# 20190326, Ch2 Quantum Dynamics

Tuesday, March 26, 2019 2:48 PM

HW: Sakurai 2.14, 2.22

Recap:

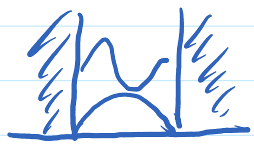
Postulates of QM

Ch2 Quantum Dynamics

§1. Time evolution and H

§2. Static Schrödinger's equation

① 1-D infinitely deep square well




$$\begin{cases} E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2} \\ \phi_n = \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{n\pi}{a}\left(x+\dfrac{a}{2}\right)\right), \quad n=1,2,\cdots \end{cases}$$

note: degeneracy? sign?

$\phi_n = -\phi_{-n} = e^{i\pi}\phi_{-n}$

physically $\phi_n$ is the same as $\phi_{-n}$.

if we have $\psi = e^{i\phi}\psi'$, we treat them to be the same.

$|\psi\rangle = e^{i\phi}|\psi'\rangle$, $\phi$ is a constant

observable $A$, $\langle A\rangle = \langle\psi|A|\psi\rangle$

$= \langle\psi'|A|\psi'\rangle$

$\{|a_i\rangle\}$ : $|\psi\rangle = \sum_i c_i|a_i\rangle$, $P_i = |c_i|^2$

$|\psi'\rangle = \sum_i c_i e^{i\phi}|a_i\rangle$, $P_i = |c_i|^2$

$\boxed{\text{we always throw out overall phase}}$.

(we always throw out overall phase).

- potential barrier and probability flux

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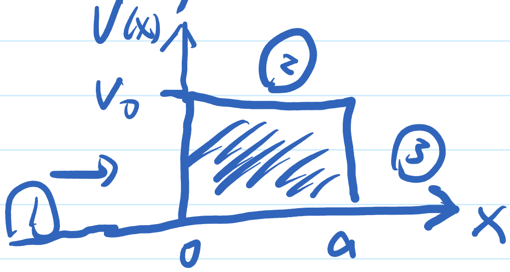



$$V(x) = \begin{cases} 0 & x<0,\ x>a \\ V_0 & 0<x<a \end{cases}$$

$x<0$ $\quad \psi_1(x) = A_1 e^{ikx} + B_1 e^{-ikx}$

$$\begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x) \\ k = \sqrt{\frac{2mE}{\hbar^2}} \quad \checkmark \end{cases}$$

$x<0$, $V=0$ $\qquad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$

$$\psi''(x) + k^2\psi(x) = 0$$

$x>a$ $\quad \psi_3(x) = A_3 e^{ikx} + B_3 e^{-ikx}$

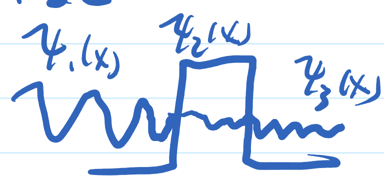
$0<x<a$, $V=V_0$ $\qquad -\frac{\hbar^2}{2m}\psi'' + V_0\psi = E\psi$

$$k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

① case 1. if $E>V_0$ $\quad k'$ real.

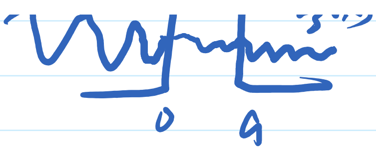
② case 2. if $E<V_0$ $\quad k'$ imaginary

$$\psi_2(x) = A_2 e^{ik'x} + B_2 e^{-ik'x}$$




continuous $\psi_1(x=0) = \psi_2(x=0)$

continuous $\begin{cases} \psi_1(x=0) = \psi_2(x=0) \\ \psi_2(x=a) = \psi_3(x=a) \end{cases}$




$$\Rightarrow \boxed{\begin{cases} A_1 + B_1 = A_2 + B_2 \\ A_2 e^{ik'a} + B_2 e^{-ik'a} = A_3 e^{ika} + B_3 e^{-ik'a} \end{cases}}$$

$\psi'(x)$ should also be continuous

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x).$$

do an integral between $x_0 \pm \epsilon$, $\epsilon$ is a small number.

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\psi'(x_0+\epsilon) - \psi'(x_0-\epsilon)\right) + \underbrace{\int_{x_0-\epsilon}^{x_0+\epsilon} dx\, V(x)\psi(x)}_{\to 0}$$

$$= E\underbrace{\int_{x_0-\epsilon}^{x_0+\epsilon} \psi(x)\, dx}_{\to 0}.$$

since $\psi(x)$ is finite, $\int_{x_0-\epsilon}^{x_0+\epsilon} \psi(x)\, dx \to 0$

$V(x)\psi(x)$ also finite

$$\Rightarrow \boxed{\begin{array}{l} \psi'(x_0+\epsilon) = \psi'(x_0-\epsilon) \\ \text{if } V(x) \text{ is finite} \end{array}}$$

$$\Rightarrow \psi_1'(0) = \psi_2'(0),\ \psi_2'(a) = \psi_3'(a)$$

$$\Rightarrow \begin{cases} ikA_1 - ikB_1 = ik'A_2 - ik'B_2 \\ ik'A_2 e^{ik'a} - ik'B_2 e^{-ik'a} \end{cases}$$

$$\boxed{ik' A_2 e^{ik'a} - ik' B_2 e^{-ik'a} = ik A_3 e^{ika} - ik B_3 e^{-ika}}$$

$$\begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik' & -ik' \end{pmatrix}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix}$$

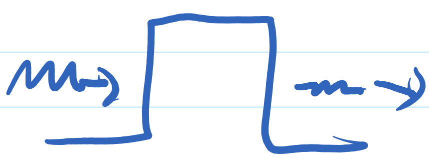
$$\underbrace{\begin{pmatrix} e^{ik'a} & e^{-ik'a} \\ ik' e^{ik'a} & -ik' e^{-ik'a} \end{pmatrix}}_{M_3}\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = \underbrace{\begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{ika} & -ike^{-ika} \end{pmatrix}}_{M_4}\begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$$

$$M_1 = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}, \quad M_2 = \begin{pmatrix} 1 & 1 \\ ik' & -ik' \end{pmatrix}$$

$$M_1 \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M_2 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad M_3 \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M_4 \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$$

$$M_2^{-1} M_1 \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M_3^{-1} M_4 \begin{pmatrix} A_3 \\ B_3 \end{pmatrix}$$

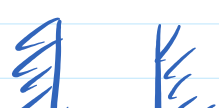
$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \underbrace{M_4^{-1} M_3 M_2^{-1} M_1}_{\text{transformation matrix.}} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$



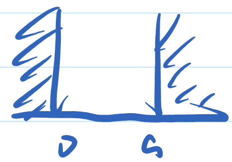
{ tunneling if $E < V_0$

## §3. 1D Harmonic Oscillator.

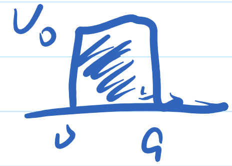
$$V(x) = \begin{cases} \infty & x<0,\ x>a \end{cases} \Rightarrow$$



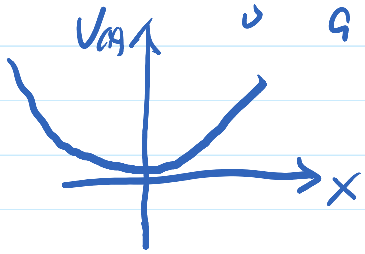
$$V(x) = \begin{cases} \infty & x<0,\ x>a \\ V_0 & 0<x<a \end{cases} \Rightarrow$$



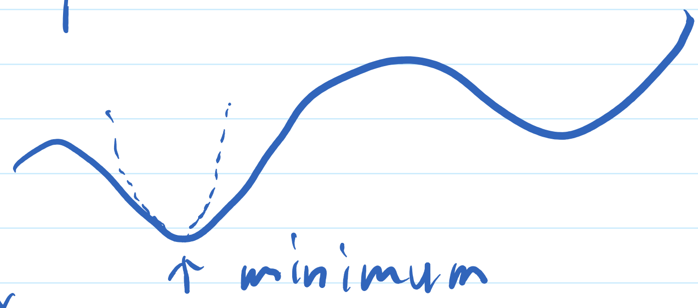
$$V(x) = \begin{cases} 0 & x<0,\ x>a \\ V_0 & 0<x<a \end{cases}$$



$$V(x) = \frac{1}{2}kx^2, \quad k>0$$



for a general potential



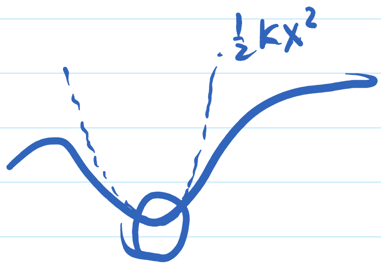
at minimum $x = x_0$

for a general potential

$$V(x) = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 \cdots$$

at minimum $V'(x_0) = 0$

$$V(x) = \underbrace{V(x_0)}_{\text{offset}} + \frac{1}{2}V''(x_0)(x-x_0)^2 + O(x-x_0)^3.$$



1D Harmonic oscillator

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

$k = m\omega^2$

① $\hat{p} \leftrightarrow -i\hbar \frac{\partial}{\partial x} \Rightarrow -\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2 x^2 \psi(x)$
$= E\psi(x)$

solving this eq. gives $\psi(x)$
but it is complicated.

② observe structure of $H$

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2$$

$\begin{cases} a^2 + b^2 = (a+ib)\cdot(a-ib) \leftarrow \text{classical cas} \\ \text{if } a, b \text{ are real numbers.} \end{cases}$

$$H \overset{?}{=} \underline{\left(-i\frac{\hat{p}}{\sqrt{2m}} + \sqrt{\frac{1}{2}m\omega^2}\,\hat{x}\right)\left(i\frac{\hat{p}}{\sqrt{2m}} + \sqrt{\frac{1}{2}m\omega^2}\,\hat{x}\right)}$$

$$= \frac{\hat{p}^2}{2m} \underline{- i\frac{\hat{p}}{\sqrt{2m}}\sqrt{\frac{1}{2}m\omega^2}\,\hat{x} + \sqrt{\frac{1}{2}m\omega^2}\,\hat{x}\left(i\frac{\hat{p}}{\sqrt{2m}}\right)}$$
$$+ \frac{1}{2}m\omega^2\hat{x}^2$$

$$-i\frac{1}{2}\omega\underbrace{[\hat{p},\hat{x}]}_{-i\hbar} = -\frac{\hbar\omega}{2}$$

$$= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \frac{\hbar\omega}{2}$$

define $\hat{a} = \frac{1}{\sqrt{\hbar\omega}}\left(i\frac{\hat{p}}{\sqrt{2m}} + \sqrt{\frac{1}{2}m\omega^2}\,\hat{x}\right)$, $\hat{a}^+ = \left(-i\frac{\hat{p}}{\sqrt{2m}} + \sqrt{\frac{1}{2}m\omega^2}\,\hat{x}\right)\frac{1}{\sqrt{\hbar\omega}}$

$\hbar\omega\,\hat{a}^+\hat{a} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \frac{\hbar\omega}{2} = \hat{H} - \frac{\hbar\omega}{2}$

$$\hbar\omega\hat{a}^{+}\hat{a} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \frac{\hbar\omega}{2} = \hat{H} - \frac{\hbar\omega}{2}$$

$$\Rightarrow \quad \hat{H} = \hbar\omega a^{+}a + \frac{\hbar\omega}{2} = \hbar\omega(\hat{a}^{+}a + \frac{1}{2})$$

since $\underbrace{[\hat{H}] = [\hbar\omega]}_{\text{unit}}$, this definition

makes $\hat{a}$, $\hat{a}^{+}$ to be unitless 无量纲

$$[a, a^{+}] = \frac{1}{\hbar\omega}\left[ i\frac{\hat{p}}{\sqrt{2m}} + \sqrt{\frac{1}{2}m\omega^2}\hat{x}, -i\frac{\hat{p}}{\sqrt{2m}} + \sqrt{\frac{1}{2}m\omega^2}\hat{x} \right]$$

$$= \frac{-i}{2\hbar}\left( [\hat{x}, \hat{p}] - [\hat{p}, x] \right) = 1$$

$\boxed{[\hat{a}, \hat{a}^{+}] = 1}$ $\longleftrightarrow$ in analog of $[\hat{x}, \hat{p}] = i\hbar$

also since $\hat{H} = \hbar\omega(\hat{a}^{+}\hat{a} + \frac{1}{2})$

$$[\hat{H}, a] = -\hbar\omega a. \checkmark \quad [\hat{H}, \hat{a}^{+}] = \hbar\omega a^{+}.$$

$$[\hat{H}, a] = [\hbar\omega(a^{+}a + \tfrac{1}{2}), a]$$

$$= \hbar\omega \underbrace{[a^{+}a, a]} = -\hbar\omega a.$$

$aa^{+} - a^{+}a = 1$

$[a, a^{+}] = 1 \leftarrow aa^{+} = 1 + a^{+}a$

$$a^{+}aa - \underline{aa^{+}}a \Longrightarrow a^{+}aa - (1 + a^{+}a)a$$

$$= \cancel{a^{+}aa} - a - \cancel{a^{+}aa}$$

$$= -a$$

$$[\hat{x}, \hat{p}] = i\hbar \longrightarrow xp - px = i\hbar$$

$$xp = i\hbar + px$$

recap. $\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$

$$[\hat{a}, \hat{a}^\dagger] = \mathbb{1}$$

$$[\hat{H}, \hat{a}] = -\hbar\omega\hat{a}, \quad [\hat{H}, a^\dagger] = \hbar\omega a^\dagger.$$

now try to solve S-eq.

$H|u\rangle = E|u\rangle \leftarrow$ we have $|u\rangle$ eigenstate

apply $\hat{a}$ on both side $\qquad E$ energy

$$\underline{aH|u\rangle} = Ea|u\rangle$$

left $\quad [H, a] = -\hbar\omega a \Rightarrow Ha - aH = -\hbar\omega a$

we have $\quad aH = Ha + \hbar\omega a.$

$$\Rightarrow (Ha + \hbar\omega a)|u\rangle = Ea|u\rangle$$

$$\underline{Ha|u\rangle = (E - \hbar\omega)a|u\rangle}.$$

$\uparrow$ $a|u\rangle$ also an eigenstate

$E - \hbar\omega$ is eigenenergy.

$\Big\{$ applying $\hat{a}$ on $|u\rangle$ lowers the energy by $\hbar\omega$. but the state remains eigenstate.

$\hat{a}$ : annihilating operator 湮灭算符.

lowering operator.

$\hat{a}^{+}$ increasing energy by $\hbar\omega$.

creating operator

or raising operator