<u>Particle in a potential</u>

$$E = T + V = \underbrace{\frac{p^2}{2m}}_{\text{non rel.}} + V(x) \qquad \text{[recall Bohr model]}$$

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

[What is $\hat{V}$?]

Power series expansion of $V(x) = V_0 + V_1 x + V_2 x^2 + \ldots$

$$\Rightarrow \hat{V} = V_0 + V_1 \hat{X} + V_2 \hat{X}^2 + \ldots$$

$\hat{p}$, $\hat{x}$ are hermitian

$\hat{V}$ is hermitian if $V(x)$ is a real function, ie $V_0, V_1 \ldots$ are real

$$\hat{V}^\dagger = V_0^* + V_1^* \hat{X}^\dagger + V_2^* (\hat{X}^2)^\dagger + \ldots$$

But $(\hat{X}^n)^\dagger = \hat{X}^\dagger \hat{X}^\dagger \ldots \hat{X}^\dagger = \hat{X}^n$

$\Rightarrow \hat{V}^\dagger = \hat{V}$ if V

$\Rightarrow \hat{H}$ is hermitian

Recall
Ehrenfest theorem
~~Heisenberg eqns~~

$$\frac{d}{dt}\langle A\rangle = \frac{1}{i\hbar}\langle [A,H]\rangle$$

Consider $\frac{d}{dt}\langle p\rangle$

$$[p,H] = [p, \frac{p^2}{2m} + V(x)] \overset{\text{HW}}{=} -i\hbar\frac{dV}{dx}$$

$$\Rightarrow \frac{d}{dt}\langle p\rangle = -\left\langle \frac{dV}{dx}\right\rangle \quad \text{(Ehrenfest's theorem)}$$

Classically $\frac{dp}{dt} = F_x = -\frac{dV}{dx}$

[HW: for free particle $\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m}$

$\frac{d}{dt}\langle p\rangle = 0$.]

Can alternatively compute commutator in position space

$$[p, V(x)]_{pos}\psi(x) = p_{pos}V(x)_{pos}\psi - V(x)_{pos}p_{pos}\psi$$

$$= \frac{\hbar}{i}\frac{d}{dx}(V(x)\psi) - V(x)\frac{\hbar}{i}\frac{d\psi}{dx}$$

$$= -i\hbar\frac{dV}{dx}\psi$$

$$= -i\hbar\left(\frac{dV}{dx}\right)_{pos}\psi$$

Energy eigenvalue eqn

$$\hat{H}|E\rangle = E|E\rangle$$

$$\left(\frac{\hat{p}^2}{2m} + \hat{V}\right)|E\rangle = E|E\rangle$$

In position space, energy eigenstates are $\langle x|E\rangle \equiv u_E(x)$

$u(x)$ is commonly used for energy eigenstates

$$(\hat{H})_{pos} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right) + V(x)$$

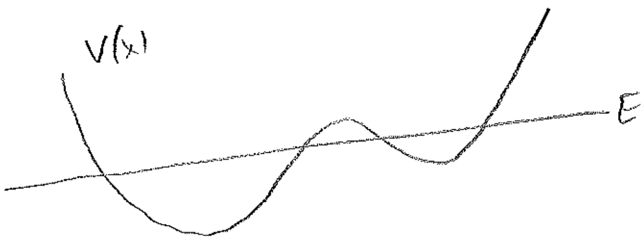
$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$\Rightarrow$ energy eigenfunctions satisfy

$$-\frac{\hbar^2}{2m}\frac{d^2u_E}{dx^2} + V(x)\,u_E = E\,u_E \qquad (\text{t.i. S.e})$$

$$\frac{d^2u_E}{dx^2} = -\frac{2m}{\hbar^2}\left(E - V(x)\right)u_E(x)$$

$$\Rightarrow \boxed{\frac{1}{u_E}\frac{d^2 u_E}{dx^2} = -\frac{2m}{\hbar^2}\left(E - V(x)\right)}$$

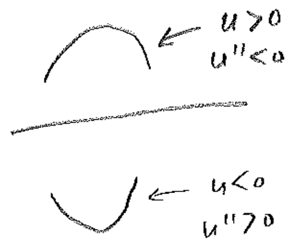


classically allowed regions $\Rightarrow E - V(x) > 0 \Rightarrow \frac{u''}{u} < 0 \Rightarrow$ concave toward x-axis

classically forbidden regions $\Rightarrow E - V(x) < 0 \Rightarrow \frac{u''}{u} > 0 \Rightarrow$ concave away from axis

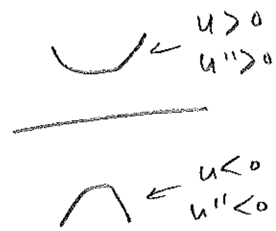
turning point $\Rightarrow E - V(x) = 0 \Rightarrow \frac{u''}{u} = 0 \Rightarrow$ point of inflection

concave toward axis



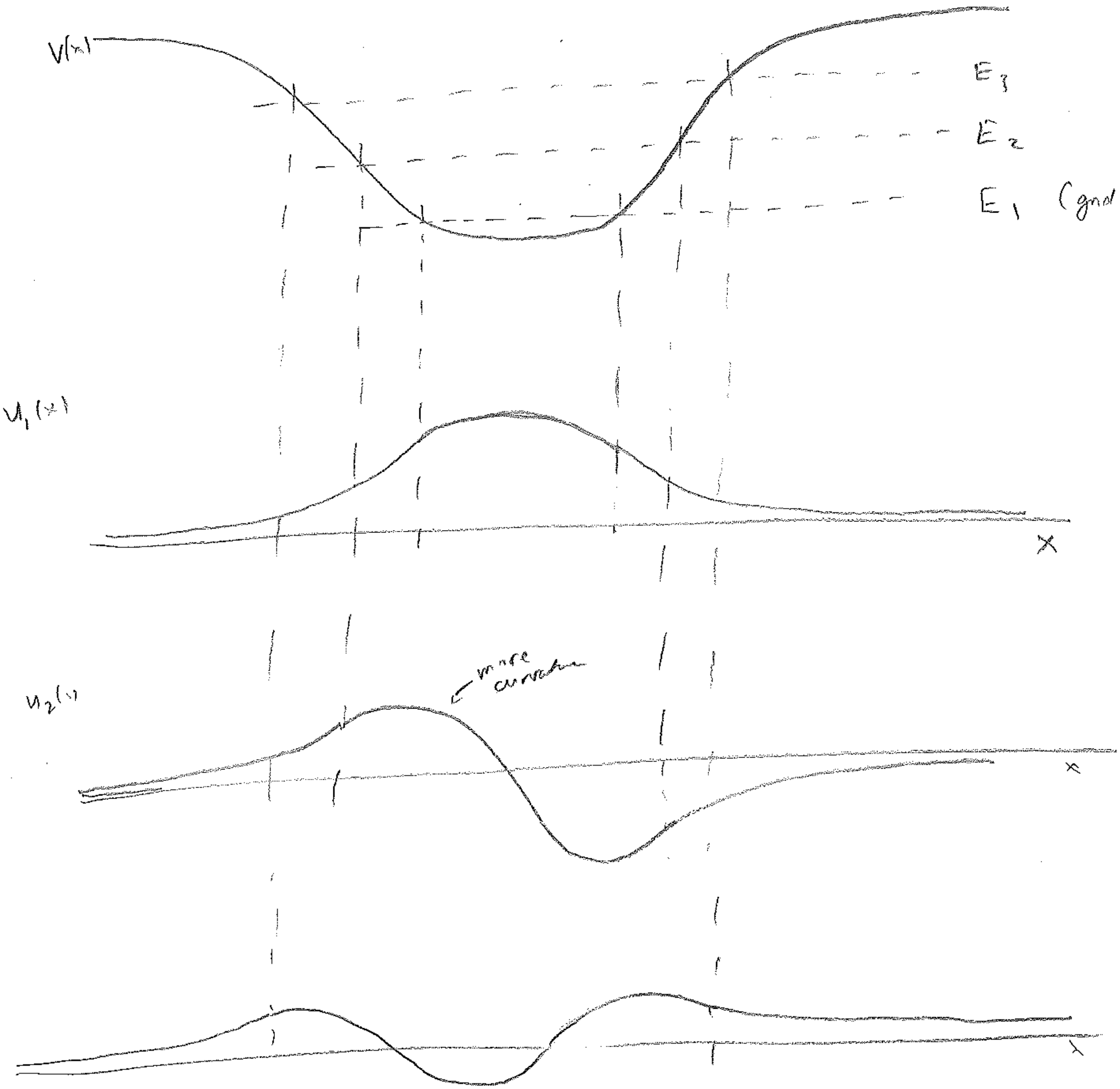
$\frac{u''}{u} < 0$

concave away from axis



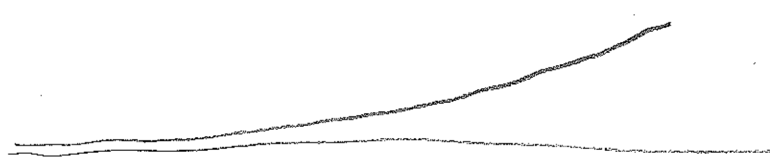
$\frac{u''}{u} > 0$

Suppose the potential has the shape



For energies between the eigenvalues, $u(x) \not\to 0$ as $x \to \infty$

Suppose $E < V_{min} \Rightarrow$ all regions forbidden
$\Rightarrow$ always concave away $\Rightarrow u(x) \not\to 0$
not normalizable



$\Rightarrow \exists$ no energy eigenvalues
$\forall E < V_{min}$

Let's assume the Hamiltonian $\hat{H} = \frac{p^2}{2m} + V(x)$

has a <u>discrete</u> spectrum $\{E_n\}$ and that the

eigenstates $|E_n\rangle$ are non degenerate (true in 1 dimension)

Completeness relation $\sum |E_n\rangle\langle E_n| = 1$

orthonormality $\langle E_n | E_m\rangle = \delta_{nm}$

Expand the initial state in the energy basis

$$|\psi(0)\rangle = \sum_n |E_n\rangle \underbrace{\langle E_n|\psi(0)\rangle}_{c_n = \text{coeffs}} = \sum c_n |E_n\rangle \text{ in energy basis}$$

Then $$|\psi(t)\rangle = e^{-\frac{iHt}{\hbar}} |\psi(0)\rangle = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} |E_n\rangle$$

each energy eigenstate picks up a complex phase

[That was all review]

In position space

$$\psi(x,t) = \langle x|\psi(t)\rangle = \sum c_n e^{-\frac{iE_n t}{\hbar}} \underbrace{\langle x|E_n\rangle}$$

$u_n(x)$ = energy eigenstate in position space

$$\boxed{\psi(x,t) = \sum c_n e^{-\frac{iE_n t}{\hbar}} u_n(x)}$$

Coefficients given by

$$c_n = \langle E_n|\psi(0)\rangle = \int dx \underbrace{\langle E_n|x\rangle}_{u_n^*(x)} \underbrace{\langle x|\psi(0)\rangle}_{\psi(x,0)}$$

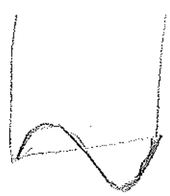
$$\boxed{c_n = \int dx\, u_n^*(x)\, \psi(x,0)}$$

Review of particle in a box

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu \quad \text{for} \quad 0<x<L$$

$$u(x) = 0 \quad \text{for} \quad \begin{cases} x<0 \\ x>L \end{cases}$$

$$\begin{cases} u_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi n x}{L}\right) \\ E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2} \end{cases}$$



- concave toward x-axis
- continuous u
- $\frac{du}{dx}$ discontinuous only where $V \to \infty$

[can skip]

(skip)

If $\psi(x,0)$ consists of a single energy eigenstate

eg $\psi(x,0) = u_n(x)$

then $\psi(x,t) = u_n(x) e^{-\frac{iE_n t}{\hbar}}$ [separable solution of t.d.S.e.]

and $|\psi|^2 = |u_n(x)|^2$ is indep of time $\Rightarrow$ stationary state

all observables for this state do not depend on time

If $\psi(x,0)$ consists of several eigenstates (of different energies)

$\psi(x,0) = \sum c_n u_n(x)$

then $\psi(x,t) = \sum c_n u_n(x) e^{-\frac{iE_n t}{\hbar}}$ is not a stationary state

$$|\psi(x,t)|^2 = \left(\sum c_n^* u_n^*(x) e^{+\frac{iE_n t}{\hbar}}\right)\left(\sum c_m u_m(x) e^{-\frac{iE_m t}{\hbar}}\right)$$

$$= \underbrace{\sum_n |c_n|^2 |u_n(x)|^2}_{\text{indep of time}} + \sum_{n \neq m} c_n^* c_m \underbrace{u_n^*(x) u_m(x) e^{\frac{i(E_n - E_m)t}{\hbar}}}_{\text{cross-terms carry time dependence}}$$

(change / motion requires interference)

[unless degenerate]

Time independent Schrodinger eqn

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

SKIP

~~necessary?~~ Let's skip this 32-1

Boundary conditions on wavefunction $u(x)$

① $u(x) \longrightarrow 0$ as $x \to \pm\infty$ (square integrability)

② $u(x)$ continuous at all points

③ $\frac{du}{dx}(x)$ continuous, except if $V(x)$ is infinite

necessary?

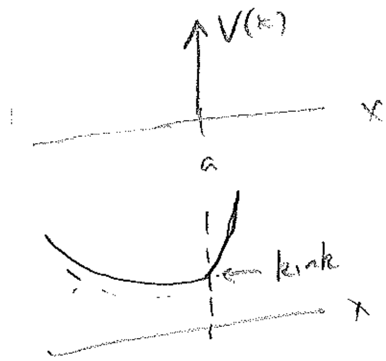
Consider $$\int_{a-\epsilon}^{a+\epsilon} \frac{d^2u}{dx^2}\,dx = \int_{a-\epsilon}^{a+\epsilon} \frac{d}{dx}\left(\frac{du}{dx}\right) dx = \frac{du}{dx}\bigg|_{a-\epsilon}^{a+\epsilon} = \text{discontinuity in } \frac{du}{dx}$$

But $$\int_{a-\epsilon}^{a+\epsilon} \frac{d^2u}{dx^2}\,dx = -\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} (E - V(x))\,u(x)\,dx$$

If $V(x)$, $u(x)$ finite, the integral $\propto \epsilon$ $\Rightarrow \frac{du}{dx}(a+\epsilon) - \frac{du}{dx}(a-\epsilon) \xrightarrow[\epsilon\to 0]{} 0$

Suppose $V(x) = +\alpha\,\delta(x-a)$ then $-\frac{2m}{\hbar^2}\int (E - \alpha\,\delta(x-a))\,u(x)\,dx$

$$\frac{du}{dx}(a+\epsilon) - \frac{du}{dx}(a-\epsilon) = \frac{2m\alpha}{\hbar^2}\,u(a)$$



Perhaps we don't need to review solving 1d t.i.s.e since we did so much in PHY40 (skip: discussed in [illegible]) previously?)

Theorem:

If the potential is even: $V(x) = V(-x)$

then nondegenerate eigenfunctions are either even or odd

Proof: Let $u(x)$ obey

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

Let $x \to -x$

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

$$\downarrow$$

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

ie $u(-x)$ obeys the same eqn as does $u(x)$

Since $u(x)$ is nondegenerate, $u(-x)$ must be prop. to $u(x)$

$$u(-x) = \lambda u(x)$$

Let $x \to -x$

$$u(x) = \lambda u(-x) = \lambda^2 u(x) \implies \lambda^2 = 1$$

$$\lambda = \pm 1$$

$\lambda = 1$: $u(-x) = u(x)$ even

$\lambda = -1$ $u(-x) = -u(x)$ odd

Recall: ptcl in box