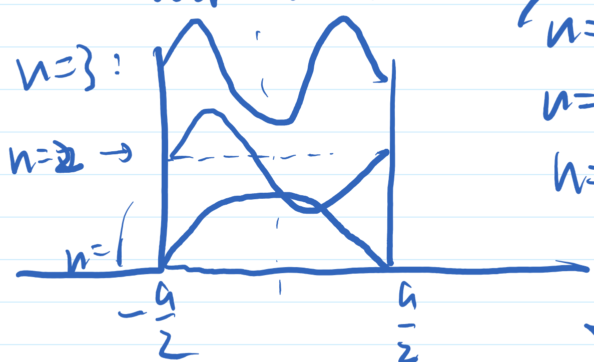
$\left\{ 2\varphi = (n+n')\pi \right.$ ↳ φ = half int. $\times \pi$

↳ notice ka & 2φ are both even or both odd.

$l \leftrightarrow n$ $\quad E = \frac{n^2\pi^2\hbar^2}{2ma^2}$,

$$\phi(x) = A\sin(kx+\varphi) = A\cos(kx) = A\cos\left(\frac{n\pi}{a}x\right)$$

now sketch wavefunction → ground state



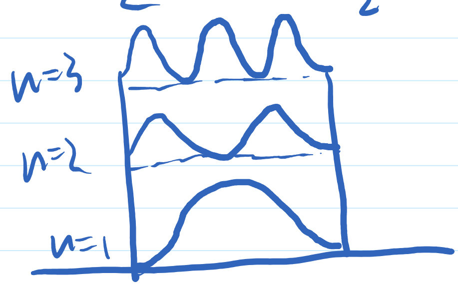
$n=1$, $\phi_1(x) = A_1\cos(\frac{\pi}{a}x)$

$n=2$, $\phi_2(x) = A_2\sin(\frac{2\pi}{a}x)$

$n=3$, $\phi_3(x) = A_3\cos(\frac{3\pi}{a}x)$

$\left\{ \int_{-\infty}^{+\infty} \phi_n^* \phi_m \, dx = 0 \right.$ if $n\neq m$.

$|\phi(x)|^2$



$$\phi(x) = A\sin\left(k(x+\frac{a}{2})+\varphi\right)$$

$\left\{ \begin{array}{l} \phi(\frac{a}{2}) = 0 \\ \phi(-\frac{a}{2}) = 0 \end{array} \right. \Rightarrow$ $A\sin(\varphi) = 0 \Rightarrow \varphi = n\pi$; $\quad A\sin(ka+\varphi) = 0 \Rightarrow ka = m\pi$.

$\phi(x) = A\sin\left(k(x+\frac{a}{2})\right)$ at $-\frac{a}{2}<x<\frac{a}{2}$

$$\boxed{\begin{cases} \phi(x) = A\sin\left(k\left(x+\frac{a}{2}\right)\right) \\ k = \frac{n\pi}{a}, \ n \in \mathbb{N}, \quad E = \frac{n^2\pi^2\hbar^2}{2ma^2} \end{cases}}$$ at $-\frac{a}{2} < x < \frac{a}{2}$

$\phi(x) = 0$ outside.

physical $\phi(x)$, $\int_{-\infty}^{+\infty} |\phi(x)|^2 dx = 1$

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} \underline{|A|^2} \sin^2\left(kx + \frac{ka}{2}\right) dx = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

$$\phi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} + \frac{ka}{2}\right), & -\frac{a}{2} < x < \frac{a}{2} \\ 0 & \text{outside.} \end{cases}$$

$\phi(x)\underline{e^{i\phi}}$ this constant $e^{i\phi}$ won't change any physical result, as well as the Schrödinger's equation.

show orthonormal condition.

$$\int_{-\infty}^{+\infty} dx \, \phi_n^*(x) \phi_m(x) = \int_{-\frac{a}{2}}^{\frac{a}{2}} dx \, \sqrt{\frac{2}{a}} \underline{\sin}\left(\frac{n\pi x}{a} + \frac{ka}{2}\right) \underline{\sin}\left(\frac{m\pi x}{a} + \frac{ka}{2}\right)$$

$= 0$, if $m \neq n$.

$$\boxed{\sin(\eta)\sin(\xi) = \frac{1}{2}\left(\cos(\eta-\xi) - \cos(\eta+\xi)\right)}$$

$\eta = \frac{\pi}{2}, \xi = 0$

$\eta = \frac{\pi}{2}, \xi = \frac{\pi}{2}$ $\quad \frac{1}{2}(1 - (-1)) = 1$ ✓

$\{\phi_n(x)\}$ form a basis. $\Leftarrow$ Hilbert space

we can expand a function

$$\psi(x) = \sum_i c_i \underline{\phi_i(x)}$$

If $\psi(x)$ is within this Hilbert space if $\psi(x)$ is within this Hilbert space

$\Rightarrow \psi(\pm\frac{a}{2}) = 0, \quad \psi(x > \frac{a}{2}, x < -\frac{a}{2}) = 0$