Lecture 8 137A ①

Time indep. Schrödinger Equation

- Assume time independent potential $V(\vec{r})$

→ look for "stationary solutions"
(aka eigenfunctions)
→ These are standing waves

Apply Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r},t) = \left[\frac{-\hbar^2}{2m} \nabla^2 + \hat{V}(\vec{r},t) \right] \psi(\vec{r},t)$$

with ansatz solution:

$$i\hbar\, \psi(\vec{r}) \frac{d}{dt} f(t) = \left[\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + \hat{V}(\vec{r}) \psi(\vec{r}) \right] \cdot f(t)$$

Divide by $\psi(\vec{r}) f(t)$
both sides

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = \frac{1}{\psi(\vec{r})} \left[\frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) \right]$$

Method of separation of variables ②

→ Both sides must equal a constant which has dimensions of energy → call it E.

- $i\hbar \frac{d}{dt} f(t) = E f(t)$

$$f(t) = C e^{-iEt/\hbar}$$

$$\Longrightarrow \Psi(\vec{r},t) = \psi(\vec{r})\, e^{-iEt/\hbar}$$

↙ Soln of time indep. Schrödinger equation

- $$\underbrace{\left[\frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right]}_{\hat{H}} \psi(\vec{r}) = E\, \psi(\vec{r})$$

$$\longrightarrow \quad \hat{H}\psi(\vec{r}) = E\psi(\vec{r})$$

* The eigenfunctions of $\hat{H}$ are stationary states with $e^{-iEt/\hbar}$ time dep.

* Eigenvalues are E

* $\hat{H}$ is Hermitian and E is real

- E is a well defined quantity for a stationary state of Schrödinger equation.

$$\langle E \rangle = \int \psi^* \left(i\hbar \frac{\partial}{\partial t} \right) \psi \, d\vec{r} = \int \psi^* (\hat{H}) \psi \, d\vec{r} = E$$

since $\int \psi^* \psi \, d\vec{r} = 1$

For stationary states, probability (3)
density is constant in time.

$$P(\vec{r},t) = \Psi^*(\vec{r},t)\,\Psi(\vec{r},t) = |\Psi(\vec{r})|^2$$

General solution of Schrödinger Equation:

We would like to construct any solution of the Schrödinger equation as a <u>combination</u> of stationary states.

→ Just like basis vectors in geometry, require Ψ_E and $\Psi_{E'}$ to be <u>orthogonal</u>. $(E \neq E')$

$$\int \Psi^*_{E'}(\vec{r})\,\Psi_E(\vec{r})\,d\vec{r} = 0\ , \quad E \neq E'$$

<u>Proof:</u>

$$\hat{H}\Psi_E = E\,\Psi_E$$

multiply both sides by $\Psi^*_{E'}$

$$\Psi^*_{E'}\,(\hat{H}\Psi_E) = E\,\Psi^*_{E'}\,\Psi_E \qquad (1)$$

For the other function.

$$\hat{H}\Psi_{E'} = E'\,\Psi_{E'}$$

Take complex conjugate

$$(\hat{H}\psi_{E'})^* = E'\psi^*_{E'} \quad \text{since } E' \text{ is real}$$

Multiply on the right by ψ_E

$$(\hat{H}\psi_{E'})^*\psi_E = E'\psi^*_{E'}\psi_E \qquad (2)$$

Subtract (2) from (1)

$$\psi^*_{E'}(\hat{H}\psi_E) = E\psi^*_{E'}\psi_E \qquad (1)$$

$$-\ (\hat{H}\psi_{E'})^*\psi_E = E'\psi^*_{E'}\psi_E \qquad (2)$$

$$\psi^*_{E'}(\hat{H}\psi_E) - (\hat{H}\psi_{E'})^*\psi_E = (E-E')\psi^*_{E'}\psi_E$$

Integrate both sides,

$$(E-E')\int \psi^*_{E'}\psi_E\, d\vec{r} = \int \psi^*_{E'}(\hat{H}\psi_E) - \underbrace{(\hat{H}\psi_{E'})^*}_{\psi^*_{E'}\hat{H}\psi_E}\psi_E\, d\vec{r}$$

since $\hat{H} = \hat{H}^*$

$$= 0$$

Thus $\int \psi^*_{E'}(\vec{r})\psi_E(\vec{r})\, d\vec{r} = \delta_{EE'}$!

* If there is degeneracy, i.e.

different eigenfunctions have the same eigenvalue, we can use the Gram-Schmidt procedure to generate an orthonormal set.

*** We postulate that the energy spectrum obtained by solving the time-indep. Schrödinger eqn. represents all the possible realizable energies of the system.

Thus, a general state of the time dependent equation is

$$\Psi(\vec{r},t) = \sum_{E} \underbrace{C_E(t)}_{} \Psi_E(\vec{r})$$

coefficients depend on time.

- compare to a vector expanded in basis vectors (eg. $\hat{x}, \hat{y}, \hat{z}$) with time varying coefficients.

To figure out coefficients, multiply by $\psi^*_{E'}(\vec{r})$ and integrate: (6)

$$\int \psi^*_{E'}(\vec{r})\psi(\vec{r},t)\,d\vec{r} = \sum_E C_E(t) \underbrace{\int \psi^*_{E'}(\vec{r})\psi_E(\vec{r})\,d\vec{r}}_{\delta_{EE'}}$$

$$= C_{E'}(t)$$

To form the full time dependent solution, recall that each eigenfunction has a time dependence $e^{-iEt/\hbar}$.

Thus, each eigenfunction is $\psi_E(\vec{r})e^{-iEt/\hbar}$

The general solution is then.

$$\psi(\vec{r},t) = \sum_E C_E(t=0)\,\psi_E(\vec{r})\,e^{-iEt/\hbar}$$

$$C_E = \int \psi^*_E(\vec{r})\,\psi(\vec{r},t=0)\,d\vec{r}$$

Probability conservation implies $\sum_E \underbrace{|C_E|^2}_{\text{prob. to be in state with } E.} = 1$

** Note: The probability density of a sum of stationary states is time dependent! (Need to add amplitudes of functions with different E (i.e. ω)!)

- As a final check of the formalism, let's calculate $\langle E \rangle$ for a general state.

$$\langle E \rangle = \langle H \rangle = \int \psi^*(\vec{r},t)\,\hat{H}\,\psi(\vec{r},t)\,d\vec{r}$$

$$= \sum_E \sum_{E'} c^*_{E'} c_E\, e^{-i(E-E')t/\hbar} \int \psi^*_{E'}(\vec{r})\,\hat{H}\,\psi_E(\vec{r})\,d\vec{r}$$

$$= \sum_E \sum_{E'} c^*_{E'} c_E\, e^{-i(E-E')t/\hbar}\, E \underbrace{\int \psi^*_{E'}(\vec{r})\,\psi_E(\vec{r})\,d\vec{r}}_{\delta_{EE'}}$$

$$= \sum_E \underbrace{|c_E|^2}_{\text{probability that a measurement will yield } E} E$$

Lecture 9 1-D problems & Energy quantization

Recall the time independent Schrödinger equation:

$$\hat{H}\psi = E\psi$$

The eigenfunctions and eigenenergies are different for different types of potential functions $\hat{V}(\vec{r})$

Consider 1-D problems:

$$\psi(x,t) = \psi(x)\, e^{-iEt/\hbar}$$

The Schrödinger equation thus reads

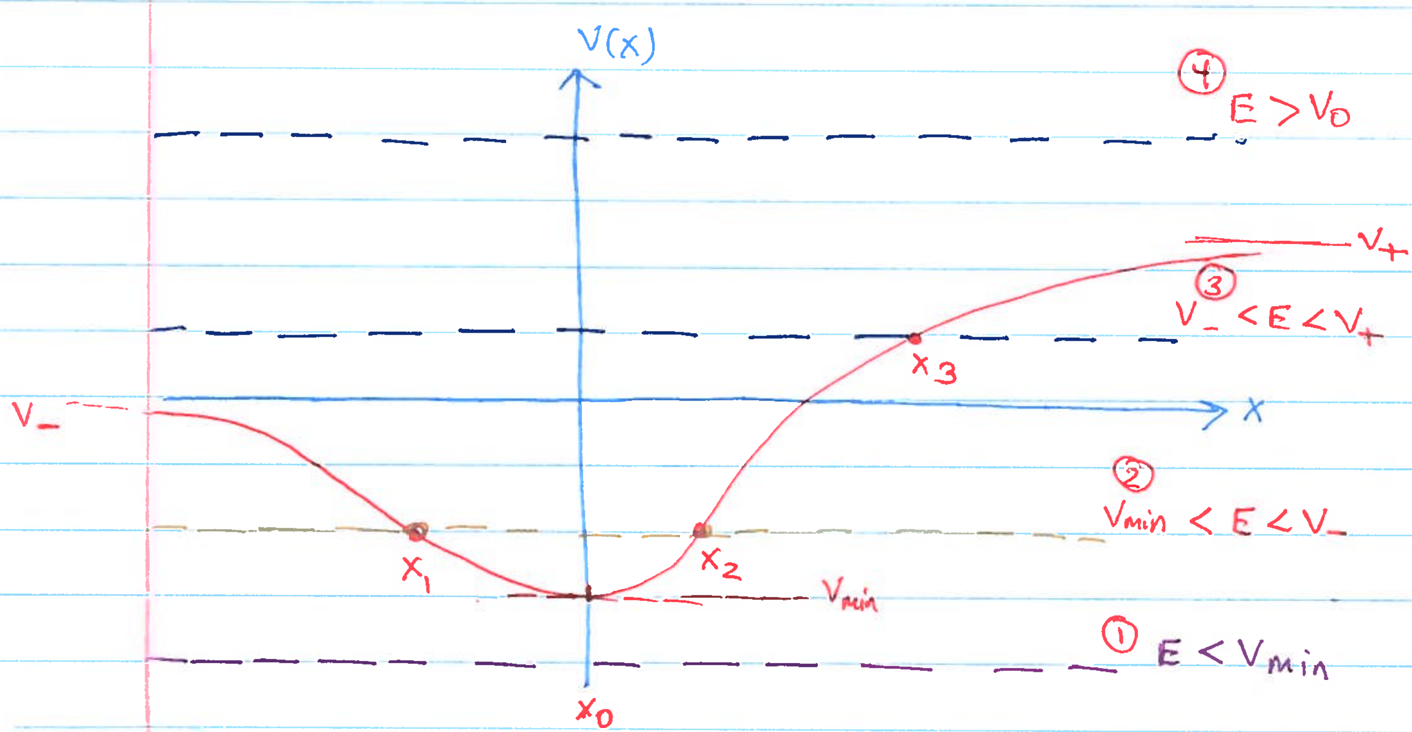
$$\left[\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\,\psi(x)$$

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

$\Longrightarrow$ • Two linearly indep. solutions for each E

• Form of solution depends on whether $V-E > 0$ or $V-E < 0$.

Consider a generic $V(x)$



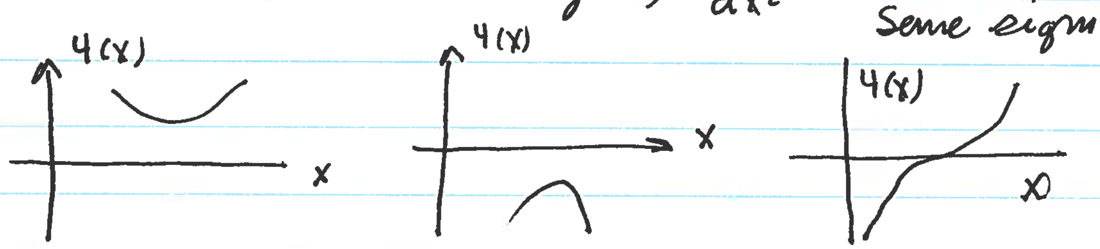
- Require $\psi(x)$ to be finite and single valued to maintain probabilistic interpretation

$\rightarrow$ $\psi(x)$ is finite, continuous, and has a continuous derivative

Case 1 $E < V_{min}$

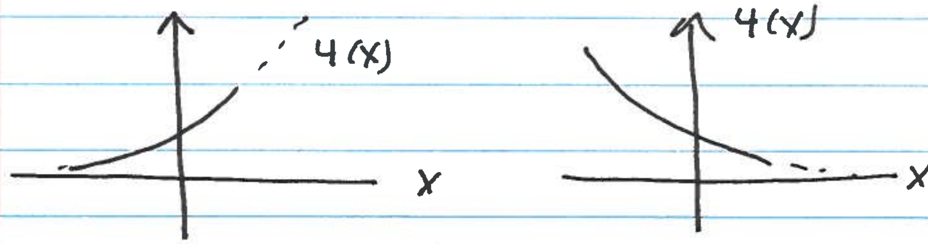
$V(x) - E > 0$ always, $\frac{d^2\psi}{dx^2}$ and ψ have same sign

egs:



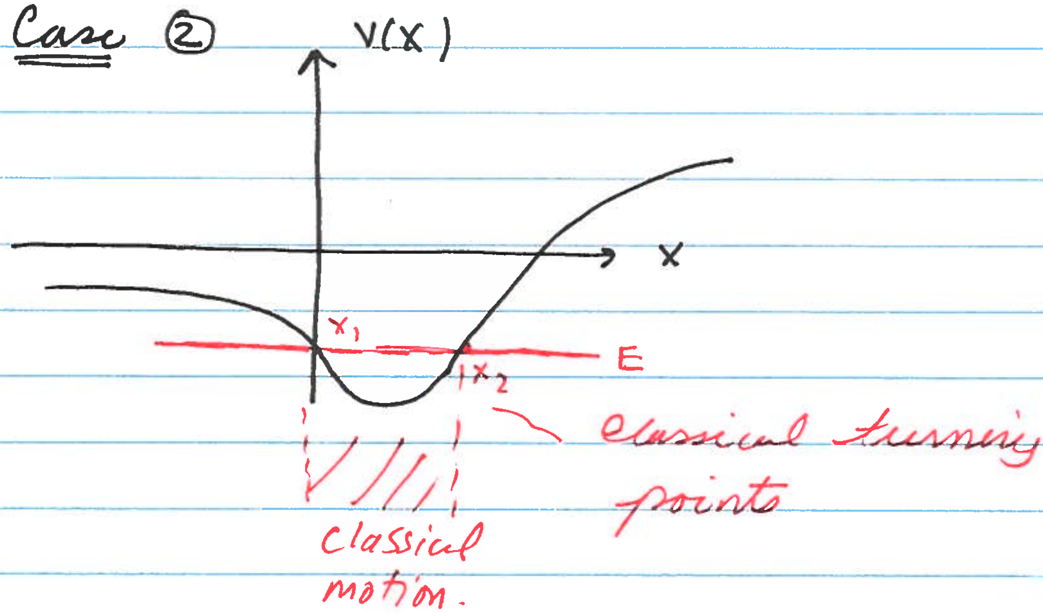
Thus, we cannot find a solution which is finite everywhere b/c $|\psi| \to \infty$ as $x \to \pm\infty$

We could try to pick functions that approach the x-axis, but they blow up at $+\infty$ or $-\infty$



$\Longrightarrow$ * No physically allowed solution when $E < V(x)$ for all x.

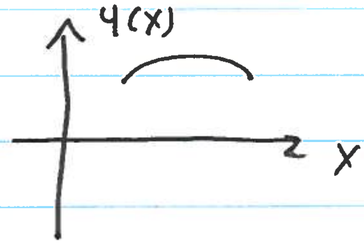
Case ②

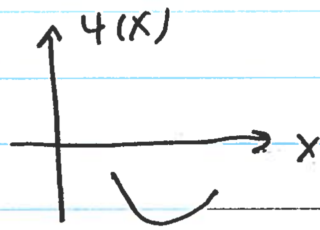


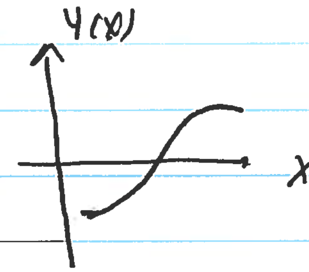
Quantum Mechanically: Solutions exist for certain, discrete E's.

- In the internal region $x \in [x_1, x_2]$,

$\frac{d^2\psi}{dx^2}$ and ψ have opposite sign.





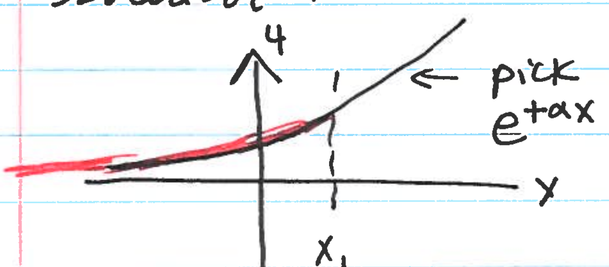


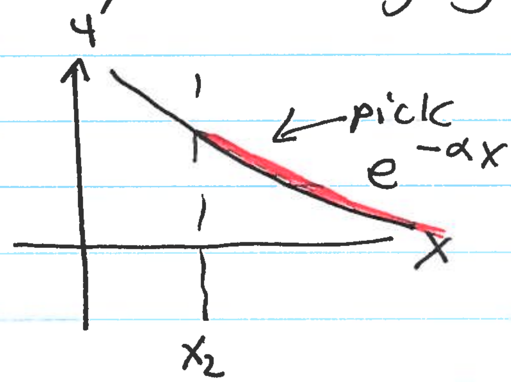
→ always concave towards x → axis
→ oscillatory function
→ Solutions could be $e^{\pm i\alpha x}$

- In the external region $x < x_1$, $x > x_2$,

$\frac{d^2\psi}{dx^2}$ and ψ have same sign.

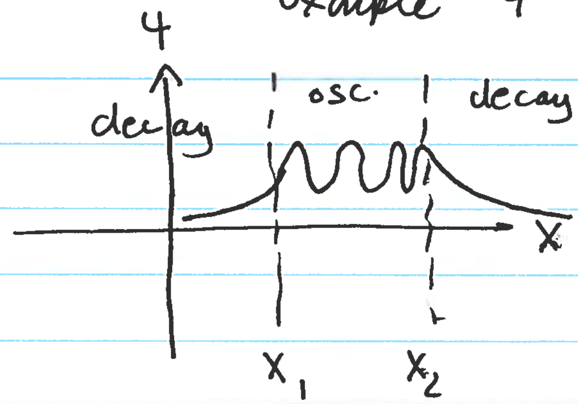
We can use $e^{\pm \alpha x}$ and pick decaying solution.





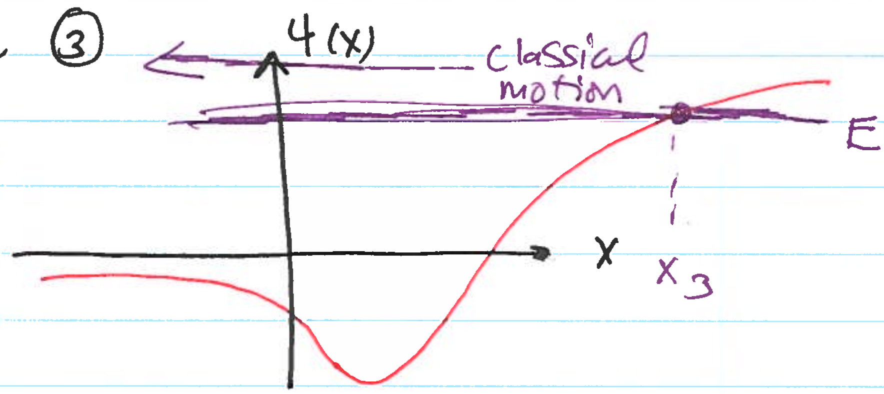
* Condition that $|\psi| \to 0$ as $|x| \to \infty$ and $\frac{d\psi}{dx}$ be continuous at x_1, x_2 only satisfied for certain E → BOUND STATES

Example 4

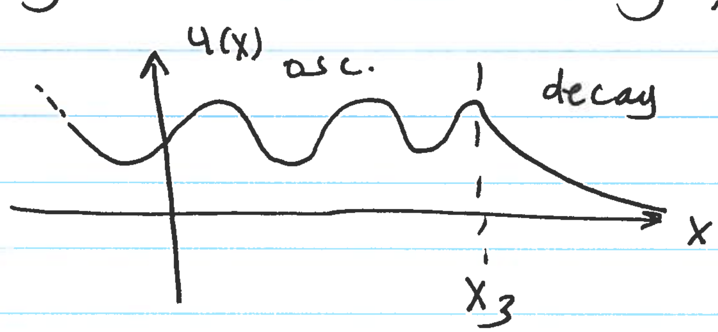


→ Thus, QM allows only certain discrete energies, but they are <u>not</u> confined to region with $E > V$!

Case 3



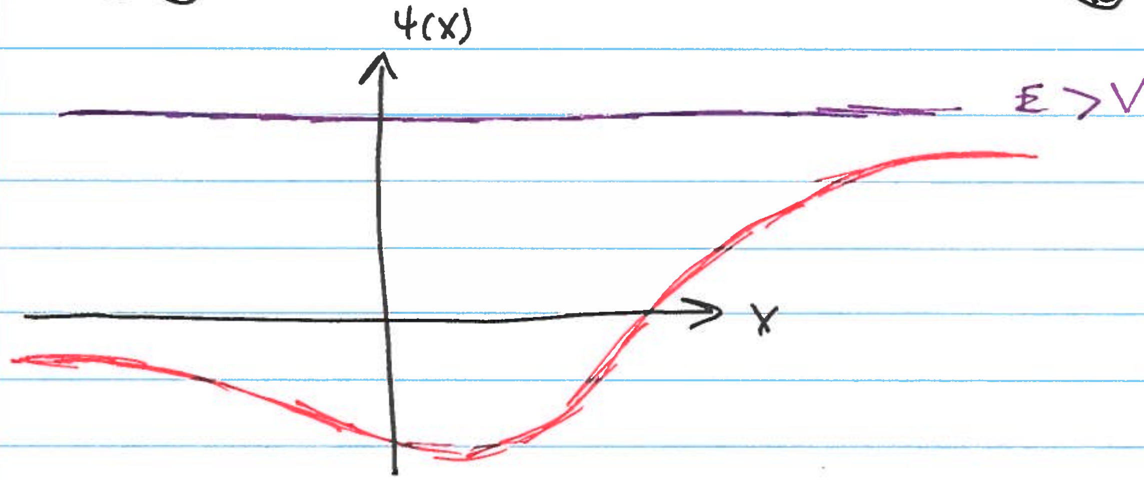
Only one classical turning point at x_3



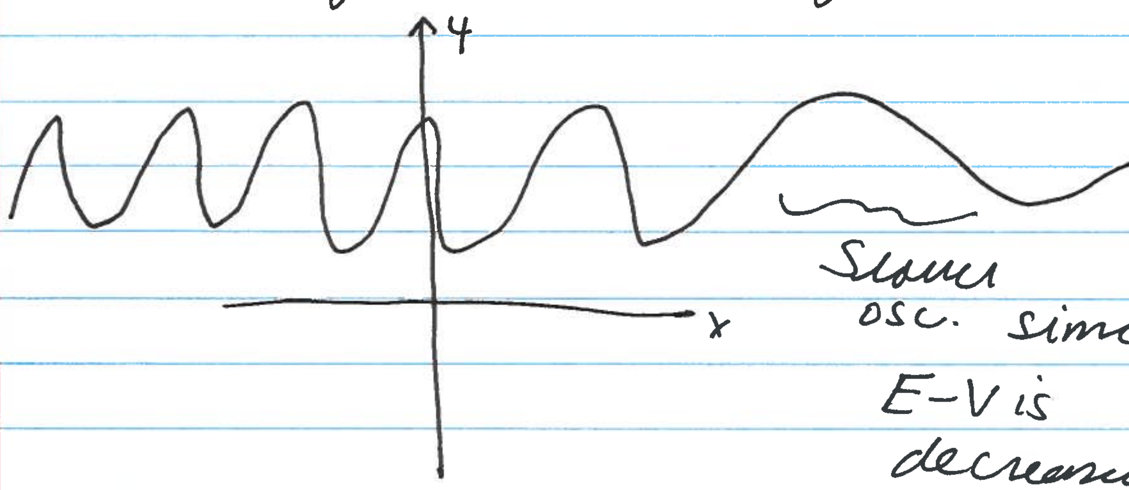
SCATTERING STATES

* <u>Note</u>: We can always find a solution for every E since we have only to match at x_3. Continuous spectrum!

Case 4

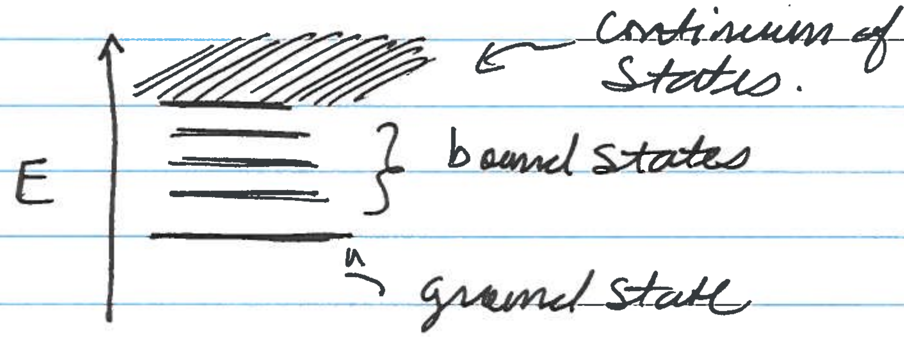


Oscillating solutions everywhere



Slower osc. since E−V is decreasing

Thus, the energy spectrum looks like



Lecture 10 Formal solution to 1-D problems: free particle and potential step

The Free Particle

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\,\psi(x)$$ for eigenfunctions $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$

let $k = \left(\frac{2mE}{\hbar}\right)^{1/2}$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

$\rightarrow$ General solution: $\psi(x) = Ae^{+ikx} + Be^{-ikx}$

k must be a real # or $\psi \to \infty$ as $x \to \pm\infty$

- $E = \frac{\hbar^2 k^2}{2m} \geq V = 0$ so E is continuous and can take any value from 0 to ∞

- E is doubly degenerate since $e^{\pm ikx}$ have same energy (i.e. particle moving left or right)

• Note $e^{\pm ikx}$ also eigenfunctions of $\hat{P}_x = -i\hbar \frac{d}{dx}$ (Note $\hat{H} \sim \hat{P}_x^2$
$[\hat{H}, \hat{P}_x] = 0$)

General time dependent solution

$$\psi(x,t) = \left(Ae^{ikx} + Be^{-ikx}\right) e^{-iEt/\hbar}$$

$$= Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

Consider different possible boundary conditions.

a. $\underline{B=0}$

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

→ particle moving to the right and momentum $\hbar k$.

Probability density $P = |\psi(x,t)|^2 = |A|^2$
(indep. of space + time)

→ Remember, a plane wave is an idealized, simple approx to a real wavepacket

Let's calculate the probability current j at $t=0$

$$j = \frac{\hbar}{2mi}\left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right]$$

③

$$= \frac{\hbar}{2mi}\left(A^* e^{-ikx} A(ik) e^{ikx} - A e^{ikx} A^*(-ik) e^{-ikx}\right)$$

$$= \frac{\hbar k}{m}|A|^2 = \frac{p}{m}|A|^2 = \underbrace{v}_{\text{velocity}}\,\underbrace{|A|^2}_{\text{prob density}}$$

b. $A=0$

Same as case a alone but moving to the left.

c. $A=B$

$$\psi(x,t) = A\left(e^{ikx} + e^{-ikx}\right)e^{-i\omega t}$$

$$= 2A\cos(kx)\,e^{-i\omega t}$$

$\longrightarrow$ Standing wave with nodes at

$$x_n = \frac{\pm\left(\frac{\pi}{2} + n\pi\right)}{k}, \quad n = 0, 1, 2, \ldots$$

Probability density $P(x) = \underbrace{|2A|^2}_{C}\cos^2(kx)$

$$j = \frac{\hbar}{2mi}\left(-C^*\cos(kx)\,C\,k\sin(kx) + C\cos(kx)\,C^*k\sin(kx)\right) = 0$$

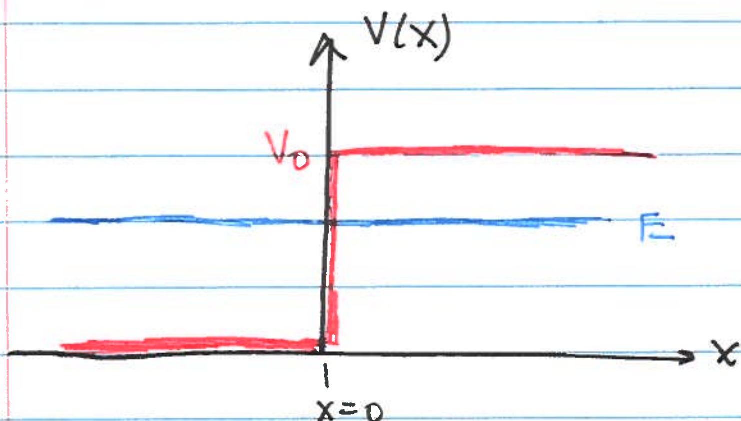
→ No probability current!
→ ψ vanishes at nodes

If we want to normalize ψ,
we can use the def. of the δ function.

We can use $\int_{-\infty}^{\infty} e^{i(k-k')x} dx = 2\pi\delta(k-k')$

Thus $\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$

The Potential Step



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

→ Consider different values of E
• No solution for $E<0$

Case 1: $E < V_0$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \qquad k = \left(\frac{2mE}{\hbar^2}\right)^{1/2} \text{ for } x<0$$

require ψ and $\frac{d\psi}{dx}$ to be finite and continuous and

$$\frac{d^2\psi(x)}{dx^2} - K^2\psi(x) = 0 \quad K = \left[\frac{2m}{\hbar^2}(V_0 - E)\right]^{1/2}$$

for $x > 0$

For $x<0$: Free particle

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

For $x>0$:

$$\psi(x) = Ce^{Kx} + De^{-Kx}$$

Require ψ and $\frac{d\psi}{dx}$ to be finite and continuous at all x

- We can consider a particle coming from the left. Thus $C=0$
- Now, we have to have continuity in ψ and $\frac{d\psi}{dx}$ at $x=$

Continuity of $\psi(x)$

@ $x=0 \rightarrow A+B=D$

Continuity of $\frac{d\psi}{dx}$ @ $x=0$

$$ik(A-B) = -KD$$

Combine equations,

$$A = \left(\frac{1 + iK/k}{2}\right)D \qquad B = \left(\frac{1 - iK/k}{2}\right)D$$

Note that $\frac{B}{A} = \frac{1 - iK/k}{1 + iK/k}$ is a # of modulus 1

and can be written as

$$\frac{B}{A} = e^{i\alpha} \quad \text{where } \alpha = 2\tan^{-1}\left[-\left(\frac{V_0}{E} - 1\right)^{1/2}\right]$$

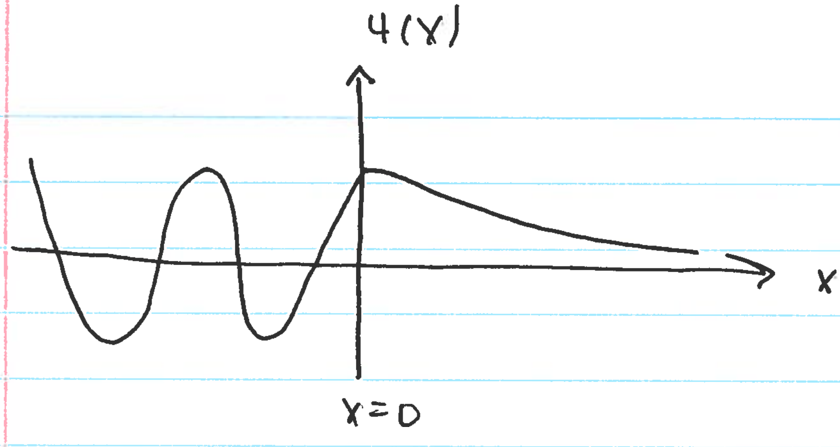
We have used the definitions of K, k in terms of V_0, E

$$\frac{D}{A} = \frac{2}{1 + iK/k} = 1 + e^{i\alpha}$$

We can then write ψ as:

$$\psi(x) = \begin{cases} 2Ae^{i\alpha/2}\cos\left(kx - \alpha/2\right), & x<0 \\ 2Ae^{i\alpha/2}\cos\left(\frac{\alpha}{2}\right)e^{-Kx}, & x>0 \end{cases}$$

⑦



Ae^{ikx} is the right moving wave

Be^{-ikx} is the reflected wave.

Reflection coefficient $R = \frac{|B|^2}{|A|^2} = 1$ → agrees with classical physics for $E < V_0$.

↓

ratio of probabilities

But... probability density...

$P(x) = 4|A|^2 \cos^2(kx - \alpha/2)$ for $x < 0$

$= |D|^2 e^{-2Kx}$ for $x > 0$

<u>Note</u>: We cannot experimentally determine wave-like character in the region $x > 0$.

Justification: To have appreciable probability in this region, need to localize $\Delta x \sim \frac{1}{K}$

Uncertainty principle says

$$\Delta P_x \gtrsim \frac{\hbar}{\Delta x} \simeq \hbar k = \left[2m(V_0 - E)\right]^{1/2}$$

The energy would thus be uncertain by

$$\Delta E = \frac{(\Delta P_x)^2}{2m} \gtrsim V_0 - E. \longrightarrow \text{Thus, if you}$$ ✱

measure the particle at $x > 0$, you cannot say with certainty that it is under the barrier!

Consider the limit of an infinite step.

let $V_0 \to \infty$ (E is kept constant)

$K \to \infty$, thus $\psi(x) \to 0$ in classically forbidden region

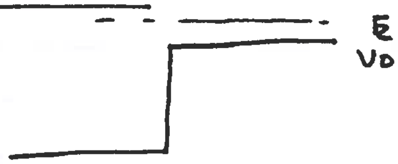
$$\lim_{V_0 \to \infty} \frac{B}{A} = -1 \qquad \lim_{V_0 \to \infty} \frac{D}{A} = 0$$

Thus
$$\psi(x) = \begin{cases} A(e^{ikx} - e^{-ikx}), & x < 0 \\ 0, & x > 0 \end{cases}$$

ψ goes to 0 at $x = 0$

✱ Note, there is a discontinuity of the slope of ψ at 0, but "smooth" joining is only needed for

Case 2 $E > V_0$



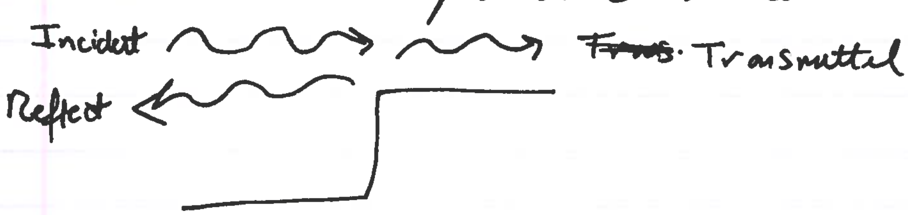
$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \qquad k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}, \quad x<0$$

$$\frac{d^2\psi(x)}{dx^2} + k'^2\psi(x) = 0 \qquad k' = \left[\frac{2m}{\hbar^2}(E-V_0)\right]^{1/2}, \quad x>0$$

$\longrightarrow$ oscillatory solutions everywhere

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x<0 \\ Ce^{ik'x} + De^{-ik'x}, & x>0 \end{cases}$$

Consider particle incident from left, Thus $D=0$



Note: Classical physics says particle is always transmitted. QM says there is a probability of reflection!

Apply BC:

@ $X=0$ continuity of ψ

$$A+B=C$$

continuity of $\frac{d\psi}{dX}$

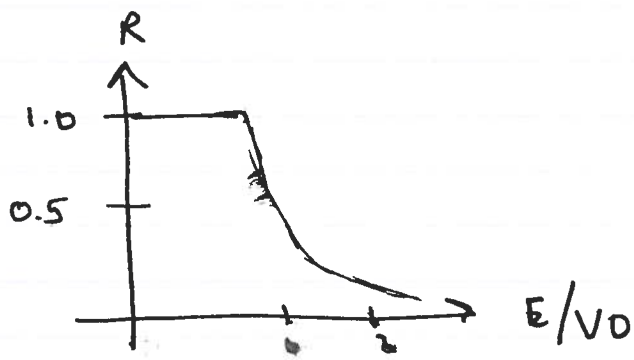
$$k(A-B) = k'C$$

$$\frac{B}{A} = \frac{k-k'}{k+k'} \qquad \frac{C}{A} = \frac{2k}{k+k'}, \quad \text{; works for all values of } E$$

$$j = \underbrace{\frac{\hbar k}{m}}_{v}\left[|A|^2-|B|^2\right], \quad X<0$$

$$= \underbrace{\frac{\hbar k'}{m}}_{v'}|C|^2, \quad X>0$$

$$R = \frac{|B|^2}{|A|^2} = \frac{(k-k')^2}{(k+k')^2} = \frac{\left[1-(1-V_0/E)^{1/2}\right]^2}{\left[1+(1-V_0/E)^{1/2}\right]^2}, \quad E>V_0$$



Transmission Coefficient = Ratio of $\frac{\text{transmitted prob.}}{\text{incident prob.}}$ (11)

$$T = \frac{v'|C|^2}{v|A|^2} = \frac{4kk'}{(k+k')^2} = \frac{4\left(1-V_0/E\right)^{1/2}}{\left[1+\left(1-V_0/E\right)^{1/2}\right]^2}$$

★★ In QM, we get partial reflections at potential variations!