Part 3: Quantum Physics of Matter

Lecture 13. The Infinite Square Well

13·1 Applying Schrödingers Equation – Free Particle

TISE

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\,\psi(x) \quad [13\cdot1]$$

In region where $V(x) = 0$ or 'free space':

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

$$\Rightarrow \quad \frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x) = -\left(\frac{p}{\hbar}\right)^2\psi(x) \quad [13\cdot2]$$

General solutions:

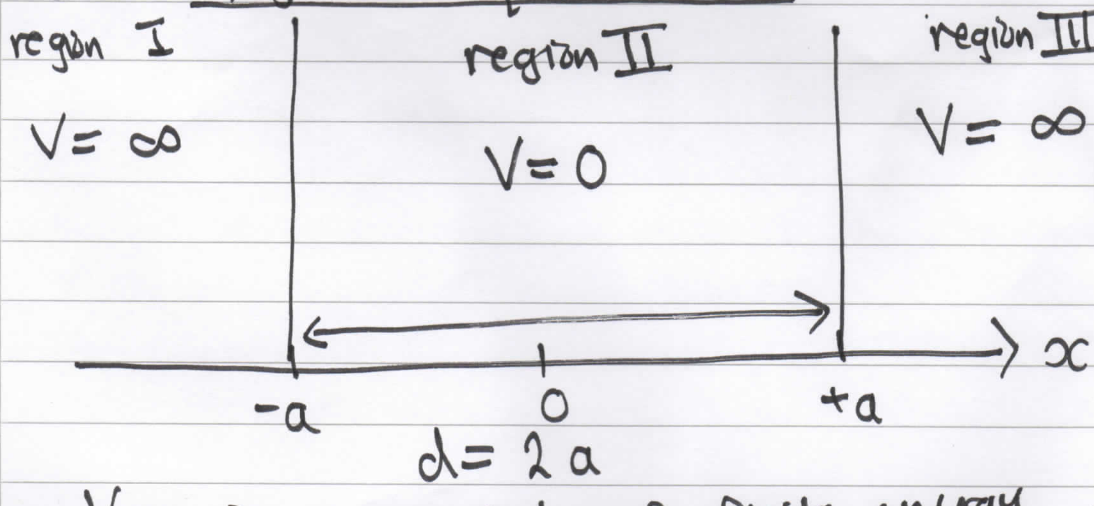
$$\psi(x) = C_1 e^{+i\frac{p}{\hbar}x} + C_2 e^{-i\frac{p}{\hbar}x} \quad [13\cdot3]$$

or

$$= C_1' \sin\left(\frac{p}{\hbar}x\right) + C_2' \cos\left(\frac{p}{\hbar}x\right)$$

- no constraints on p & E in free space (continuous)
- quantisation will come from boundary conditions (note $+p$ or $-p$ for a given E satisfy eqns)

13·2 Infinite Square Well



- $V = \infty$ a particle of finite energy cannot penetrate into this region $\Rightarrow \psi_{I,III}(x) = 0$
- $V(x) = 0$ solutions $\psi_{II}(x)$ as for 13·3

$$\psi(x) = A\cos kx + B\sin kx \qquad [13.4]$$

where $k = \frac{p}{\hbar} = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$ [13.5]

$\sqrt{2mE}/\hbar$

Boundary conditions:—
(i) $\psi(x)$ should be continuous and single valued
(ii) $\psi(x) \to 0$ lim $x \to \infty$ to ensure normalisation
(iii) $\frac{d}{dx}\psi(x)$ should be continuous for finite $V(x)$

Here $\psi(a) = \psi(-a) = 0$

$$\left.\begin{array}{ll} x = a & A\cos ka + B\sin ka = 0 \\ x = -a & A\cos ka - B\sin ka = 0 \end{array}\right\} \quad [13.6]$$

two ways to satisfy:

case 1 $B = 0$ $\therefore$ $\cos ka = 0$

$\Rightarrow$ $ka = \frac{n\pi}{2}$ n-odd integer

case 2 $A = 0$ $\therefore$ $\sin ka = 0$

$\Rightarrow$ $ka = \frac{n\pi}{2}$ n-even integer

- as before energy quantised with quantum number n
- two families of solution

$$\left.\begin{array}{ll} \sin\left(\frac{n\pi}{2a}x\right) & n \text{ even} \\ \cos\left(\frac{n\pi}{2a}x\right) & n \text{ odd} \end{array}\right\} \quad [13.7]$$

$p = \hbar k$

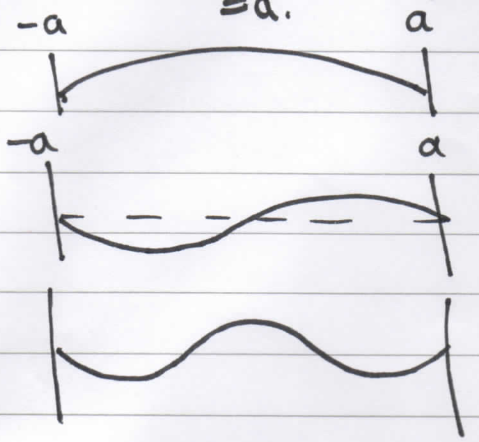
$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2 n^2}{8ma^2} \qquad [13.8]$$

$$= \frac{h^2 n^2}{8 \cdot 4 \cdot ma^2} = \frac{n^2 h^2}{8md^2} \quad \text{as before}$$

$$\psi(x) = C \begin{bmatrix} \cos \\ \sin \end{bmatrix} \left(\frac{n\pi}{2a} x \right) \qquad [13.9]$$

C normalisation

$$C^2 \underbrace{\int_{-a}^{a} \sin^2\left(\frac{n\pi}{2a}\right) dx}_{=a} = 1 \Rightarrow C = \frac{1}{\sqrt{a}} \qquad [13.10]$$



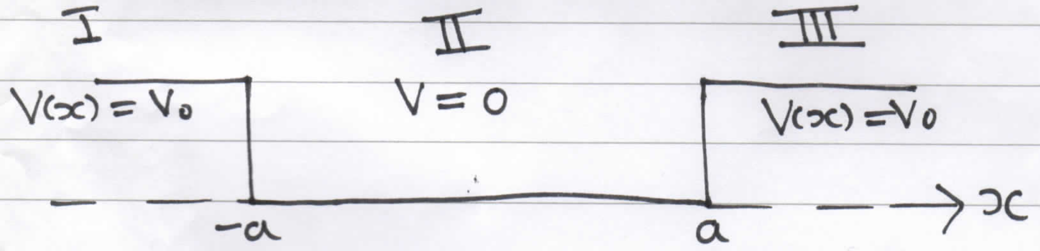
$\psi_1(x)$ $n=1$ $\frac{1}{\sqrt{a}} \cos\left(\frac{\pi x}{2a}\right)$

$\psi_2(x)$ $n=2$ $\frac{1}{\sqrt{a}} \sin\left(\frac{\pi}{a} x\right)$

$\psi_3(x)$ $n=3$ $\frac{1}{\sqrt{a}} \cos\left(\frac{3\pi}{2a} x\right)$

⋮

13.3 Finite Square Well

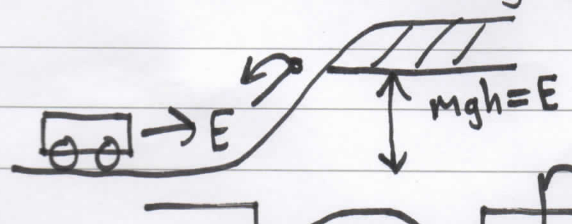


More like 'real' potential (nuclear or quantum well structure)

$E > V_0 \longrightarrow$ free particle (energy continuum)

$E < V_0 \longrightarrow$ bound particle (energy quantised)

for $E < V_0$ classically forbidden



but in QM w.f may exist as a <u>decaying exponential</u>

continuity of $\psi(x)$ & $\frac{d}{dx}\psi(x)$