Review of basic systems (ctd.)

Work in the position space $\hat{H}\varphi_E(x) = E\varphi_E(x)$

- free particle

$V = 0$ at all x

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

$\hat{X} \doteq x$

$\hat{P} \doteq -i\hbar\frac{d}{dx}$

$\Downarrow$

$\hat{P}^2 \doteq -\hbar^2\frac{d^2}{dx^2}$

$\Downarrow$

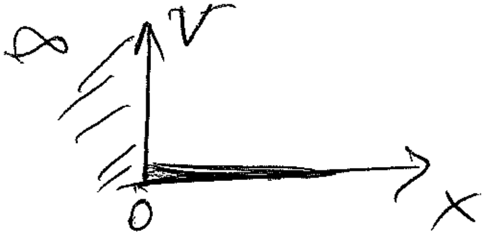
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi_E(x) = E\varphi_E(x) \Rightarrow$$

$$\varphi_E''(x) + k^2\varphi_E(x) = 0 \quad \text{with } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\varphi_E(x) = Ae^{ikx} + Be^{-ikx} \leftarrow \text{plane waves moving} \rightarrow, \leftarrow$$

- any k is possible
- energy $E = \frac{\hbar^2 k^2}{2m}$ is continuous

- introduce one boundary $\Rightarrow V = \begin{cases} 0 & \text{at } x > 0 \\ \infty & x < 0 \end{cases}$



$\Downarrow$

- same solution $\varphi_E(x)$ as above for $x > 0$
- $\varphi_E(0) = 0 \leftarrow$ boundary condition also for $x < 0$

$$A + B = 0 \Rightarrow A = -B \Rightarrow \varphi_E(x) = A(e^{ikx} - e^{-ikx}) =$$

$= C \sin kx$

$\uparrow$

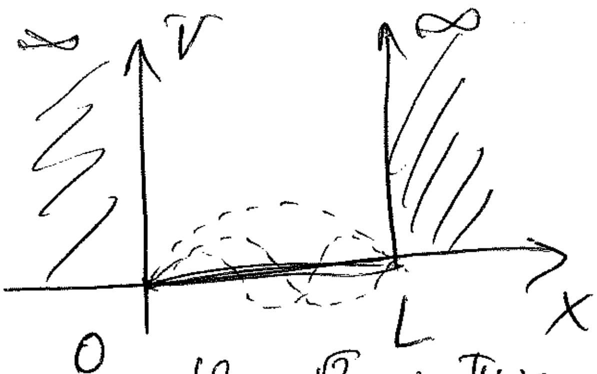
$$\frac{e^{ikx} - e^{-ikx}}{2i} = \sin kx$$

$E = \frac{\hbar^2 k^2}{2m}$, still continuous since no restriction on k

• introduce the second boundary $\Rightarrow$ now have a box

$\Downarrow$

another boundary condition!



$\varphi_n = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}$

$$\varphi_E(L) = 0 \Rightarrow$$

$$C \sin kx \Big|_{x=L} = 0 \Rightarrow$$

$$\sin kL = 0 \Rightarrow k = \frac{\pi n}{L}$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{L}\right)^2$$

Now the energy is quantized! $(n = 1, 2, \ldots)$

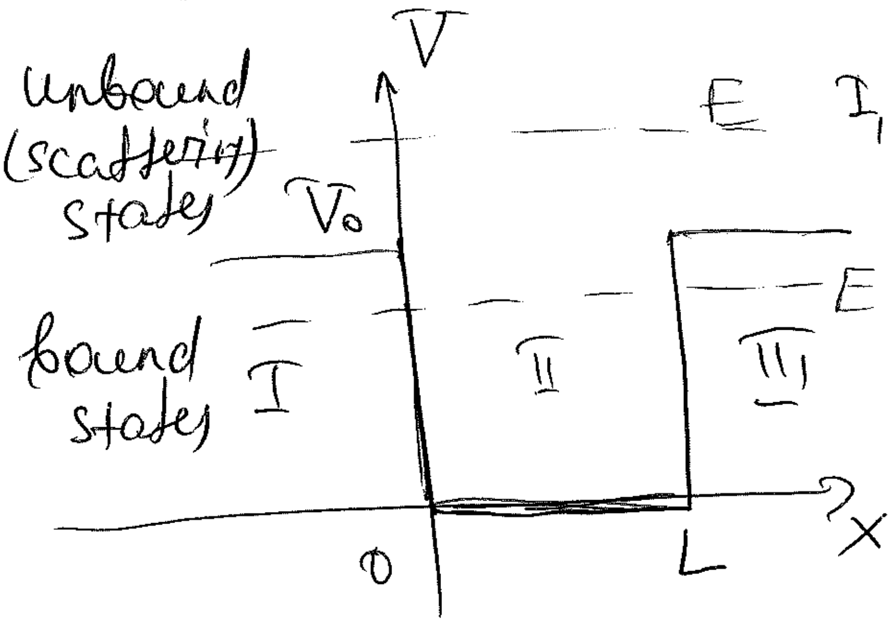
So the particle <u>confinement</u> led to the energy quantization!

What exactly defines this "confinement"?

$\Downarrow$

Consider a finite well

• finite well



I, III: $-\frac{\hbar^2}{2m}\varphi_E''(x) + V_0\varphi_E(x) = E\varphi_E(x)$

II: $-\frac{\hbar^2}{2m}\varphi_E''(x) = E\varphi_E(x)$

as before!

so general solution for II would be

$\varphi_E(x) = Ae^{ikx} + Be^{-ikx}$ or (more convenient here)

$k = \sqrt{\frac{2mE}{\hbar^2}} \longleftrightarrow \varphi_E(x) = C\sin kx + D\cos kx$

region II: oscillatory solution for any E

I, III: $\varphi_E'' - q^2\varphi_E = 0, \quad q = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$

$(E < V_0)$ $\quad \varphi_E(x) = \hat{A}e^{qx} + \tilde{B}e^{-qx}$ ← decaying exp

$(E > V_0)$ $\quad \varphi_E'' + q^2\varphi_E = 0, \quad q = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$

$\varphi_E(x) = \tilde{C}e^{iqx} + \hat{D}e^{-iqx}$

oscillatory

Need: - physical solution ④

→ φ_E does not blow up as $x \to \pm\infty$

spatial period $= \frac{2\pi}{q}$

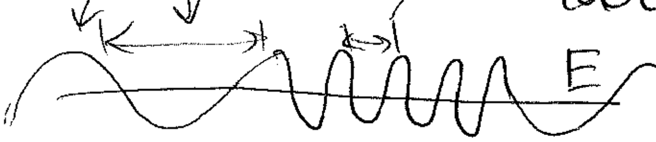
$\sim\sqrt{E-V_0}$

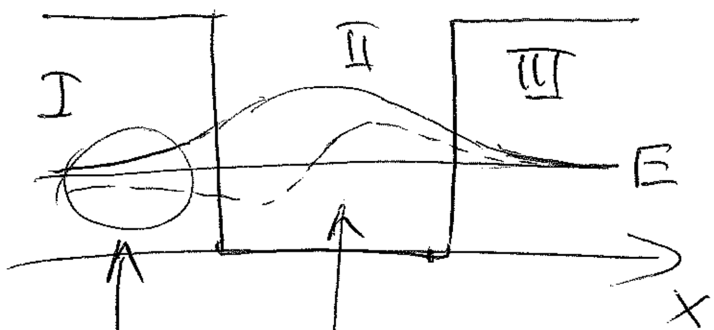
$\frac{2\pi}{K} \leftarrow \sim\sqrt{E}$

high E = high K

- boundary condition

continuity of $\varphi_E(x)$ & $\varphi_E'(x)$





oscillatory

how fast this decay is determined by $q \sim \sqrt{V_0 - E}$ $\Rightarrow$ the closer E to V_0 $\Rightarrow$ the longer the decay

$(e^{\pm qx})$

more prob. to find the particle well outside of the box ⇐

Important:

- "confinement" here $(E < V_0)$

$\Updownarrow$

$\varphi_E(x) \to 0$ at $x \to \pm\infty$

$\Downarrow$

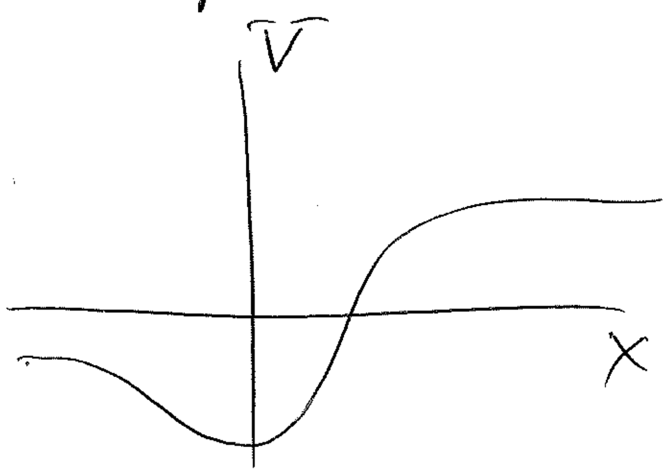
quantization of energy at $E < V_0$

$\Downarrow$

discrete spectrum

- $E > V_0 \Rightarrow$ continuous energy spectrum

Can we predict the behaviour of $\varphi_E(x)$ & energy spectra (continuous vs discrete) for a potential which doesn't have a simple solution?



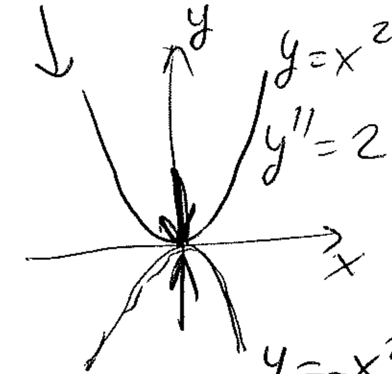
Schrödinger equation (2nd-order) $\Rightarrow$ diff. eqn

$$\varphi_E'' = \frac{2m}{\hbar^2}\left(V(x)-E\right)\varphi_E$$

2nd derivative is related to curvature

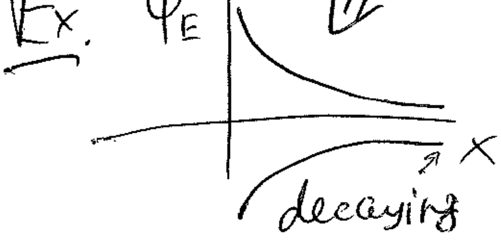
• depending on whether $V(x)-E$ is >0 or <0 $\Rightarrow$ $\Leftarrow$

Ex.



φ_E'' either has the same sign as φ_E or the opposite sign as φ_E

Ex.



φ_E, φ_E'' have same sign (i.e. if $\varphi_E \gtrless 0$, φ_E'' is also $\gtrless 0$)

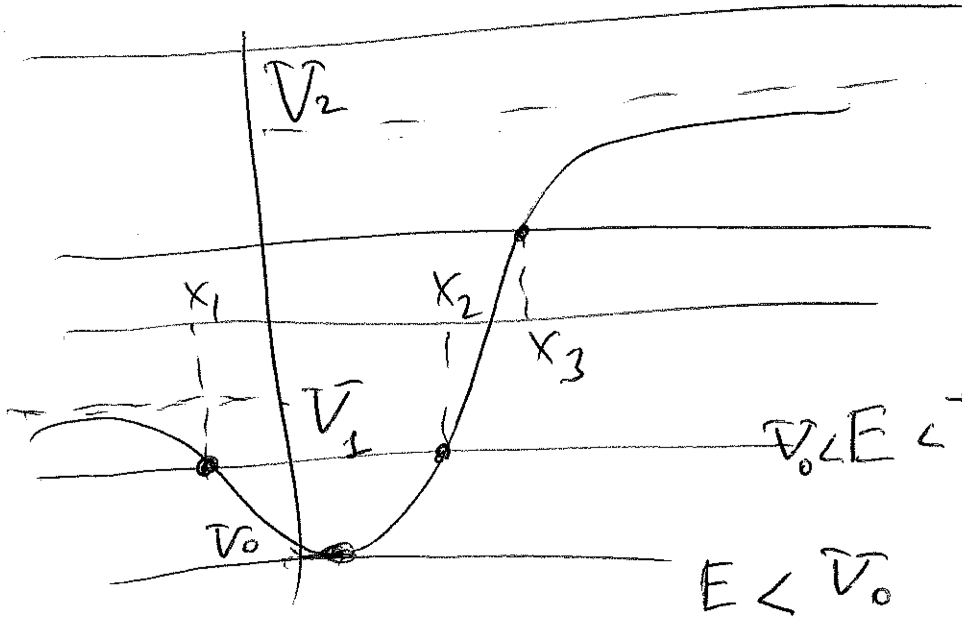
$E < V(x)$

If φ_E, φ_E'' have opposite signs $\Rightarrow$ $\varphi_E \gtrless 0$, $\varphi_E'' \lessgtr 0$

<u>Ex.</u>

oscillating

$\Downarrow$ use this to predict behaviour!



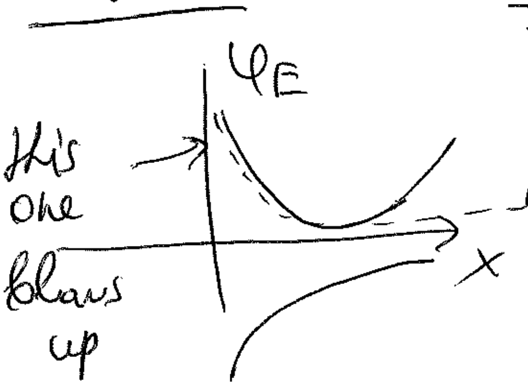
$E > V_2$ case 4

$V_1 < E < V_2$ $\Rightarrow$ case 3

$V_0 < E < V_1$ $\Rightarrow$ case 2

$E < V_0$ $\Rightarrow$ case 1

<u>Case 1</u> For <u>all x</u>, $V(x) - E > 0 \Rightarrow \varphi_E, \varphi_E''$ have same sign



this one blows up

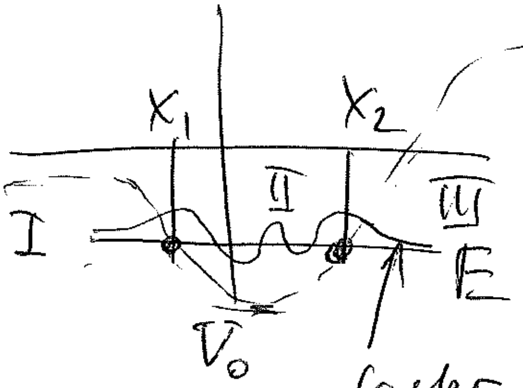
even if this end decays as $x \to \infty$

can't construct a physical solution!

Also, if $E < V_0$ everywhere $\Rightarrow$ negative kinetic energy

Case 2 $V_0 < E < V_1$

$x_1, x_2 \to$ turning points (classical motion is possible only between x_1 & x_2)



classically forbidden regions

I, III : $E < V(x) \Rightarrow$ decay

II : $E > V(x) \Rightarrow$ oscillations

(φ_E, φ_E'' have opposite signs)

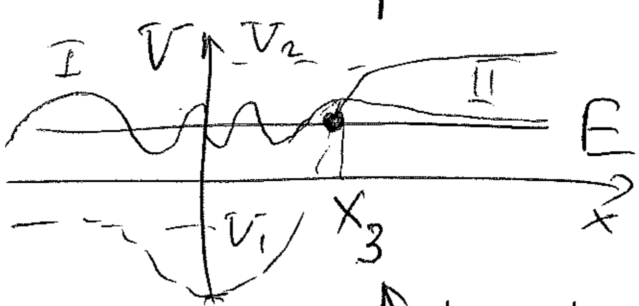
faster decay since $V - E$ is large

Note: $\varphi_E \to 0$ at $x \to \pm\infty$ $\Rightarrow$ bound states

$\Downarrow$

discrete energy spectrum!

Case 3 $V_1 < E < V_2$



turning point

I: $E > V(x) \Rightarrow$ oscillations

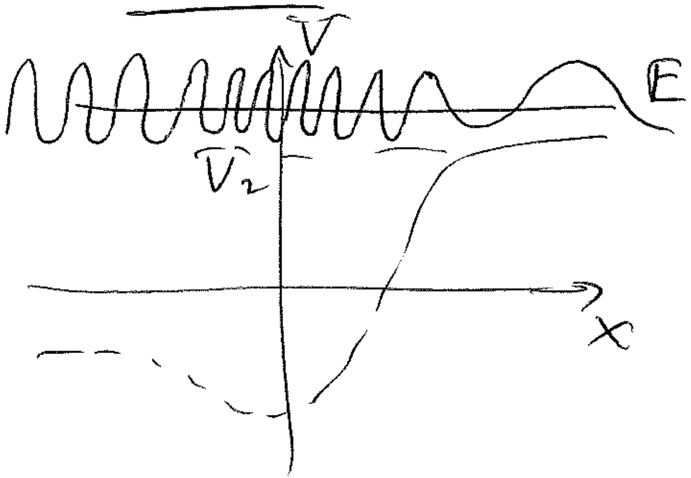
II : $E < V(x) \Rightarrow$ decay

$\varphi_E \to 0$ at $x \to \infty$

but not at $x \to -\infty$

unbound states (scattering) $\Rightarrow$ continuous energy spectra

Case 4 $E > V_2$



$E > V(x)$ everywhere!

$\Downarrow$

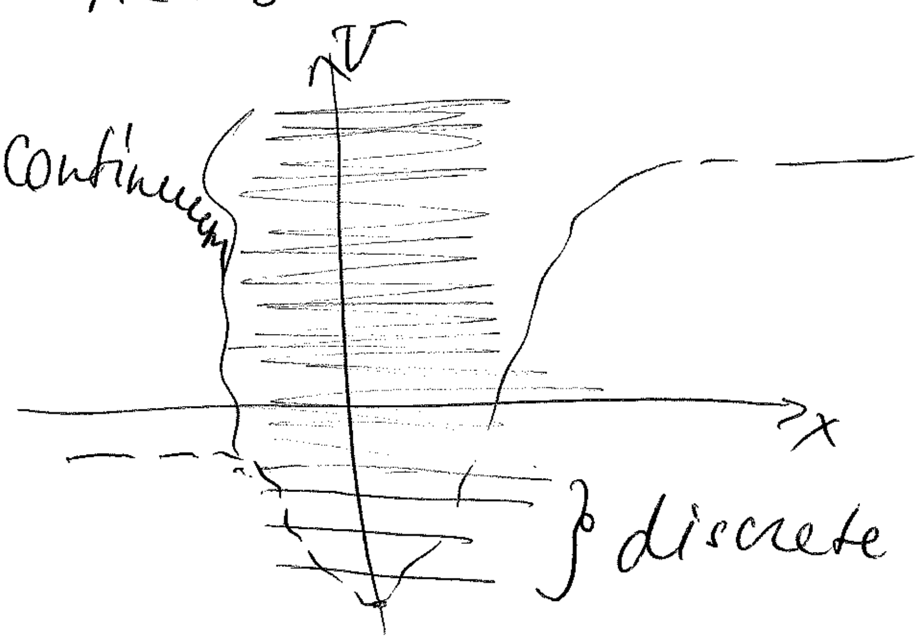
oscillations!

$\Downarrow$

spatial frequency/ period change with $\sqrt{E - V(x)}$

φ_E does not go to 0 at either $+\infty$ or $-\infty$ $\Rightarrow$ unbounded (scattering) states $\Rightarrow$ continuous energy spectra

Altogether:



Also: see McIntyre 5.10.1 for summary