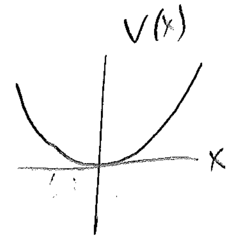
Harmonic oscillator:

(eg diatomic molecule)



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

Natural frequency $\omega = \sqrt{\frac{k_s}{m}}$ $\Rightarrow$ $E = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2 = \hbar\omega \left[\frac{m\omega}{2\hbar} \hat{X}^2 + \frac{1}{2m\hbar\omega} \hat{p}^2 \right]$$

Operator approach

Define $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{X} + \frac{i}{\sqrt{2m\hbar\omega}} \hat{p}$ non hermitian! (not an observable)

$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \hat{X} - \frac{i}{\sqrt{2m\hbar\omega}} \hat{p}$

$[\hat{a}, \hat{a}^\dagger] = \mathbb{1}$ using $[\hat{X}, \hat{p}] = i\hbar \mathbb{1}$

Define $\hat{N} = \hat{a}^\dagger \hat{a} = \frac{m\omega}{2\hbar} \hat{X}^2 + \frac{1}{2m\hbar\omega} \hat{p}^2 - \frac{1}{2}\hat{\mathbb{1}} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\hat{\mathbb{1}}$

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2}\hat{\mathbb{1}}\right)$$

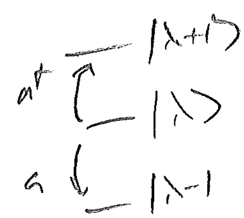
$[N, a^\dagger] = a^\dagger \Rightarrow N a^\dagger = a^\dagger (N+1)$

$[N, a] = -a \Rightarrow N a = a(N-1)$

Let $\hat{N}|\lambda\rangle = \lambda|\lambda\rangle$ be eigenstates of $\hat{N}$ (normalized)

Then $\hat{N}(a^\dagger|\lambda\rangle) = (\lambda+1)(a^\dagger|\lambda\rangle)$ re $\quad a^\dagger|\lambda\rangle \sim |\lambda+1\rangle$ raising

$\hat{N}(a|\lambda\rangle) = (\lambda-1)(a|\lambda\rangle)$ re $\quad a|\lambda\rangle \sim |\lambda-1\rangle$ lowering



$|\lambda\rangle$ are also energy eigenstates

$$\hat{H}|\lambda\rangle = \underbrace{\hbar\omega(\lambda+\tfrac{1}{2})}_{E}|\lambda\rangle$$

From analysis of Schrodinger eqn $\Rightarrow E > V_{min} = 0$

$$\Rightarrow \lambda > -\tfrac{1}{2}$$

$\exists \, \lambda_{min} \ni \quad a|\lambda_{min}\rangle = 0$

$$\langle\lambda_{min}|a^\dagger = 0$$

$$0 = \langle\lambda_{min}|a^\dagger a|\lambda_{min}\rangle = \langle\lambda_{min}|N|\lambda_{min}\rangle = \lambda_{min}$$

$$E_{min} = \hbar\omega(\lambda_{min}+\tfrac{1}{2}) = \tfrac{1}{2}\hbar\omega \leftarrow \text{ground st energy of harmonic oscillator}$$

$|0\rangle$ = ground state

All other states obtained by raising λ by 1 $\Rightarrow |n\rangle$

n = non-neg integers

$a^\dagger|1\rangle \propto |2\rangle$

$\vdots$

Eigenstate $|n\rangle$ has energy $E = \hbar\omega(n+\tfrac{1}{2})$

one can show:
$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$
$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

Mnemonic: $\sqrt{\text{larger}}$

$|1\rangle = a^\dagger|0\rangle$

$|2\rangle = \frac{1}{\sqrt{2}}a^\dagger|1\rangle$

$|3\rangle = \frac{1}{\sqrt{3}}a^\dagger|2\rangle$

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

In position space

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\, x + \sqrt{\frac{\hbar}{2m\omega}}\, \frac{d}{dx}$$

$$= \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right) \qquad y = \sqrt{\frac{m\omega}{\hbar}}\, x$$

$$\therefore \hat{a}^{\dagger} = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)$$

Ground state obeys $\quad a\,|0\rangle = 0$

$$\left(y + \frac{d}{dy}\right) u_0(y) = 0$$

$$\frac{du_0}{dy} = -y\, u_0$$

$$\frac{du_0}{u_0} = -y\, dy$$

$$\ln u_0 = -\frac{1}{2}y^2 + \text{const}$$

$$u_0 = C e^{-\frac{1}{2}y^2}$$

$$= C e^{-\frac{m\omega x^2}{2\hbar}}$$

Normalize: $\quad u_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}$

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$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^{+})^n |0\rangle$$

$$u_n = \frac{1}{\sqrt{n!}} \left(\frac{1}{\sqrt{2}} \left[y - \frac{d}{dy} \right] \right)^n \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{1}{2}y^2}$$

$$= \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{n!\,2^n}} \underbrace{\left(y - \frac{d}{dy} \right)^n e^{-\frac{1}{2}y^2}}_{\text{this is } H_n(y)\, e^{-\frac{1}{2}y^2}}$$

eg $\left(y - \frac{d}{dy} \right) e^{-\frac{1}{2}y^2}$

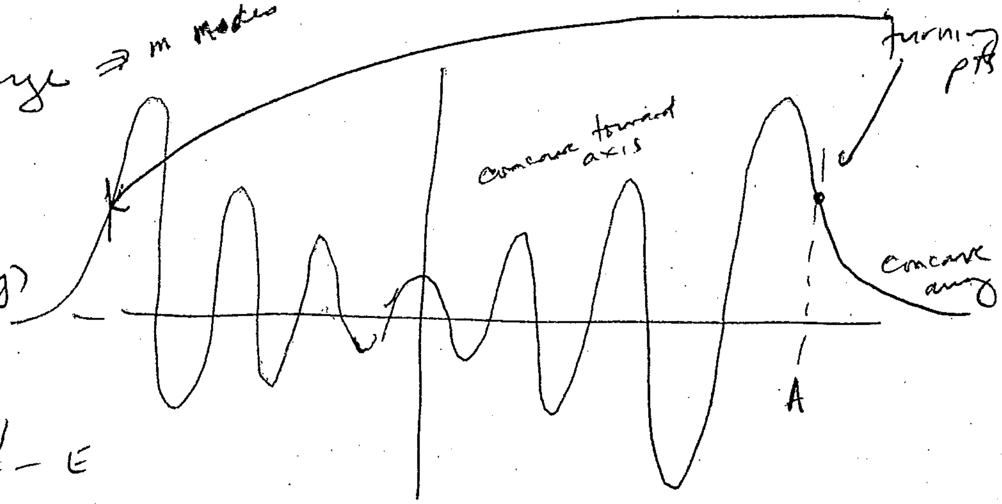
$= [y - (-y)]\, e^{-\frac{1}{2}y^2} = 2y\, e^{-\frac{1}{2}y^2}$

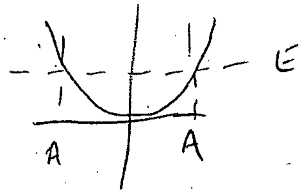
$H_1(y) = 2y$

n	$H_n(y)$
0	1
1	$2y$
2	$4y^2 - 2$
3	$8y^3 + 2y$
4	$16y^4 - 48y^2 + 12$

$$u_n = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{n!\,2^n}} H_n(y)\, e^{-\frac{1}{2}y^2}$$

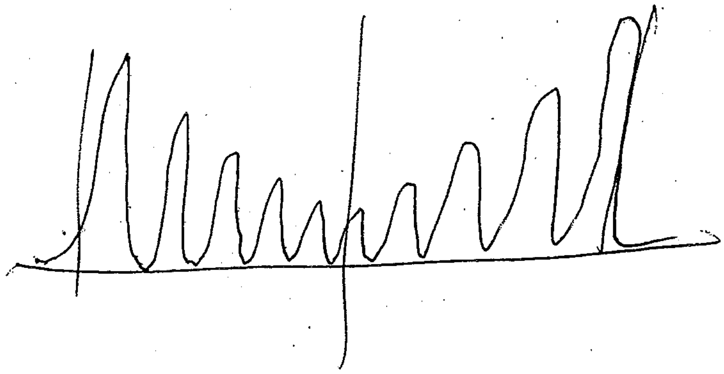
∘ m large ⇒ m nodes





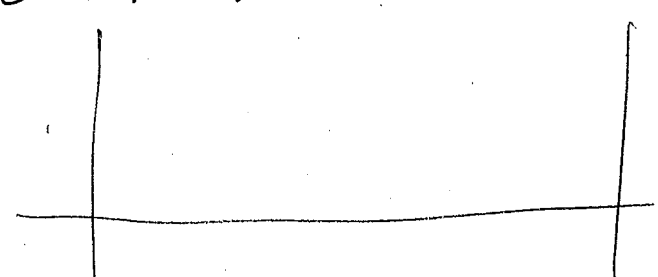
beyond turning points, $|u|^2 \neq 0$

$|u|^2$



Why is it more probable to find particle near turning points? Because particle moves more slowly there!

~~Correspondence principle~~



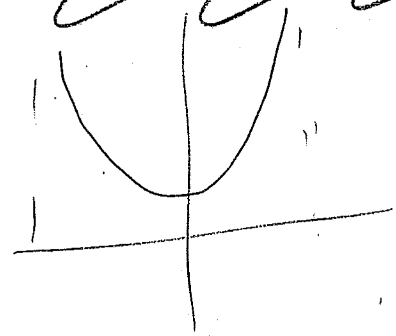
$\frac{1}{9}$ $\cancel{3/10}$ 10

[amt of time spent btw x & $x+\Delta x$ — x $x+\Delta x$ — $\Delta t = \frac{\Delta x}{v}$]

Prob ~ time spent ~ $\frac{1}{v}$

$\cancel{x = A\cos\omega t}$

$\cancel{v = -\omega A \sin\omega t = -\omega\sqrt{A^2 - A^2\cos^2\omega t} = -\omega\sqrt{A^2-x^2}}$



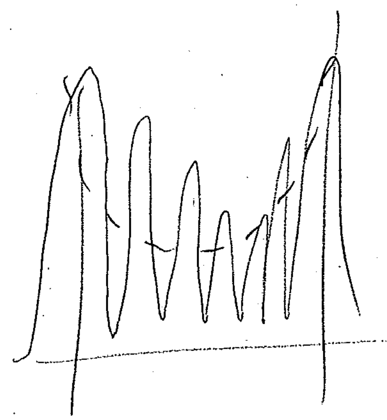
$P(x) \sim \frac{1}{v} \sim \frac{1}{\sqrt{A^2-x^2}}$

$\frac{1}{2}mv^2 = E - V(x) = \frac{1}{2}m\omega^2(A^2-x^2)$

$v = \pm\omega\sqrt{A^2-x^2}$

do a problem?

QM



Correspondence principle

QM → CM as $n \to \infty$

The power of the operator approach

$$\langle n | X^2 | n \rangle = \int dx \; \cancel{\quad} \; x^2 |u_n(x)|^2$$

$$\sim \int dy \;\; y^2 \; H_n^2(y) e^{-y^2}$$

difficult for $n = 143$!

$$X = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$$

$$\langle n | X^2 | n \rangle = \frac{\hbar}{2m\omega} \underbrace{\langle n | (a + a^\dagger)(a + a^\dagger) | n \rangle}$$

$$\underbrace{\langle n | a\,\underbrace{a | n \rangle}_{\sqrt{n}\,|n-1\rangle}}_{\underbrace{\sqrt{n}\sqrt{n-1}\,|n-2\rangle}_{0}} + \underbrace{\langle n | a \underbrace{a^\dagger | n \rangle}_{\sqrt{n+1}\,|n\rangle}}_{\underbrace{(n+1)\,|n\rangle}_{n+1}} + \underbrace{\langle n | a^\dagger \underbrace{a | n \rangle}_{\sqrt{n}\,|n-1\rangle}}_{\underbrace{n\,|n\rangle}_{n}} + \langle n | a^\dagger a^\dagger | n \rangle$$

$$= \frac{\hbar}{2m\omega} (2n + 1)$$

[Problem: show $\langle n | X | n \rangle = 0$
$\langle n | P | n \rangle = 0$]

In 2010, I skipped the following but talked about

quizer of some fol

~~phonons~~

→ zero pt energy

→ phonons

(also trans: $\sum q_i a^\dagger_i$

~~$\sum q_i a$~~

$a^2 = (a^\dagger)^2 = 0$

I9 ~~X~~ ~~X~~10

[Taste of Matrix mechanics: Heisenberg, Born....]

omitted F'05 / '06 for time reasons

Optional

Operators as ∞ dim'l matrices

Pick an operator $\hat{A}$

Pick a basis, eg energy basis $|n\rangle = |0\rangle, |1\rangle, |2\rangle, \ldots \longrightarrow \psi = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \end{pmatrix}$

~~Pick an operator~~ Then $|\psi\rangle = \sum_n c_n |n\rangle$

Form a matrix A whose matrix elements are $A_{mn} = \langle m|\hat{A}|n\rangle$

$$\begin{bmatrix} \langle 0|\hat{A}|0\rangle & \langle 0|\hat{A}|1\rangle & \langle 0|\hat{A}|2\rangle & \cdots \\ \langle 1|\hat{A}|0\rangle & \langle 1|\hat{A}|1\rangle & \langle 1|\hat{A}|2\rangle & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix}$$

eg $\hat{a}$:
$$\langle m|\hat{a}|n\rangle = \langle m|\sqrt{n}\,|n-1\rangle = \sqrt{n}\,\underbrace{\langle m|n-1\rangle}_{\delta_{m,n-1}}$$

only nonzero if $m = n-1$

$$a = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ \vdots & & & & \end{bmatrix}$$

$$a^\dagger = (a^T)^* = \begin{bmatrix} 0 & 0 & \cdots & & \\ \sqrt{1} & 0 & \cdots & & \\ 0 & \sqrt{2} & 0 & & \\ 0 & 0 & \sqrt{3} & 0 & \end{bmatrix}$$

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$$X = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^\dagger) = \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \\ & \vdots & & & \end{bmatrix}$$

$$a^\dagger a = \begin{bmatrix} 0 & 0 \\ \sqrt{1} & 0 \\ 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} 0 & \sqrt{1} & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} = N$$

$$N_{mn} = \langle m | N | n \rangle = n \underbrace{\delta_{mn}}_{\text{diagonal matrix}}$$

$$a a^\dagger = \begin{bmatrix} 0 & \sqrt{1} & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} 0 & 0 \\ \sqrt{1} & 0 \\ 0 & \sqrt{2} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

$$a a^\dagger - a^\dagger a = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mathbb{1} \qquad [a, a^\dagger] = 1$$

$$\hat{H} = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right) = \hbar\omega \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{3}{2} & 0 \\ 0 & 0 & \frac{5}{2} \end{bmatrix}$$

$\hat{H}$ is always diagonal in the energy basis!