Simple Applications III

Lecture 5: Simple Problems in 1d

solve: $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ in most convenient representation, e.g. $|r\rangle$

$$H_r \psi_n(r) = E_n \psi_n(r) \;; \quad H_r = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

require continuity of $\psi(x)$ & $\psi'(x)$ for finite $V(x)$ only.

Simple examples:

(a) $\boxed{\text{free particle}, \; V(x) = 0}$

$$\Rightarrow \; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) = E_n \psi_n(x)$$

$$\Rightarrow \; \psi_k(x) = A e^{ikx} \,, \quad E_k = \frac{\hbar^2 k^2}{2m}$$

A - normalization determined by putting a system in a box of size L.

$$1 = \int_{-L/2}^{L/2} dx\, A^2 \;\Rightarrow\; A = \frac{1}{\sqrt{L}}$$

(... more carefully, in a box with periodic b.c.

$$e^{ikL} = 1 \Rightarrow k_n = \frac{2\pi}{L} n$$

$$\sum_k \psi_k^*(x)\psi_k(x') = \sum_{k_n} \frac{1}{L} e^{ik_n(x-x')} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')}$$

$$= \delta(x-x') \; \checkmark \;)$$

relation to $U(x, x', t)$ convolution:

$$\psi(x,t) = \int dx' \; U(x, x'; t)\, \psi(x', 0)$$

$$= \int_{x'} \langle x | \hat{U}_{(t)} | x' \rangle \langle x' | \psi(0) \rangle$$

$$= \int_{x'} \varphi_E(x)\, \varphi_E^*(x')\, e^{-\frac{i}{\hbar} E t}\, \psi(x', 0)$$

$$\langle x | \psi(x,t) \rangle = \sum_E \langle x | E \rangle\, e^{-\frac{i}{\hbar} E t} \langle E | \psi(0) \rangle$$

$$| \psi(x,t) \rangle = \sum_E | E \rangle \langle E | \psi(0) \rangle\, e^{-\frac{i}{\hbar} E t}$$

More formally: $\hat{H} = \frac{\hat{p}^2}{2m}$

$\Rightarrow \hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \Rightarrow \frac{\hat{p}^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle$

where $\hat{p}|p\rangle = p|p\rangle$

$|E_p\rangle = |\pm\sqrt{2mE}\rangle \leftarrow$ 2 states $\pm p_E$ for every E.

recall for free particle:

$$U(x,t;x',0) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')^2/2\hbar t}$$

Evolution of $\psi(x',0) = e^{i\frac{p_0}{\hbar}x'} \frac{e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/2}}$
gaussian wave packet

$\Rightarrow$ see hw2.

$$\psi(x,t) = \left[\pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)\right]^{-1/2} e^{-\frac{(x-p_0t/m)^2}{2\Delta^2(1+i\hbar t/m\Delta^2)}} \times e^{i\frac{p_0}{\hbar}x - i\frac{p_0^2}{2m}t/\hbar}$$

$$\Rightarrow \langle X\rangle = \frac{p_0 t}{m} = \frac{\langle\hat{p}\rangle}{m}t$$

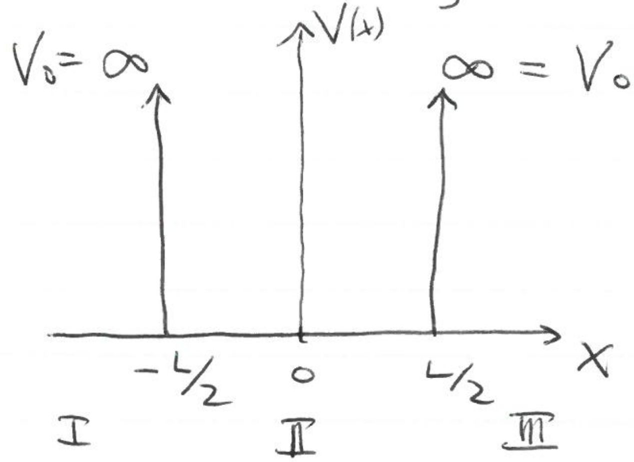
$$\langle\delta X(t)\rangle = \frac{\Delta(t)}{\sqrt{2}} = \frac{\Delta}{\sqrt{2}}\left(1+\frac{\hbar^2t^2}{m^2\Delta^4}\right)^{1/2}$$

Why? $\delta X(0) = \Delta \Rightarrow$ uncertainty grows in time

$\delta p(0) = \frac{\hbar}{\Delta} \Rightarrow \delta X(t) \sim \frac{\hbar}{\Delta m}t$ ✓

(b) $\boxed{\text{Particle in a "box" – infinite square poten.}}$

$$V(x) = 0 \quad , \quad |x| < L/2$$
$$= V_0 \to \infty \quad , \quad |x| \geq L/2$$



$\Rightarrow \partial_x \psi(\pm L/2)$ can be discontinuous.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi = 0$$

III. $$\frac{d^2\psi_{III}}{dx^2} - \frac{2m}{\hbar^2}\underbrace{(V_0 - E)}_{\text{large \& } > 0}\psi_{III} = 0$$

$$\Rightarrow \psi_{III} = Ae^{-\kappa x} + Be^{\kappa x}$$

$\Rightarrow \boxed{\psi_{III} = Ae^{-\kappa x} \underset{V_0 \to \infty}{=} 0}$ choose $B = 0$ so that $\psi_{III}(x > L/2)$ finite.

$$\kappa \equiv \sqrt{2m(V_0 - E)/\hbar^2}$$

I. $$\psi_I = Ce^{-\kappa x} + De^{\kappa x}$$

choose $C = 0$ so that $\psi_I(x < -L/2)$ finite

$$\boxed{\psi_I(x) = De^{\kappa x} \underset{V_0 \to \infty}{=} 0}$$

$$\psi_{II}(x) = A e^{ikx} + B e^{-ikx}, \quad k = \sqrt{2mE}/\hbar$$

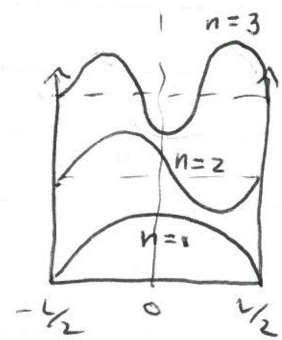
Require continuity of ψ, i.e.

$$\begin{cases} \psi_{II}(x=L/2) = \psi_{III}(x=L/2) = 0 \\ \psi_{II}(x=-L/2) = \psi_{I}(x=-L/2) = 0 \end{cases}$$

leads to energy eigenvalues quantization (c.f. notes/harmonics on a guitar string)

$$A e^{-ikL/2} + B e^{ikL/2} = 0$$

& $$A e^{ikL/2} + B e^{-ikL/2} = 0$$



$$\det\begin{pmatrix} e^{-ikL/2} & e^{ikL/2} \\ e^{ikL/2} & e^{-ikL/2} \end{pmatrix} = \sin kL = 0$$

$\sin kL = 0 \Rightarrow$ $k_n = n\pi/L, \quad n \in \mathbb{Z}.$

$$A = -e^{i\pi n} B = (-1)^n B$$

$$\Rightarrow \psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\frac{n\pi x}{L}, \quad n \text{ even} > 0$$

$$= \left(\frac{2}{L}\right)^{1/2} \cos\frac{n\pi x}{L}, \quad n \text{ odd} > 0$$

only positive as $n < 0$ are not distinct

($n=0$, boring since $\psi_0 = 0$)

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

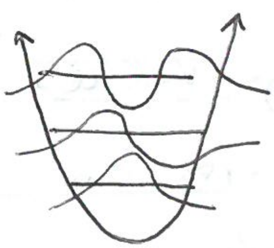
Note: in system with origin at $x=0 \Rightarrow$ (see Exerc. 5.2.5 Shankar pg 164)

$$\psi_n = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right), \quad n = 1, 2, 3, \ldots$$

• "crude" soln of S. Eqn.:

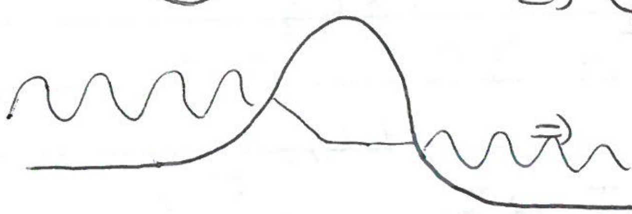
balance $\underbrace{-\frac{\hbar^2 \nabla^2}{2m}\psi \text{ with } V\psi}$ with $E\psi$

Three classes of $V(x)$ probs

• 

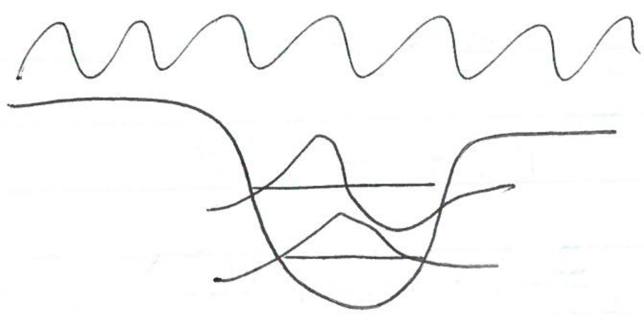
$\Rightarrow$ only discrete spectrum, since $V(x \to \pm\infty) \to \infty$

$\Rightarrow \psi(x \to \pm\infty) \to 0$

• 

$\Rightarrow$ only continuum spectrum.

$\psi(x \to \pm\infty)$ oscillates.

• 

$\Rightarrow$ discrete & continuum set of states.

- All eigenvalues are discrete, all <u>states</u> are <u>bound</u> $\rightarrow$ since $V_0 \rightarrow \infty$

  more generically a range of discrete E_n's for each bound state & for $E > E_n^{max}$ continuous spectrum
  $\simeq V_0$

- n counts # of nodes in $\psi_n(x)$
  higher n $\rightarrow$ higher k $\rightarrow$ higher E_k

- lowest $E_{n=1} = \dfrac{\hbar^2 \pi^2}{2mL^2} \Leftrightarrow \begin{cases} \delta p \sim \dfrac{\hbar}{L} \\ \delta x \sim L. \end{cases}$
  uncertainty principle

- energy discretization comes from b.c. of continuity of ψ, ψ' that is only possible at discrete set of energies E_n.

- in 1d E uniquely labels states, i.e. no degeneracy (almost $E \Rightarrow \pm p = \pm\sqrt{2mE}/\hbar$) for bound states.

- in 1d (& 2d) bound state for arbitrarily weak attractive potential. (see HW3)

▲ expect this physically $E = \dfrac{p^2}{2m}$ $\rightarrow$ in 1d no other d.o.f. for point particle.

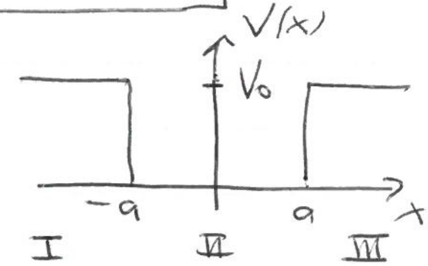
▲ $-\dfrac{\hbar^2}{2m}\psi_1'' + V\psi_1 = E\psi_1$
$-\dfrac{\hbar^2}{2m}\psi_2'' + V\psi_2 = E\psi_2$ $\Rightarrow$

$(\psi_2\psi_1' - \psi_1\psi_2')' = 0 \Rightarrow \psi_1\psi_2' - \psi_2\psi_1' = c = 0$ if $\psi_1 = 0$ at $\pm\infty$.

$\Rightarrow \underline{\psi_1 = A\psi_2}$

(c) $\boxed{\text{Finite square-well potential } V(x):}$

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

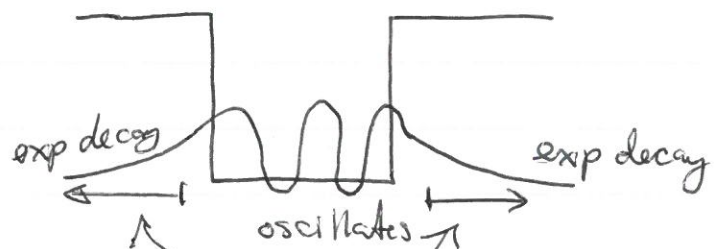


$\boxed{\text{Bound states : } E < V_0 .}$

- $$\left.\begin{aligned} \psi_I &= C e^{+\kappa x} , \\ \psi_{III} &= D e^{-\kappa x} \end{aligned}\right\} \quad \kappa = \sqrt{2m(V_0 - E)}/\hbar > 0$$

$$\psi_{II} = A e^{ikx} + B e^{-ikx} = \tilde{A} \sin kx + \tilde{B} \cos kx .$$
$$k = \sqrt{2mE}/\hbar$$

- qualitatively



leaks/tunneling into classically forbidden region.

- match at $\pm a = x$, requiring continuity of ψ, ψ'.

(i) $\psi_I(-a) = \psi_{II}(-a)$ $\quad Ce^{-\kappa a} = -\tilde{A} \sin ka + \tilde{B} \cos ka$

(ii) $\psi_I'(-a) = \psi_{II}'(-a)$ $\iff +\kappa C e^{-\kappa a} = \tilde{A} k \cos ka + \tilde{B} k \sin ka$

(iii) $\psi_{II}(a) = \psi_{III}(a)$ $\quad De^{-\kappa a} = \tilde{A} \sin ka + \tilde{B} \cos ka$

(iv) $\psi_{II}'(a) = \psi_{III}'(a)$ $\quad -\kappa D e^{-\kappa a} = \tilde{A} k \cos ka - \tilde{B} k \sin ka$

4 eqns, <u>3</u> unknown coefficients (ratios, since linear homogeneous) + 1 unknown energy E $\rightarrow$ eigenvalues!

$$
\left.\begin{aligned}
&\left.\begin{aligned}
Ce^{-\kappa a} &= -A\sin ka + B\cos ka \\
De^{-\kappa a} &= A\sin ka + B\cos ka
\end{aligned}\right] \text{(drop} \sim) \\
&\left.\begin{aligned}
C\kappa e^{-\kappa a} &= Ak\cos ka + Bk\sin ka \\
-D\kappa e^{-\kappa a} &= Ak\cos ka - Bk\sin ka
\end{aligned}\right]
\end{aligned}\right\} \det = 0 \Rightarrow \text{messy!}
$$

2 types of solns: (a) $C = D$ and $A = 0$

(b) $C = -D$ and $B = 0$

why? Parity is a good quantum #:

$$V(x) = V(-x) = P[V(x)]$$

P sends $x \to -x$

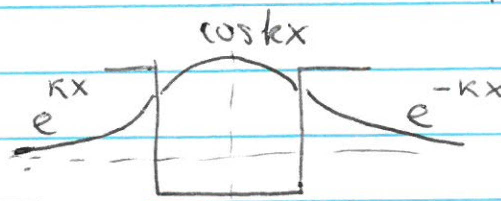
$[P, H] = 0 \Rightarrow \psi$ eigenfnc of H & P

$P\psi = \epsilon\psi$, but $P^2 = 1 \Rightarrow \epsilon = \pm 1$

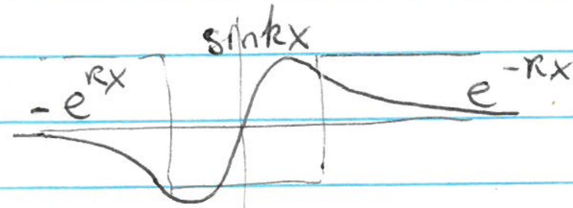
$\Rightarrow \psi(x) = \pm\psi(-x) \to \psi_{odd}(x) = -\psi_{odd}(-x)$

$\psi_{even}(x) = \psi_{even}(-x)$

ψ_{even}:



ψ_{odd}:



$\Rightarrow$ only need to look at $x > 0$

$$\psi_{even} = \begin{cases} B\cos kx, & 0 < x \le a \\ De^{-\kappa x}, & a < x \end{cases}$$

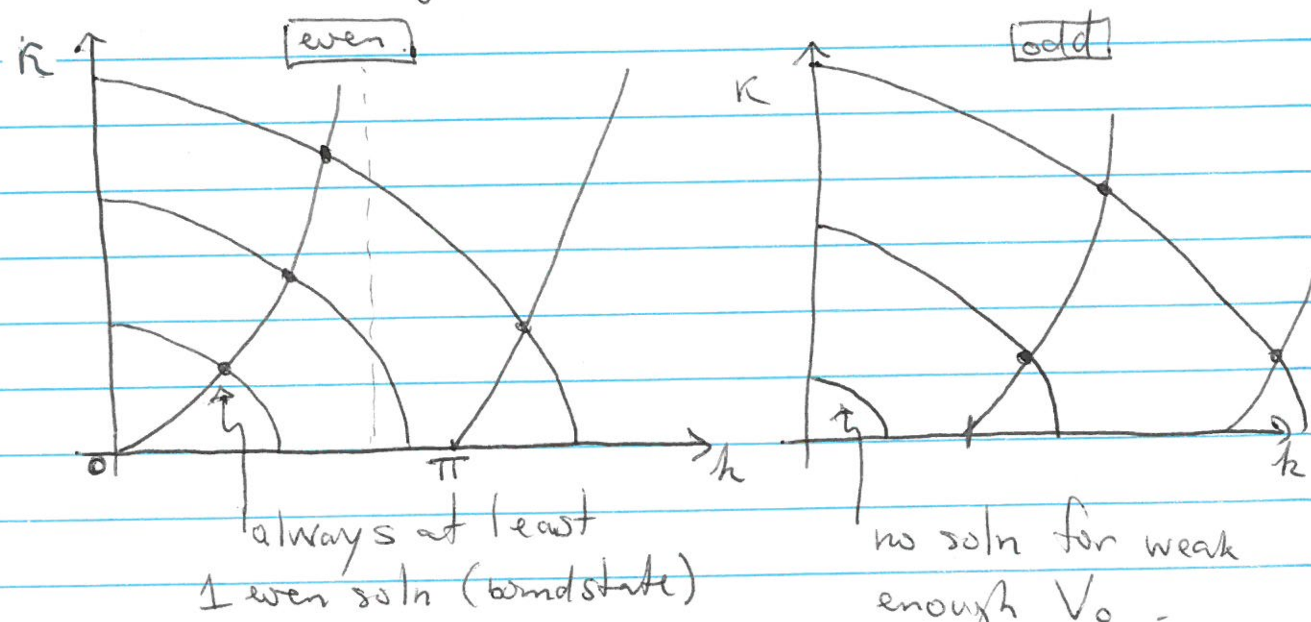
$$\Rightarrow \quad \begin{aligned} B\cos ka &= De^{-\kappa a} \\ -Bk\sin ka &= -D\kappa e^{-\kappa a} \end{aligned} \quad \Rightarrow \quad \boxed{k\tan ka = \kappa}$$

$$\psi_{odd} = \begin{cases} A\sin kx, & 0 < x \le a \\ De^{-\kappa x}, & a < x \end{cases}$$

$$\Rightarrow \quad \begin{aligned} A\sin ka &= De^{-\kappa a} \\ Ak\cos ka &= -D\kappa e^{-\kappa a} \end{aligned} \quad \Rightarrow \quad \boxed{k\cot ka = -\kappa}$$

Note: $k^2 + \kappa^2 = \frac{2mV_0}{\hbar^2}$

$\Rightarrow$ intersections of circle & $k\tan ka = \kappa$ or $k\cot ka = -\kappa$ for even & odd eigenfncs.



$\Rightarrow$ even groundstate, always at least 1 bound state.

What happens to soln's for $V = \infty$, $x < 0$
$V = 0$, $0 < x < a$, $V = V_0$, $x > a$?

<u>Note:</u> • $V_0 \to \infty$, $\kappa \to \infty$

$\Rightarrow$ even solns: $k \tan ka = \kappa \to \infty$
(cos kx)

$$\Rightarrow ka = \frac{\pi}{2}(2n+1) \Rightarrow k = \frac{\pi}{2a}(2n+1)$$

$$k = \frac{\pi}{L}(2n+1) \checkmark$$

$\Rightarrow$ odd solns: $k \cot ka \to -\infty$
(sin kx)

$$\Rightarrow ka = \pi(1+n) \Rightarrow k = \frac{\pi}{a}(n+1)$$

$$k = \frac{\pi}{L} 2(n+1) \checkmark$$

• Always bound state (at least one) even soln!

$\boxed{\text{Continuum states.}}$

$\boxed{\text{even}}$ for $x>0$: $\psi_{II}^{>} = \cos kx$, $\psi_{III}^{>} = C \sin k'x + D \cos k'x$ $= A\cos(k'x+\delta)$

$$k = \sqrt{2mE}/\hbar, \quad k' = \sqrt{2m(E-V_0)}/\hbar$$

$$\left.\begin{aligned} \cos ka &= C \sin k'a + D \cos k'a \\ -k \sin ka &= C k' \cos k'a - D k' \sin k' \end{aligned}\right\}$$

2 eqns, 2 unknowns
C, D $\Rightarrow$ k $\not\Rightarrow$ E
<u>unconstrained</u>
$\Rightarrow$ continuum.

(Note: for $x<0$: $\psi_{II}^{<} = \cos kx$, $\psi_{III}^{<} = -C \sin k'x + D \cos k'x$)

$$\underbrace{\begin{pmatrix} \sin k'a & \cos k'a \\ k'\cos k'a & -k'\sin k'a \end{pmatrix}}_{M} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \cos ka \\ -k \sin ka \end{pmatrix}$$

$$\Rightarrow M^{-1} = \begin{pmatrix} \sin k'a & \frac{1}{k'}\cos k'a \\ \cos k'a & -\frac{1}{k'}\sin k'a \end{pmatrix}$$

$$\Rightarrow \boxed{\begin{aligned} C^e &= \cos ka \sin k'a - \frac{k}{k'} \cos k'a \sin ka \\ D^e &= \cos ka \cos k'a + \frac{k}{k'} \sin ka \sin k'a \end{aligned}}$$

$$\left(\frac{D^e}{C^e} = -\cot \delta \right)$$

$\boxed{\text{odd}}$ for $x>0$: $\psi_{II}^{>} = \sin kx$, $\psi_{III}^{>} = C \sin k'x + D \cos k'x$
$= A \sin(k'x + \delta)$

(Note: for $x<0$, $\psi_{II}^{<} = \sin kx$, $\psi_{III}^{<} = C \sin k'x - D \cos k'x$)

$$\begin{pmatrix} \sin k'a & \cos k'a \\ k' \cos k'a & -k' \sin k'a \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \sin ka \\ k \cos ka \end{pmatrix}$$

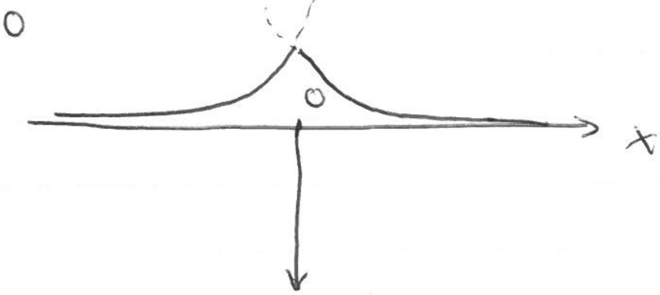
$$\Rightarrow \boxed{\begin{aligned} C^o &= \sin k'a \sin ka + \frac{k}{k'} \cos k'a \cos ka \\ D^o &= \cos k'a \sin ka - \frac{k}{k'} \sin k'a \cos ka \end{aligned}}$$

$$\left(\frac{D^o}{C^o} = \tan \delta \right)$$

Note: wavefn does something "complicated" near $V(x) \neq 0$, but far away just a phase shift.
δ ← key quantity determining scattering of particle by a potential, localized.

(d) $\boxed{\text{Attractive } \delta\text{-fnc potential}}$

$$V_0 = + \frac{U_0}{2a} \underset{a \to 0}{\Rightarrow} - U_0\, \delta(x) = V(x)$$



$\boxed{\text{Bound state(s):}}$

<u>even soln</u>:

$$\psi = \begin{cases} e^{-\kappa x} & , x > 0 \\ e^{\kappa x} & , x < 0 \end{cases} , \quad \underline{E = -\frac{\hbar^2 \kappa^2}{2m}}$$

$$\psi(0) = 1 , \quad \psi'(0\pm) = \mp \kappa$$

$$\int_{-\varepsilon}^{+\varepsilon} \left[-\frac{\hbar^2}{2m} \psi'' - U_0\, \delta(x)\, \psi = E \psi \right]$$

$$\varepsilon \to 0 \quad -\frac{\hbar^2}{2m} \Big(\underbrace{\psi'(0^+)}_{-\kappa} - \underbrace{\psi'(0^-)}_{\kappa} \Big) - U_0 \underbrace{\psi(0)}_{1} = 2E\varepsilon\, \psi(0) = 0$$

$$\frac{\hbar^2}{m} \kappa = U_0 \Rightarrow \boxed{\kappa = \frac{m U_0}{\hbar^2}}$$

$$\boxed{E = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{m U_0^2}{2\hbar^2}}$$

<u>odd soln</u>: $\quad \psi_{odd}(x)\, \delta(x) = \psi_{odd}(0)\, \delta(x) = 0$

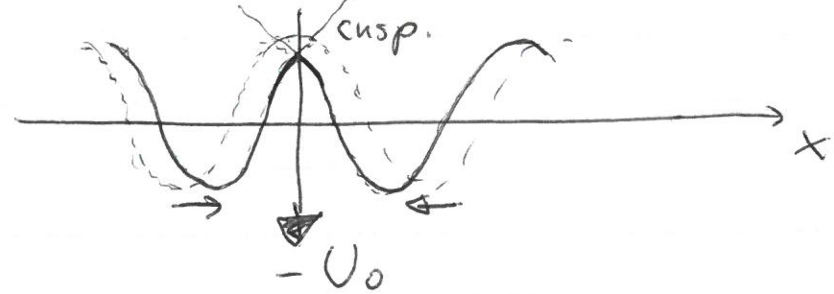
$\Rightarrow$ odd soln do not "see" $V(x) = -U_0\, \delta(x)$

$\Rightarrow$ unmodified free $\Rightarrow$ $\boxed{\psi_{odd}(x) = \sin kx}$
continuum.

Continuum states:

odd: $\psi_k^{odd}(x) = \sin kx$, $E = \dfrac{\hbar^2 k^2}{2m}$

even:



$$\psi^>(x>0) = \cos(kx+\delta) \;,\; \psi^<(x<0) = \cos(kx-\delta)$$
$$(= \psi^>(x \to -x))$$

$$\psi'_>(0^+) = -k\sin\delta \;,\; \psi'_<(0^-) = k\sin\delta$$

$$-\frac{\hbar^2}{2m}\big(\underbrace{\psi_>'(0^+) - \psi_<'(0^-)}_{-2k\sin\delta}\big) - U_0\cos\delta = 0$$

$$\boxed{\frac{\hbar^2 k}{m U_0} = \cot\delta} \equiv \left(k a_s \;,\; \Rightarrow a_s = \frac{\hbar^2}{m U_0} > 0\right)$$

for attractive V(x)

Compare to finite-size well $V_0 = \dfrac{U_0}{2a} \to \infty,\ a \to 0$

$$E = \underset{\substack{\uparrow \\ \text{finite.}}}{\frac{\hbar^2 k'^2}{2m}} = \underset{\uparrow\infty}{\frac{\hbar^2 k^2}{2m}} - \underset{\uparrow\infty}{\frac{U_0}{2a}} \Rightarrow \frac{\hbar^2 k^2}{2m} \simeq \frac{U_0}{2a} \to \infty$$

b.e. of bound state.

$$C^e \underset{a\to 0}{\simeq} 0 - \frac{k^2 a}{k'} = -\frac{\frac{\hbar^2 k^2}{m} a}{\frac{\hbar^2 k'}{m}} \overset{= U_0}{=} \boxed{-\frac{U_0}{\left(\frac{\hbar^2 k'}{m}\right)} = C^e}$$

$$D^e \underset{a\to 0}{\simeq} 1 + \underset{\to 0}{\frac{k^2 a}{k'} k' a} \longrightarrow \boxed{D^e = 1}$$

$$\Rightarrow \frac{D^e}{C^e} = -\cot\delta = -\frac{\hbar^2 k'}{m U_0} \Rightarrow \boxed{\cot\delta = \frac{\hbar^2 k'}{m U_0}}$$

Note: $\delta \to 0$ as $U_0 \to 0$

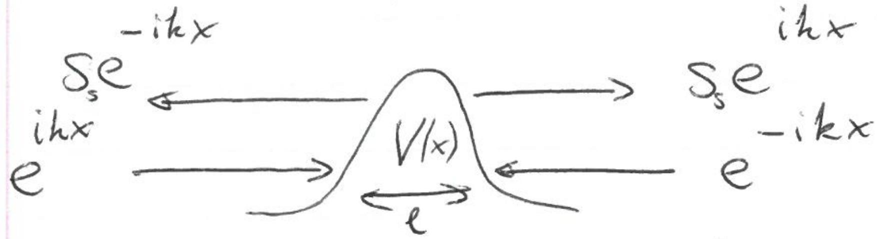
$$C^{\circ} \underset{a\to 0}{\simeq} 0 + \frac{k}{k'} \to \infty , \quad D^{\circ} \underset{a\to 0}{\simeq} 0 - ka \to 0 .$$

$$\Rightarrow \boxed{\psi = \sin kx} \quad \frac{C^{\circ}}{D^{\circ}} = \cot \delta = \infty \Rightarrow \boxed{\delta = 0}$$

General theory of 1d scattering on bounded potential $V(x)$:

even

$$\Psi_e = A\begin{cases}\cos(kx+\delta_s), & x \gg \ell\\ \cos(kx-\delta_s), & x \ll -\ell\end{cases}$$



$$\Psi_e = \frac{A}{2}\begin{cases} e^{-i\delta_s}\left(e^{-ikx} + e^{i2\delta_s} e^{ikx}\right), & x>0\\ e^{-i\delta_s}\left(e^{ikx} + \underbrace{e^{i2\delta_s}}_{\equiv S_s} e^{-ikx}\right), & x<0\end{cases}$$

$$\boxed{S_s = e^{i2\delta_s}}$$

Scattering matrix

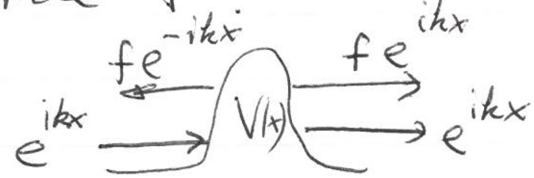
$$\Psi_o = A\begin{cases}\sin(kx+\delta_A), & x \gg \ell\\ \sin(kx-\delta_A), & x \ll -\ell\end{cases}$$

$$\Psi_o = \frac{A}{2i}\begin{cases} -e^{-i\delta_A}\left(e^{-ikx} - e^{i2\delta_A} e^{ikx}\right), & x>0\\ e^{-i\delta_A}\left(e^{ikx} - e^{i2\delta_A} e^{-ikx}\right), & x<0\end{cases}$$

$$\boxed{S_o = e^{i2\delta_A}}$$, odd, even are 1d analogs of ℓ-partial waves of 3d

In terms of scattering amplitude f:

$$\Psi_{scatt} = \begin{cases} e^{ikx} + f_s e^{+ikx} + f_A e^{ikx}, & x>0\\ e^{ikx} + f_s e^{-ikx} - f_A e^{-ikx}, & x<0.\end{cases}$$



$$t = 1 + f_s + f_A, \quad r = f_s - f_A$$

$T = |t|^2 , \quad R = |r|^2$

$$\psi_{scatt} = \begin{cases} t e^{ikx} , & x>0 \\ e^{ikx} + r e^{-ikx} , & x<0 \end{cases}$$

$\downarrow$ construct symm (even) & antisymm (odd) combinations to relates $f_{S/A}$ to $S_{S/A}$

$$\psi_e = \frac{1}{2}\left(\psi_s(x) + \psi_s(-x)\right)$$

$$= \begin{cases} \frac{1}{2}\left(t e^{ikx} + e^{-ikx} + r e^{ikx}\right) , & x>0 \\ \frac{1}{2}\left(e^{ikx} + r e^{-ikx} + t e^{-ikx}\right) , & x<0 \end{cases}$$

$$= \frac{A e^{-i\delta_s}}{2} \begin{cases} e^{-ikx} + S_s e^{ikx} , & x>0 \\ e^{ikx} + S_s e^{-ikx} , & x<0 \end{cases}$$

$$\Rightarrow \boxed{t + r = S_s = 2f_s + 1}$$

$$\psi_o = \frac{1}{2}\left(\psi_s(x) - \psi_s(-x)\right) = \frac{1}{2} \begin{cases} t e^{ikx} - e^{-ikx} - r e^{ikx} , & x>0 \\ e^{ikx} + r e^{-ikx} - t e^{-ikx} , & x<0 \end{cases}$$

$$= \frac{A}{2i} e^{-i\delta_A} \begin{cases} -e^{-ikx} + S_A e^{ikx} , & x>0 \\ e^{ikx} - S_A e^{-ikx} , & x<0 \end{cases}$$

$$\boxed{S_A = t - r = 1 + 2f_A}$$

<u>Note</u>: poles in $S_{S,A}$ with $k = i\kappa$ $(\kappa>0)$ give even/odd bound states

For $V(x) = -U_0\,\delta(x)$

$$\psi_{odd} = \sin kx = (e^{ikx} - e^{-ikx})\frac{1}{2i}$$

$$\Rightarrow S_A = e^{i2\delta_A} = 1 \Rightarrow \boxed{\delta_A = 0,\ f_A = 0.}$$

$$\Rightarrow t = 1 + r$$

$$\psi_{even} = \begin{cases} \cos(kx + \delta_s), & x > 0 \\ \cos(kx - \delta_s), & x < 0 \end{cases}$$

$$\boxed{\cot\delta_s = \frac{\hbar^2 k}{mU_0}} \quad ; \quad k \to 0,\ \delta_s \to \frac{\pi}{2}$$

$$k \to 0,\ \delta_s \to \pi/2^- \Rightarrow \boxed{\delta_s \approx \frac{\pi}{2} - \frac{\hbar^2}{mU_0}k} \ (U_0 > 0)$$

$$f_s = \frac{1}{2}(S_s - 1) = \frac{1}{2}(e^{i2\delta_s} - 1)$$

$$\cot\delta_s = ck \quad \left(c \equiv \frac{\hbar^2}{mU_0}\right)$$

$$i\,\frac{e^{i\delta_s} + e^{-i\delta_s}}{e^{i\delta_s} - e^{-i\delta_s}} = ck \Rightarrow -ick = \frac{e^{i2\delta_s} + 1}{e^{i2\delta_s} - 1} = \frac{S_s + 1}{S_s - 1}$$

$$\Rightarrow (S_s - 1)(-ick) = S_s + 1$$

$$\Rightarrow S_s(1 + ick) = -(1 - ick)$$

$$S_s \equiv e^{i2\delta_s} = -\frac{1 - ick}{1 + ick}$$

$f_s(k \to 0) \to -1$
for all 1d potent.
$\Rightarrow t = 0,\ r = -1$
complete reflection

$$\Rightarrow \boxed{f_s = \frac{1}{2}(S_s - 1) \underset{exact}{=} \frac{1}{-ika - 1}, \quad a \equiv \frac{\hbar^2}{m}\frac{1}{U_0}}$$

a: scattering length.

Note: with this defn U_0 ($V(x) < 0$ attractive), $a > 0$!

<u>Bound states</u>:

$$\psi_e = \begin{cases} e^{-ikx} + S_s e^{ikx}, & x>0 \\ e^{ikx} + S_s e^{-ikx}, & x<0 \end{cases}$$

for special k s.t. $S_s(k_*) \to \infty$ <u>drop</u>

$e^{\mp ikx}$, $x \gtrless 0$ (first term)

require $k_* = +i\kappa$. $(\kappa > 0)$

$$S_s = -\frac{1-iak}{1+iak} \to \infty, \quad \text{for } \underline{k_* = i a^{-1}}$$

$\Rightarrow$ bound state for $\underline{a>0}$, i.e. $\underline{U_0 > 0}$

i.e. attractive potential.

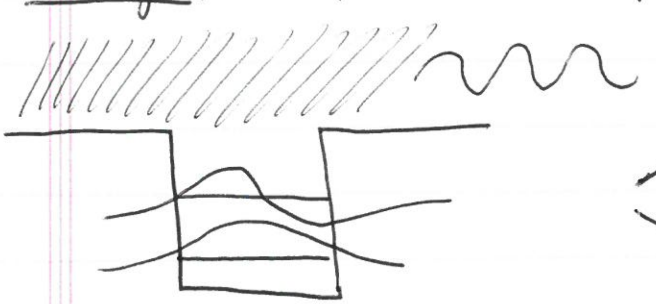
$$\Rightarrow \psi_{bound} = \begin{cases} e^{-x/a}, & x>0 \\ e^{x/a}, & x<0 \end{cases}$$

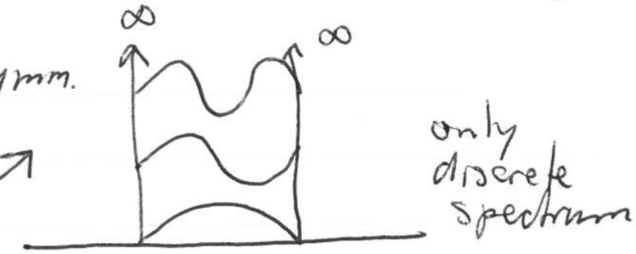
$$\boxed{a = \kappa^{-1} = \frac{\hbar^2}{mU_0}}$$

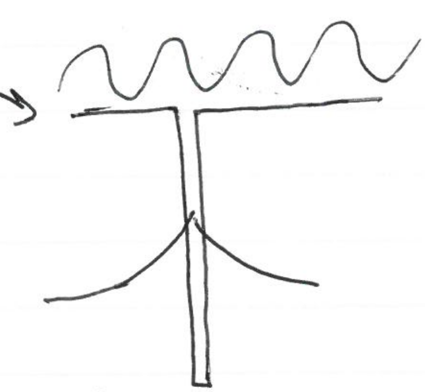
$$\boxed{E_{bound} = \frac{\hbar^2 k^2}{2m} = -\frac{\hbar^2}{2ma^2} = -\frac{mU_0^2}{2\hbar^2}}$$

5.18

Recap: important use of parity symm.







... more generically

special to 1d:

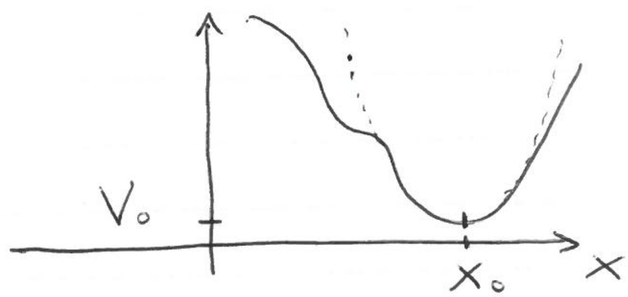
- nondegenerate states if $\psi(x \to \infty) \to 0$
  see proof in Shankar
- bound state (in 1d & 2d) for arbitrarily weak attractive potential (hw3)
- for localized potential $\quad \psi = Ae^{ikx} + Be^{-ikx} = \tilde{A}\cos(kx+\delta)$
  δ – scattering phase shift
  key ingredient in scattering
- crude estimate of spectrum & size of bound states: $\quad E = \frac{p^2}{2m} + V(x)$, $\quad p_n = \frac{\hbar}{x} n$.
  $\frac{\partial E}{\partial x} = 0 \Rightarrow p_n, \; x, \; E(p_n, x) = E_n.$

Lecture 6: Harmonic Oscillator

- one mass

work-horse of theoretical physics.

$$H = \frac{p^2}{2m} + V(x)$$



if $V(x)$ has a minimum at x_0

$$\Rightarrow \quad V(x) \simeq V(x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2$$

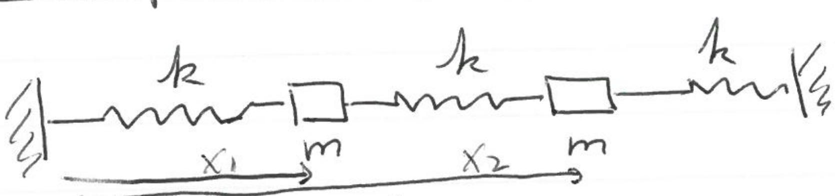
$$\equiv V_0 + \frac{1}{2}k(x-x_0)^2$$

shift origin, drop const.

$$\Rightarrow \underline{H \simeq \frac{p^2}{2m} + \frac{1}{2}kx^2} \quad \leftarrow \text{simple harmonic oscillator.}$$

$$x(t) = A\cos(\omega_0 t + \varphi), \quad \omega_0 = \sqrt{\frac{k}{m}}$$

- two coupled oscillators



$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 + \frac{1}{2}k(x_1-x_2)^2$$

decouple via normal mode analysis via a canonical transformation:

$$T = \frac{p_1^2}{2m} + \frac{p_2^2}{2m}$$

$$V(x_1,x_2) = k(x_1^2+x_2^2) - kx_1x_2$$

$$V(x_1, x_2) = k(x_1^2 + x_2^2) - k x_1 x_2$$

Canon. transf $\rightarrow$ <u>rotation</u> by $\pi/4$

$$\bar{X}_1 = \frac{1}{\sqrt{2}}(X_1 + X_2) \,, \quad \bar{X}_2 = \frac{1}{\sqrt{2}}(X_1 - X_2)$$

$$\begin{pmatrix} \bar{X}_1 \\ \bar{X}_2 \end{pmatrix} = \begin{pmatrix} \cos\pi/4 & \sin\pi/4 \\ -\sin\pi/4 & \cos\pi/4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$x_1^2 + x_2^2 = \bar{X}_1^2 + \bar{X}_2^2$$

$$x_1 x_2 = (\bar{X}_1^2 - \bar{X}_2^2)\frac{1}{2}$$

$$p_1^2 + p_2^2 = \bar{p}_1^2 + \bar{p}_2^2$$

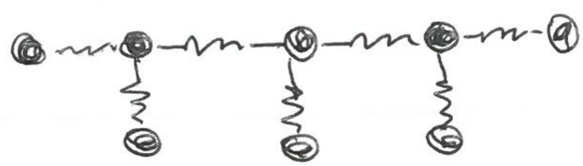
$$H(p, x) \longrightarrow H(\bar{p}, \bar{x}) = \underbrace{\frac{\bar{p}_1^2}{2m} + \frac{1}{2}k\bar{X}_1^2}_{H_1} + \underbrace{\frac{\bar{p}_2^2}{2m} + \frac{3}{2}k\bar{X}_2^2}_{H_2}$$

decoupled into normal modes. $\Leftarrow$

$$\bar{X}_1(t) = \bar{X}_1(0)\, e^{i\omega_1 t} \,, \quad \omega_1 = \sqrt{k/m}$$

$$\bar{X}_2(t) = \bar{X}_2(0)\, e^{i\omega_2 t} \,, \quad \omega_2 = \sqrt{\frac{3k}{m}}$$

- $\boxed{\text{N coupled oscillators}}$ e.g. crystal of atoms.



$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \underbrace{V(x_1, x_2, \ldots x_N)}_{V(0) + \frac{1}{2}\sum_{i=1,\, j=1}^{N} x_i \underbrace{\partial_i \partial_j V}_{\equiv V_{ij}}(0)\, x_j}$$

$$H = \sum_{i,j=1}^{N} p_i \frac{\delta_{ij}}{2m} p_j + \sum_{i,j=1}^{N} x_i V_{ij} x_j$$

symmetric $V_{ij} = V_{ji}$

$\Rightarrow$ V_{ij} diagonalizable by an orthogonal transformation $\rightarrow$ canonical transf.

$$\underline{\bar{x}_\alpha = O_{\alpha i} x_i}, \qquad O^T O = \mathbb{1}$$

$$H = \frac{1}{2m} p^T \mathbb{1}\, p + x^T V\, x$$

$$= \frac{1}{2m} \bar{p}^T \underbrace{O \mathbb{1} O^T}_{\mathbb{1}} \bar{p} + \frac{1}{2} \bar{x}^T \underbrace{O V O^T}_{k_\alpha \delta_{\alpha\beta}} \bar{x}$$

$$H = \sum_\alpha \left(\frac{\bar{p}_\alpha^2}{2m} + \frac{1}{2} k_\alpha \bar{x}_\alpha^2 \right)$$

$$= \sum_\alpha H(p_\alpha, x_\alpha) \leftarrow N \text{ decoupled H.O.'s.}$$

Quantization of oscillator in coord. repr.

single oscillator

$$\hat{H}|\psi\rangle = i\hbar\partial_t|\psi\rangle$$

$$|\psi\rangle = \sum_n c_n e^{-i/\hbar E_n t}|E_n\rangle$$

$$\Rightarrow \hat{H}|E_n\rangle = E_n|E_n\rangle \Rightarrow \langle x|E_n\rangle \equiv \psi_n(x)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\psi_n'' + \frac{1}{2}m\omega_0^2 x^2\psi_n = E_n\psi_n$$

N decoupled oscillators

$$\psi(x_1, x_2, x_3, \ldots x_N)$$

$$\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} + \cdots \frac{d^2}{dx_N^2}\right) + \sum_{i=1}^{N} V(x_i)\right]\psi = E\psi$$

product state

$$\psi(x_1, \ldots, x_N) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)\cdots\psi_N(x_N)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx_i}\psi_i(x_i) + V(x_i)\psi_i(x_i) = E_i\psi_i(x_i)$$

$$E = E_1 + E_2 + \cdots + E_N = \sum_{i=1}^{N} E_i$$

$\Rightarrow$ just focus on one harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega_0^2 x^2\psi = E\psi$$

solve with b.c. $\psi(x\to\infty)\to 0$, continuous etc...

well studied eqn, everything is known.

... but since H.O. is so important let's look in more detail to learn about soln.

6.5

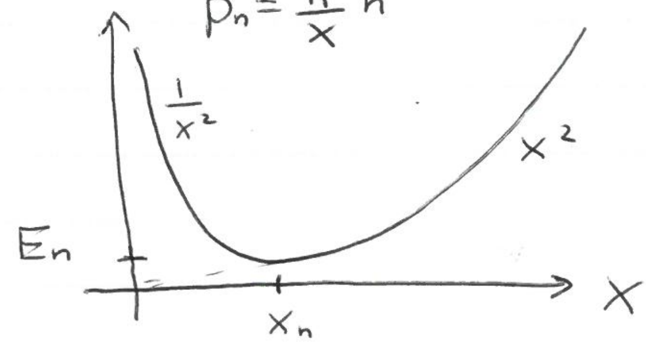
A. crude, dimensional analysis estimate:

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

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega_0^2 x^2$$

$$E(x) \simeq + \frac{\hbar^2 n^2}{2m}\frac{1}{x^2} + \frac{1}{2} m\omega_0^2 x^2$$

$$p_n = \frac{\hbar}{x} n$$



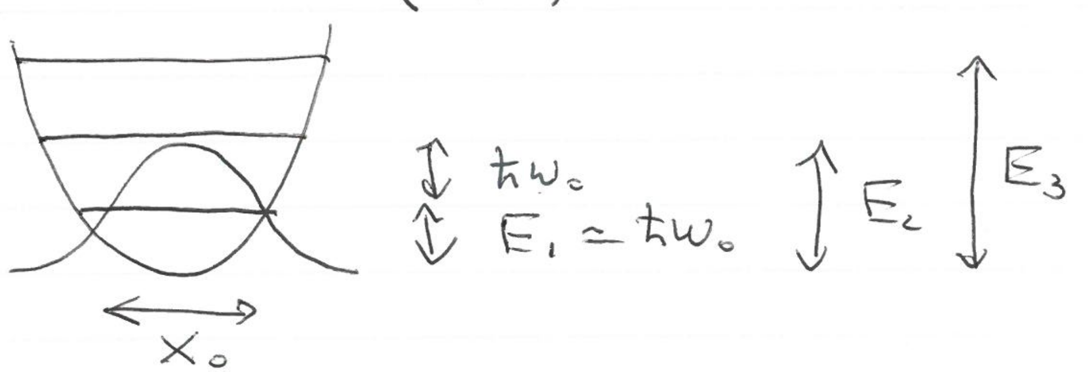
$$\frac{\partial E}{\partial x} = -\frac{\hbar^2 n^2}{m}\frac{1}{x^3} + m\omega_0^2 x = 0$$

$$\Rightarrow \boxed{x_n = \sqrt{n}\, x_0 = \sqrt{n}\left(\frac{\hbar}{m\omega_0}\right)^{1/2}}$$

$$E(x_n) = \frac{\hbar^2 n^2}{2m}\frac{1}{n x_0^2} + \frac{1}{2} m\omega_0^2\, n x_0^2$$

$$= n\left(\frac{\hbar^2 \cancel{m}\omega_0}{2\cancel{m}\hbar} + \frac{\cancel{m}\omega_0^{\cancel{2}}}{2}\frac{\hbar}{\cancel{m}\cancel{\omega_0}}\right)$$

$$\boxed{E_n = \hbar\omega_0 n} \simeq \left(\frac{\hbar^2}{2m x_0^2}\right) n$$



B. transform to dimensionless form.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi - \underbrace{\frac{m^2\omega_0^2}{\hbar^2}}_{\frac{1}{x_0^4}} x^2\psi = 0$$

$$x_0^2\frac{d^2\psi}{dx^2} + \underbrace{\frac{2m}{\hbar^2}Ex_0^2}\psi - \left(\frac{x}{x_0}\right)^2\psi = 0$$

$$y \equiv \frac{x}{x_0} \qquad 2\varepsilon \equiv \frac{2E}{\hbar\omega_0}$$

natural length scale

natural energy scale.

$$\frac{d^2\psi}{dy^2} + (2\varepsilon - y^2)\psi = 0$$

- look at $y \to \infty$ limit: $\psi'' - y^2\psi = 0$

$$\Rightarrow \psi \approx A y^m e^{\pm y^2/2} \rightarrow \underset{\text{any. at } y\to\infty}{y^m} e^{-y^2/2}$$

- look at $y \to 0$ limit: $\psi'' + 2\varepsilon\psi = 0$

$$\Rightarrow \psi(y) \underset{y\to 0}{\sim} A\cos(\sqrt{2\varepsilon}\,y) + B\sin(\sqrt{2\varepsilon}\,y)$$

$$\rightarrow A + cy + \ldots$$

$\Rightarrow$ Ansatz: $\psi(y) = H(y)e^{-y^2/2}$

$$\Rightarrow H'' - 2yH' + (2\varepsilon - 1)H = 0$$

$$H(y) = \sum_{n=0}^{\infty} c_n y^n$$

must be regular as $y \to 0$.

$$\Rightarrow \sum_{n=0}^{\infty} c_n\left[n(n-1)y^{n-2} - 2ny^n + (2\varepsilon-1)y^n\right] = 0$$

6.7

$n = 2k$

$$\frac{\frac{n}{2}!}{(\frac{n}{2}+1)!} = \frac{1}{\frac{n}{2}+1} \simeq \frac{2}{n} \checkmark$$

<u>Shift indices</u>:

$$\sum_{n=0}^{\infty} y^n \left[C_{n+2}(n+2)(n+1) + C_n(2\varepsilon - 1 - 2n) \right] = 0$$

$$\Rightarrow \quad \underline{C_{n+2} = C_n \frac{2n+1-2\varepsilon}{(n+2)(n+1)}} \xrightarrow[n\to\infty]{} C_n \frac{2}{n} \approx y^m e^{y^2}$$

<u>two independent solns</u>

$$\Rightarrow \begin{cases} C_0 \to C_2 \to C_4 \to C_6, \ \ldots & \text{even powers.} \\ C_1 \to C_3 \to C_5 \to C_7, \ \ldots & \text{odd powers} \end{cases}$$

but must require that $u(y) \xrightarrow[y\to\infty]{} y^m$

well behaved $(y \to \infty)$ soln if <u>series terminates</u>:

$$\varepsilon_n = n + \tfrac{1}{2}, \quad n = 0, 1, 2, \ldots \in \mathbb{Z}$$

$\Rightarrow C_{n+2}$ vanishes.

$$\Rightarrow \Psi(y) = H_n(y)\, e^{-y^2/2} = \begin{Bmatrix} C_0 + C_2 y^2 + C_4 y^4 + \ldots + C_n y^n \\ C_1 y + C_3 y^3 + C_5 y^5 + \ldots C_n y^n \end{Bmatrix} \times e^{-y^2/2}$$

$$\Rightarrow \boxed{E_n = (n + \tfrac{1}{2})\hbar\omega_0}$$

zero-point energy (due to Heisenberg uncert. princ. $[x, p] = i\hbar$)

$$\underline{H_n'' - 2y H_n' + 2n H_n = 0}$$

Hermite Eqn for n^{th} Hermite polynomial

odd/even n

$[P, H] = 0$

$$\begin{cases} H_0(y) = 1 \\ H_1(y) = 2y \\ H_2(y) = -2(1 - 2y^2) \\ H_3(y) = -12(y - \frac{2}{3}y^3) \\ \vdots \end{cases}$$

$H_n' = 2n H_{n-1}$

$H_{n+1} = 2y H_n - 2n H_{n-1}$

generating fnc: $Z(y, s) = e^{-s^2 + 2sy}$

Generating fnc: $\boxed{\left.\frac{\partial^n Z}{\partial s^n}\right|_{s=0} = H_n(y) = (-1)^n e^{y^2} \frac{\partial^n}{\partial y^n}(e^{-y^2})}$

$$Z(y,s) = e^{-s^2+2sy} = \sum_n \frac{s^n}{n!} H_n(y)$$

extremely useful to compute with H_n's.

$$\Psi_n(x) = A_n H_n\left(\tfrac{x}{x_0}\right) e^{-\frac{1}{2}x^2/x_0^2}, \quad E_n = \hbar\omega_c\left(n+\tfrac{1}{2}\right)$$

Normalization A_n:

$$1 = \int_{-\infty}^{\infty} |\Psi_n(x)|^2 = x_0 A_n^2 \int_{-\infty}^{\infty} H_n^2(y) e^{-y^2} dy$$

Look at more general form.

$$\int_{-\infty}^{\infty} dy\, e^{-y^2} e^{-s^2+2sy} \cdot e^{-t^2+2ty} = \sum_{n,m} \frac{s^n t^m}{n!m!} \int_{-\infty}^{\infty} H_n(y) H_m(y) e^{-y^2} dy$$

$\downarrow$ Gaussian integral

$$= e^{-s^2-t^2+(2(s+t))^2\frac{1}{4}} \sqrt{\pi}$$

$$= \pi^{1/2} e^{2st} = \sum_{n,m} \frac{s^n t^m}{n!\,m!} \int_{-\infty}^{\infty} H_n(y) H_m(y) e^{-y^2} dy$$

$$= \pi^{1/2} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!}$$

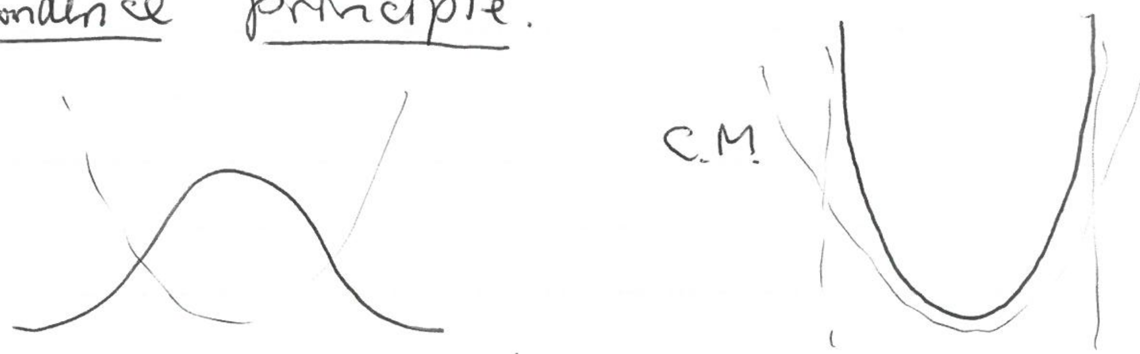
$$\Rightarrow \int_{-\infty}^{\infty} H_n(y) H_m(y) e^{-y^2} dy = \delta_{nm} \pi^{1/2} 2^n \sqrt{n!}$$

$$\Rightarrow \boxed{A_n = \left(\frac{x_0^{-1}}{\pi^{1/2} 2^n n!}\right)^{1/2}} \sim \frac{1}{\sqrt{x_0}} \checkmark$$

similarly evaluate: $\langle x \rangle$, $\langle x^2 \rangle$, $\langle n|x|m \rangle$, etc.

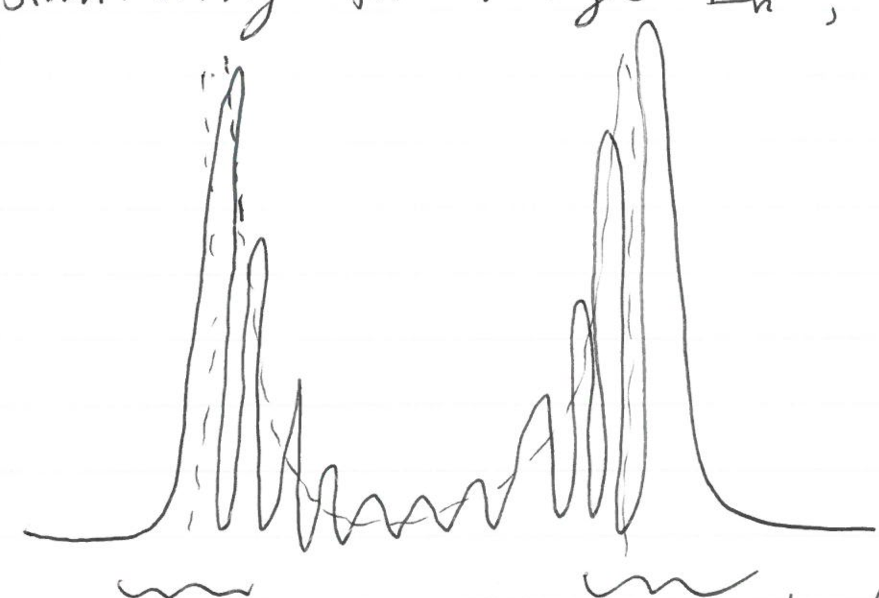
Correspondence principle.

Q.M. C.M.



very different at low E_n (small n)

Similarity for large E_n, as expected



spends a lot of time at classical turning point.

$\frac{1}{2} m v^2 = E - \frac{1}{2} m \omega_0^2 x^2$

$$v_{cl} = \omega_0 \sqrt{x_0^2 - x^2} \longleftarrow v = \sqrt{\frac{2E}{m} - \omega_0^2 x^2}$$

$x_0^2 = \frac{2E}{m\omega_0^2}$

Even with this eigenstates are very counter-intuitive / nonclassical – nothing is oscillating or even changing in time!

(6.10)

- Evolution operator:

$$U(x,t;x',t') = \sum_n \psi_n^*(x)\,\psi_n(x')\,e^{-\frac{i}{\hbar}E_n t}$$

$$= \sum_n A_n^2\, H_n\!\left(\tfrac{x}{x_0}\right) H_n\!\left(\tfrac{x'}{x_0}\right) e^{-\frac{1}{2x_0^2}(x^2+x'^2) - i\omega_c(n+\frac{1}{2})(t-t'}$$

- matrix elements.

$$\langle n|\hat{x}|n'\rangle = x_0 \frac{1}{\sqrt{2}}\left(\sqrt{n+1}\,\delta_{n',n+1} + \sqrt{n}\,\delta_{n',n-1}\right)$$

$$\langle n|\hat{p}|n'\rangle = \frac{\hbar}{x_0}\frac{-i}{\sqrt{2}}\left(\sqrt{n+1}\,\delta_{n',n+1} - \sqrt{n}\,\delta_{n',n-1}\right)$$

$$\begin{pmatrix} 0 & \sqrt{1} & & \\ \sqrt{1} & 0 & \sqrt{2} & 0 \\ & \sqrt{2} & 0 & \sqrt{3} \\ 0 & & \sqrt{3} & \end{pmatrix}$$

- Correspondence principle:

large mass $\langle E\rangle \simeq \frac{1}{2} m\omega^2 x_0^2 \simeq 1$ erg

$\Delta E = \hbar\omega \simeq 10^{-27}$ erg $\quad$ 2g $\quad$ 1 rad/s $\quad$ 1 cm

$\Rightarrow \quad \Delta E \ll E \quad \rightarrow \quad n \simeq 10^{27} \gg 1$

(Konrad Lehnert) cantelever exp's. $\quad$ impossible to notice quantization of E_n for macroscopic objects.

- E_n's equally spaced $\Rightarrow$ think of $|n\rangle$ as an oscillator state with n-quanta of excitations $\Leftrightarrow$ n-"particles" of vibrations $\Rightarrow$ identical bosonic particles

$|n\rangle \rightarrow$ state of n-quanta of excitations

$\rightarrow$ phonons $\rightarrow$ quanta of vibration of a crystal field u.

$\rightarrow$ photons $\rightarrow$ quanta of vibration of E&M fields $\vec{A}$.

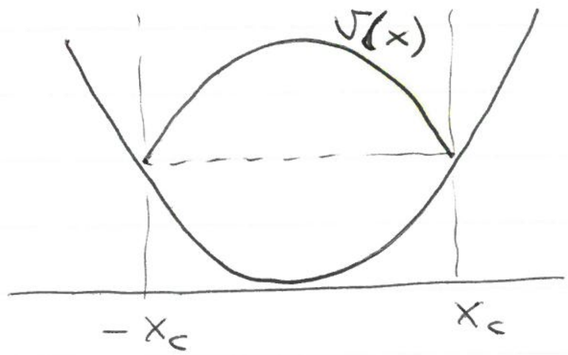
- $\psi_n(x)$ extends outside classical turning pnt.

$$E = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2$$

turning point: $p = 0$

$$\frac{1}{2} m\omega_c^2 x_c^2 = \hbar\omega_0 (n+\tfrac{1}{2}) = E_n$$

$$\Rightarrow x_c = \left(\frac{\hbar}{m\omega_c}\right)^{1/2} \sqrt{2n+1} = x_0\sqrt{2n+1}$$



$$\frac{1}{2} m v^2 + \frac{1}{2} m\omega_0^2 x^2 \stackrel{?}{=} E$$

$$\sqrt{\frac{2E}{m} - \omega_0^2 x^2} = v(x)$$

$$v(x) = \omega_0 \sqrt{x_c^2 - x^2}$$

$$P_{cl}(x) \sim \frac{1}{v(x)} = \frac{1}{\omega_0\sqrt{x_c^2 - x^2}}$$

- duality between p & x

$$H = \frac{1}{2} m^{-1} p^2 + \frac{1}{2} m\omega_0^2 x^2$$

$$\psi_n(x) \rightarrow \tilde{\psi}_n(p) = \psi_n(x)$$

$m\omega_0 \leftrightarrow \frac{1}{m\omega_0}$

$x \leftrightarrow p$.

$$\text{e.g. } \tilde{\psi}_0(p) = \left(\frac{1}{m\hbar\omega_0\pi}\right)^{1/4} \times$$

$$\times\, e^{-\frac{p^2}{2m\hbar\omega_0}}$$

$m\hbar\omega_0 \equiv p_0^2$

$$x_0 \rightarrow p_0 = \frac{\hbar}{x_0} = (\hbar m\omega_0)^{1/2}$$

$$\left(\frac{\hbar}{m\omega_0}\right)^{1/2}$$

C. Energy & number basis – Fock states
(due to Dirac)

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega_0^2 x^2 , \quad [x, p] = i\hbar$$

$$H = \hbar\omega_0 \left[\frac{1}{2}\frac{p^2}{p_0^2} + \frac{1}{2}\frac{x^2}{x_0^2} \right]$$

$$\equiv \hbar\omega_0 \hat{h}(\hat{p}, \hat{x})$$

$$\hat{h}(\hat{p}, \hat{x}) = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 ; \quad \hat{p} \equiv \frac{p}{p_0}, \hat{x} = \frac{x}{x_0}$$

$$p_0 = \frac{\hbar}{x_0}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega_0}}$$

Note: $[\hat{x}, \hat{p}] = \underbrace{[x, p]}_{i\hbar} \underbrace{\frac{1}{p_0 x_0}}_{\frac{1}{\hbar}}$

$$\Rightarrow [\hat{x}, \hat{p}] = i$$

$$\hat{h} = \underbrace{\frac{1}{\sqrt{2}}(\hat{x} - i\hat{p})\frac{1}{\sqrt{2}}(\hat{x} + i\hat{p})}_{\frac{1}{2}\hat{x}^2 + \frac{1}{2}\hat{p}^2 + \underbrace{\frac{i}{2}[\hat{x}, \hat{p}]}_{-\frac{1}{2}}} - \frac{i}{2}[\hat{x}, \hat{p}]$$

Unitary transf.

$$\boxed{\hat{h} = a^+ a + \frac{1}{2}}$$

cf
$$f = \frac{1}{2}x^2 + \frac{1}{2}y^2 = \frac{1}{\sqrt{2}}(x - iy)\frac{(x + iy)}{\sqrt{2}}$$

$$\Rightarrow H = \hbar\omega_0 \left(a^+ a + \frac{1}{2} \right)$$

$$\left.\begin{aligned} a &= \left(\frac{m\omega_0}{2\hbar}\right)^{1/2} x + i\left(\frac{1}{2m\omega_0\hbar}\right)^{1/2} p \\ a^+ &= \left(\frac{m\omega_0}{2\hbar}\right)^{1/2} x - i\left(\frac{1}{2m\omega_0\hbar}\right)^{1/2} p \end{aligned}\right\} \text{not Hermitian}$$

$$a = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + i\frac{p}{p_0}\right)$$

Note: $[a, a^+] = \frac{1}{2}[(\hat{x}+i\hat{p}), (\hat{x}-i\hat{p})]$

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

$\Rightarrow \boxed{[a, a^+] = 1}$ ← Key result:

Note: a, a^+ act like $a, -\frac{\partial}{\partial a}$ wrt fns of $f(a, a^+)$ → representation of a, a^+.

Why? $[a, -\frac{\partial}{\partial a}] = 1$

$\Leftrightarrow a, a^+ \rightarrow \frac{\partial}{\partial a^+}, a^+ \Rightarrow [\frac{\partial}{\partial a^+}, a^+] = 1$

c.f. $[x, p] = i\hbar \Rightarrow [x, -i\hbar\partial_x] = i\hbar$.

$\Rightarrow [f(a), a^+] = \frac{\partial f}{\partial a}\underbrace{[a, a^+]}_{1} = \frac{\partial f}{\partial a}$ ← true for any two ops whose [,] = = const c.#.

So what?

Note: $H = \hbar\omega_0(a^+a + \frac{1}{2})$ and $[H, a^+] = \hbar\omega_0 a^+$

suppose $|0\rangle$ ← groundstate of H, i.e.,

$H|0\rangle = E_0|0\rangle$ ← not normalized

look at $|\tilde{1}\rangle \equiv a^+|0\rangle$ – also eigenstate:

$H|\tilde{1}\rangle = Ha^+|0\rangle = a^+\underbrace{H|0\rangle}_{E_0|0\rangle} + \hbar\omega_0 a^+|0\rangle$

$\Rightarrow \boxed{H(a^+|0\rangle) = (\mathcal{E}_0 + \hbar\omega_0)(a^+|0\rangle)}$

$\Rightarrow \quad a^+|0\rangle \equiv |\tilde{1}\rangle$ is an energy eigenstate too.
i.e. excited state with energy $\hbar\omega_0$ above ground state E_0.

$(a^+)^n|0\rangle \equiv |\tilde{n}\rangle \rightarrow n^{\text{th}}$ excited state

with energy $\underline{E_n = E_0 + n\hbar\omega_0}$!

Similarly, because $[H, a] = -\hbar\omega_0 a$

$$H a|\tilde{n}\rangle = -\hbar\omega_0(a|\tilde{n}\rangle) + E_n(a|\tilde{n}\rangle)$$

$$\Rightarrow H(a|\tilde{n}\rangle) = (E_n - \hbar\omega_0)(a|\tilde{n}\rangle)$$

$\Rightarrow \quad a|n\rangle \equiv |\widetilde{n-1}\rangle$ eigenstate of H with eigenvalue $E_{n-1} = E_n - \hbar\omega_0$.

$$= E_0 + (n-1)\hbar\omega_0$$

(used the fact that there is no degeneracy in 1d)

$a^+, a \longrightarrow$ raising & lowering ops.
$\Leftrightarrow$ creation & annihilation ops.

Ground state has lowest energy $E_0 \Rightarrow$ cannot be lowered $\Rightarrow$

$$a|0\rangle = 0 \Rightarrow H|0\rangle = \tfrac{1}{2}\hbar\omega_0|0\rangle$$

$$\Rightarrow \underbrace{\boxed{E_n = \hbar\omega_0(n + \tfrac{1}{2})}}_{\text{eigenenergies.}} \;\&\; \underbrace{\boxed{|\hat{n}\rangle = (a^+)^n|0\rangle}}_{\text{eigenstates}}$$

Normalized states: $|n\rangle \equiv \mathcal{N}_n |\tilde{n}\rangle$

Define number operator: $\hat{N} = a^+ a$

$$= \frac{\hat{H}}{\hbar\omega_0} - \frac{1}{2}$$

$$\langle n|\hat{N}|n\rangle = n\underbrace{\langle n|n\rangle}_{1}$$

$\langle n|\hat{N}|n\rangle = n$ ← counts # energy quanta $\hbar\omega_0$ in state $|n\rangle$

$\hat{N}|n\rangle = n|n\rangle$

↳ $\hat{N}$ eigenstate. (Fock state)

$\hat{H} = \hbar\omega_0(\hat{N} + \frac{1}{2})$

$a|n\rangle = A_n|n-1\rangle$;

$$\langle n|a^+ a|n\rangle = |A_n|^2 \langle n-1|n-1\rangle =$$

$$n = |A_n|^2$$

$$\Rightarrow \boxed{A_n = \sqrt{n}}$$

(chose $\phi = 0$)

Equivalently:

$\langle n|a a^+|n\rangle = |B_n|^2$

$= \langle n|a^+a+1|n\rangle = (n+1)\langle n+1|n+1\rangle = |B_n|^2$.

$a^+|n\rangle = B_n|n+1\rangle$

$$\underbrace{a a^+}_{(a^+a+1)}|n\rangle = B_n a|n+1\rangle = B_n A_{n+1}|n\rangle$$

$$\Rightarrow (n+1)|n\rangle = B_n A_{n+1}|n\rangle$$

$$\Rightarrow \boxed{B_n = \sqrt{n+1}}$$

$$\Rightarrow \boxed{a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^+|n\rangle = \sqrt{n+1}|n+1\rangle}$$

$$\Rightarrow \boxed{|n\rangle = \frac{1}{\sqrt{n!}} a^{+n}|0\rangle}$$

• Matrix elements.

$$\langle n'|a|n\rangle = \sqrt{n}\,\langle n'|n-1\rangle = \sqrt{n}\,\delta_{n',n-1}$$

$$\langle n'|a^+|n\rangle = \sqrt{n+1}\,\langle n'|n+1\rangle = \sqrt{n+1}\,\delta_{n',n+1}$$

$\Rightarrow$ Much easier (than using coord. repr. $H_n e^{-\frac{x^2}{2}}$) to compute any matrix element involving a, a^+. e.g. $\langle n|p^2|n\rangle$, $\langle n|x^4|n'\rangle$

$\Rightarrow$ $\langle V(x,p)\rangle$ easy since:

$$\underline{x = \frac{1}{\sqrt{2}} x_0 (a^+ + a)}\,; \quad \underline{p = \frac{i}{\sqrt{2}} \frac{\hbar}{x_0} (a^+ - a)}$$

In matrix form a^+:

$$(a^+)_{n,n'} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 1^{1/2} & 0 & 0 & 0 & 0 & \cdots \\ 0 & 2^{1/2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & 3^{1/2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 4^{1/2} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

$(a)_{nn'}$ is just Hermitian conjugate, since real $\Rightarrow$ just transpose.

$X_{nn'}$, $P_{nn'}$ easy.

$$H_{nn'} = \hbar\omega_0 \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 5/2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 7/2 & 0 & \\ 0 & 0 & 0 & 0 & 9/2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

diagonal in $|n\rangle$ basis

Note: in Heisenberg representation

$$\hat{a}(t) \equiv e^{+\frac{i}{\hbar}\hat{H}t}\, a\, e^{-\frac{i}{\hbar}\hat{H}t}$$

$$\frac{d\hat{a}(t)}{dt} = \frac{1}{i\hbar}[\hat{a}, \hat{H}] = \frac{\hbar\omega_0}{i\hbar}[\hat{a}, \hat{a}^+\hat{a} + \tfrac{1}{2}]$$

$$\frac{d\hat{a}}{dt} = -i\omega_0 \hat{a} \Rightarrow \boxed{\hat{a}(t) = a e^{-i\omega_0 t}}$$

and $\boxed{\hat{a}^+(t) = a^+ e^{i\omega_0 t}}$

- <u>Passage</u> <u>from $|n\rangle \to |x\rangle$ basis</u>:

i.e. connection with $\psi_n(x) = A_n H_n e^{-x^2/2}$

Why? useful to obtain $P(x) = |\psi(x)|^2$

<u>Recall</u>: $\psi_n(x) = \langle x | n \rangle$

Look at ground state first: $a|0\rangle = 0$

$$\langle x | a | 0 \rangle = 0$$

$$\int_{x'} |x'\rangle\langle x'| = 1$$

$$\Rightarrow \int_{x'} \langle x | a | x' \rangle \underbrace{\langle x' | 0 \rangle}_{\psi_0(x)} = 0$$

use $a = \frac{1}{\sqrt{2}}\left(\frac{X}{X_0} + i\frac{P}{P_0}\right)$

(6.18)

$$\int dx' \langle x | a | x' \rangle \psi_0(x') = 0 \quad ?$$

$$\frac{1}{\sqrt{2}} \int dx' \langle x | \frac{X}{x_0} + i \frac{P}{p_0} | x' \rangle \psi_0(x') = 0$$

$$\int dx' \left(\frac{x}{x_0} \delta(x-x') + \frac{i(-i\hbar)}{p_0} \partial_x \delta(x-x') \right) \psi_0(x') = 0$$

$$\left(\frac{x}{x_0} + \frac{\hbar}{p_0} \frac{\partial}{\partial x} \right) \psi_0(x) = 0$$

i.e. derive coord. repr. of a:

$$a_{xx'} = \frac{1}{\sqrt{2}} \left(\frac{1}{x_0} x + x_0 \frac{\partial}{\partial x} \right) \delta(x-x')$$

$$\left(\hat{x} + \frac{\partial}{\partial \hat{x}} \right) \psi_0(\hat{x}) = 0$$

$$x \psi_0(x) + \psi_0' = 0$$

$$\Rightarrow \int \frac{d\psi_0}{\psi_0} = -\frac{1}{2} x^2 \quad \Rightarrow \quad \underline{\psi_0(x) = e^{-\frac{x^2}{2x_0^2}}}$$

$$\Rightarrow \quad \psi_0(x) = \left(\frac{m\omega_0}{\pi\hbar} \right)^{1/4} e^{-\underbrace{\frac{m\omega_0 x^2}{2\hbar}}}$$

Note: $= \frac{1}{2} \frac{m\omega_0^2 x^2}{\hbar\omega_0} = \frac{V(x)}{\hbar\omega_0}$

What about: $\psi_n(x) = ?$

$$|n\rangle = \frac{(a^+)^n}{\sqrt{n!}}|0\rangle$$

$$\Rightarrow \psi_n(x) \equiv \langle x|n\rangle = \langle x|\frac{a^{+n}}{\sqrt{n!}}|0\rangle$$

$$= \int_{x'} \langle x|\frac{a^{+n}}{\sqrt{n!}}|x'\rangle \underbrace{\langle x'|0\rangle}_{\psi_0(x)}$$

$$\psi_n(x) = \int_{x'} \left(\frac{1}{\sqrt{2}}\right)^n \left(\frac{1}{x_0}x - x_0\frac{\partial}{\partial x}\right)^n \frac{1}{(n!)^{1/2}} \delta(x-x')\, \psi_0(x')$$

$$\psi_n(\hat{x}) = \frac{1}{(n!)^{1/2}}\left[\frac{1}{2^{1/2}}\left(\hat{x} - \frac{\partial}{\partial \hat{x}}\right)\right]^n \psi_0(\hat{x})$$

$$\psi_n(x) = \frac{1}{\pi^{1/4} x_0^{1/2}}\left(\frac{1}{n!\,2^n}\right)^{1/2}\left(\hat{x} - \frac{\partial}{\partial \hat{x}}\right)^n e^{-\frac{\hat{x}^2}{2}}$$

$$\Rightarrow \underline{H_n(\hat{x}) = e^{\hat{x}^2/2}\left(\hat{x} - \frac{\partial}{\partial \hat{x}}\right)^n e^{-\hat{x}^2/2}}$$

see applications in Shankar Exercises:

- $a|n\rangle = n^{1/2}|n-1\rangle \Rightarrow H_n'(x) = 2n\,H_{n-1}(x)$
- $(a + a^+) = 2^{1/2} x \Rightarrow H_{n+1} = 2x\,H_n - 2n\,H_{n-1}$
- harmonic oscillator thermodynamics
  - Planck's black-body radiation
  - Bose - Einstein & Fermi - Dirac dist's.
  - phonons in a solid/crystal
- QED & QFT

D. Coherent states:

$|n\rangle$ Fock states are $\hat{H}$ eigenstates, but highly non-classical, e.g.:

$$\langle n| x |n\rangle = 0 \quad !?!$$

AND

"Nothing" oscillates (since eigenstates) !?!
(physical)

Consider (a seemingly complicated) "coherent" state

$$|z\rangle = e^{za^+}|0\rangle = \sum_{n=0}^{\infty} \frac{z^n}{n!} a^{+n}|0\rangle$$

$$= \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle$$

not normalized

labeled by complex # z.

different states for different z's
but not orthonormal & over-complete
i.e. too many z's (∞ #) vs. compared to integer labels $|n\rangle$ Fock states.

Why $|z\rangle$ coherent states important/useful ?

$$e^{za^\dagger}|0\rangle = |z\rangle$$

displacement operator; displaces eigenvalue of a, namely $z=0$ to z via

$$e^{za^\dagger}$$

canonically conjugate to a.

<u>Note analogy</u> $\hat{x}|x_0\rangle = x_0|x_0\rangle$

$$e^{-\frac{i}{\hbar}d\hat{p}}|x_0\rangle = |x_0+d\rangle$$

displacement op of eigenvalue of $\hat{x}$ by d as exp. of $e^{-d\frac{\partial}{\partial x}}$

$[x, \frac{\partial}{\partial x}] = -1$

cf $[a, a^\dagger] = 1$

$$\hat{x}\left(e^{-\frac{i}{\hbar}d\hat{p}}|x_0\rangle\right)$$
$$= e^{-\frac{i}{\hbar}d\hat{p}}(\hat{x}+d)|x_0\rangle$$
$$= (x_0+d)\left(\underbrace{e^{-\frac{i}{\hbar}d\hat{p}}|x_0\rangle}\right)$$
$$\Rightarrow \quad = |x_0+d\rangle \checkmark$$

$$e^{-\frac{i}{\hbar}d\hat{p}}|\psi\rangle = |\psi'\rangle$$

$$\underline{\psi'(x) \equiv \langle x|\psi'\rangle = \langle x-d|\psi\rangle \equiv \psi(x-d)}$$

<u>Actually</u>:

$$\frac{\hat{p}}{p_0} = +\frac{i}{\sqrt{2}}(a^\dagger - a) \Rightarrow e^{-\frac{i}{\hbar}d\hat{p}} = e^{-\frac{i}{\hbar}\frac{i d p_0}{\sqrt{2}}(a^\dagger - a)}$$

$$D \equiv e^{\frac{d}{x_0\sqrt{2}}(a^\dagger - a)}$$

Note: $$D|0\rangle \propto e^{\frac{d}{x_0\sqrt{2}}a^\dagger}|0\rangle$$
$$= \left|z = \frac{d}{x_0\sqrt{2}}\right\rangle$$

$|z\rangle$ is eigenstate of $\hat{a}$ with eigenvalue z! i.e.

$$\underline{a|z\rangle = z|z\rangle}$$

Easy to prove:

$$a|z\rangle = a\, e^{za^+}|0\rangle = \big(e^{za^+}a + \underbrace{[a, e^{za^+}]}_{z e^{za^+}}\big)|0\rangle$$

(recall $a, a^+ \leftrightarrow \frac{\partial}{\partial a^+}, a^+$)

$$= 0 + z\underbrace{e^{za^+}|0\rangle}_{|z\rangle}$$

$$\Rightarrow a|z\rangle = z|z\rangle \quad \checkmark$$

<u>equival.</u> $$a|z\rangle = \sum_{n=0}^{\infty} \frac{a\, z^n}{\sqrt{n!}}|n\rangle$$

$$= \sum_{n=1}^{\infty} \frac{z^n}{\sqrt{n!}}\sqrt{n}\,|n-1\rangle$$

$$= \sum_{n=0}^{\infty} \frac{z^{n+1}}{\sqrt{n!}}|n\rangle$$

$$\Rightarrow \underline{a|z\rangle = z|z\rangle} \quad \checkmark$$

<u>Note:</u> $\langle z| = \langle 0| e^{z^* a}$ with $\langle z|a^+ = \langle z|z^*$.

<u>Normalization</u>: $\langle z_2|z_1\rangle = \langle 0| e^{z_2^* a} e^{z_1 a^+}|0\rangle$

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

valid for A, B s.t. $[A,B]$ commutes with A & B. $\Longrightarrow$ Baker-Hausdorff formula.

(not difficult to derive, motivate by Taylor exp).

$$\underline{\text{Note:}} \bullet\ \psi_z(x) = \langle x | z \rangle = \overset{\text{normalized}}{\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}} \underbrace{e^{-\frac{z^2}{2}} e^{-\frac{x^2}{2x_0^2}} e^{\sqrt{2}\frac{zx}{x_0}}}_{e^{-\frac{1}{2}\left(\frac{x}{x_0}-\sqrt{2}z\right)^2}}$$

$$\bullet\ U(z_N, z_0; t) = \langle z_N | \underbrace{\hat{U}(t)|z_0\rangle}_{|z_0 e^{-i\omega_0 t}\rangle}$$

$$\underline{U(z_N, z_0; t) = e^{z_N^* z_0 e^{-i\omega_0 t}}}$$

$$\underline{\text{see hw4}}: \langle x | \tilde{z} \rangle = \sum_n \langle x | \frac{z^n a^{+n}}{n!} | 0 \rangle = \sum_n \frac{\overbrace{\langle x | n \rangle}^{A_n H_n(\frac{x}{x_0}) e^{-\frac{x^2}{2x_0^2}}}}{\sqrt{n!}} z^n e^{-|z|^2/2}$$

$$\psi_z(x) = \langle x | \tilde{z} \rangle = \sum_n \frac{1}{x_0^{1/2}} \left(\frac{1}{\pi^{1/4} 2^{n/2} \sqrt{n!}}\right) \frac{z^n}{\sqrt{n!}} H_n(x/x_0) e^{-x^2/2x_0^2} e^{-|z|^2/2}$$

$$= \frac{1}{\pi^{1/4}\sqrt{x_0}} \sum_n \frac{z^n}{2^{n/2}} \frac{1}{n!} H_n(x/x_0) e^{-x^2/2x_0^2} \Rightarrow s = \frac{z}{\sqrt{2}}$$

$\underline{\text{Note}}$: Evolution op. $\hat{U} = e^{-\frac{i}{\hbar} H(a^+, a) t}$

is really simple in coherent state basis: ...

$$\langle z_N | \hat{U}(t) | z_0 \rangle \equiv \hat{U}(z_N, z_0; t)$$

$$= \langle z_N | z_0(t) \rangle$$

$\underline{\text{for H.O.}}$:

$$= \langle z_N | z_0 e^{-i\omega_0 t} \rangle = e^{z_N^* z_0 e^{-i\omega_0 t}} \checkmark$$

$$\underline{\text{For H.O.}} \Rightarrow \underline{\hat{U}(z_N, z_0; t) = e^{z_N^* z_0 e^{-i\omega_0 t}}}$$

$$\Rightarrow \langle z_2 | z_1 \rangle = \langle 0 | e^{z_2^* a} e^{z_1 a^+} | 0 \rangle$$
$$= \langle 0 | e^{z_1 a^+} e^{z_2^* a} | 0 \rangle e^{[z_2^* a, z_1 a^+]}$$
$$\underline{\langle z_2 | z_1 \rangle = e^{z_2^* z_1}}$$

Resolution of identity:

$$1 = \int \frac{dx\,dy}{\pi} |z\rangle\langle z| e^{-|z|^2} \equiv \int \underbrace{\frac{dz\,dz^*}{2\pi i}}_{\text{Jacobian.}} |z\rangle\langle z| e^{-z^* z}$$

use $|z\rangle = e^{z a^+}|0\rangle = \sum_0^\infty \frac{z^n}{\sqrt{n!}}|n\rangle$

<u>Note</u>: $\langle z | : f(a^+, a) : | z \rangle = f(z^*, z)$!

where $: f(a^+, a) :$ is f of a^+, a where all a's are to the <u>right</u> of a^+'s.

called <u>Normal-ordered</u> e.g.

$a^+ a^2$ is "N.O"'ed but $a^2 a^+$ is <u>not</u>.

Normal order by commuting a's to right.

<u>Note</u> simple, classical-like evolution of $|z\rangle$

$$|z(t)\rangle = U(t)|z\rangle = \underbrace{U(t) e^{z a^+} U^+(t)}_{e^{z a^+(t)}} \underbrace{U(t)|0\rangle}_{|0\rangle}$$

For h.o. $a^+(t) = a^+ e^{-i\omega_0 t}$

$H = \hbar\omega_0 a^+ a$

$$= e^{(z e^{-i\omega_0 t}) a^+} |0\rangle$$

$$\Rightarrow \boxed{|z(t)\rangle = |z e^{-i\omega_0 t}\rangle}$$ oscillates !!! like classical state $\}$ remains coherent