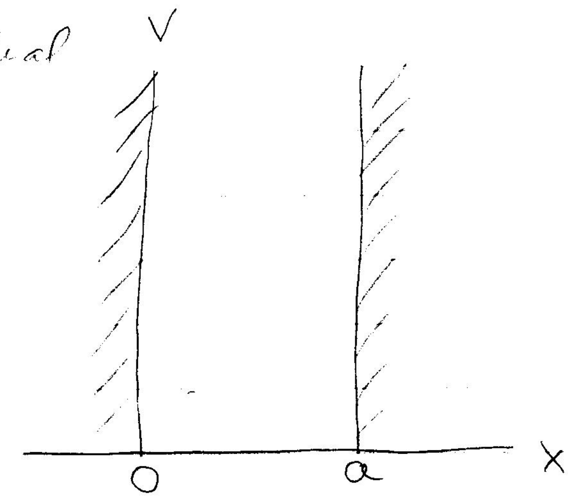
Infinite Square Well

Schroedinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2\Psi(x,t) + V(x)\,\Psi(x,t)$$

infinite square-well potential

$$V(x) = +\infty \qquad x<0$$
$$= 0 \qquad 0<x<a$$
$$= +\infty \qquad x>a$$



Schroedinger equation is a <u>linear</u> equation
(each term has one factor of Ψ)

$\Longrightarrow$ If $\psi_1(x,t)$ is a solution
and $\psi_2(x,t)$ "

then $c_1\psi_1(x,t) + c_2\psi_2(x,t)$ is a solution
for any complex constants c_1, c_2

Strategy

1. Look for simple solutions
in which dependence on x and t is separated

$$\Psi(x,t) = \psi(x)\,\chi(t)$$

$\Longrightarrow$ separate equation for $\psi(x)$ and $\chi(t)$

2. Solve differential equation for $\chi(t)$

$\Longrightarrow$ determined by arbitrary energy E

3. Solve differential equation for $\psi(t)$

$\Longrightarrow$ discrete solutions labelled by quantum number n
with energies E_n

more general solution

$$\psi(x,t) = c_1\,\chi_{E_{n_1}}(t)\,\psi_{n_1}(x) + c_2\,\chi_{E_{n_2}}(t)\,\psi_{n_2}(t)$$

quantum superposition
of state with different energies

Step 1. Look for simple solutions in which dependence on x and t is separated

$$\Psi(x,t) = \psi(x)\,\chi(t)$$

Schroedinger equation

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

$$\psi(x)\left[i\hbar\,\chi'(t)\right] = \left[-\frac{\hbar^2}{2m}\psi''(x)\right]\chi(t) + V(x)\,\psi(x)\,\chi(t)$$

divide both sides by $\psi(x)\,\chi(t)$

$$i\hbar\,\frac{\chi'(t)}{\chi(t)} = -\frac{\hbar^2}{2m}\,\frac{\psi''(x)}{\psi(x)} + V(x)$$

function of t only can be equal to function of x only
only if both are equal
to a "separation constant" E

$$\begin{cases} i\hbar\,\dfrac{\chi'(t)}{\chi(t)} = E \\[2ex] -\dfrac{\hbar^2}{2m}\,\dfrac{\psi''(x)}{\psi(x)} + V(x) = E \end{cases}$$

$$\begin{cases} i\hbar\,\chi'(t) = E\,\chi(t) \\[2ex] -\dfrac{\hbar^2}{2m}\,\psi''(x) + V(x)\,\psi(x) = E\,\psi(x) \end{cases}$$

<u>Step 2</u> Solve differential equation for $\chi(t)$

$$i\hbar \frac{\partial}{\partial t} \chi(t) = E\,\chi(t)$$

$$\Longrightarrow \quad \chi_E(t) = A\, e^{-iEt/\hbar}$$

where A is a complex constant
can choose $A=1$

<u>Step 3</u> Solve differential equation for $\psi(x)$

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\,\psi(x) = E\,\psi(x)$$

solve in 3 regions separately

Step 3a: $\quad x < 0 \qquad V(x) = +\infty$

$$\Longrightarrow \quad \psi(x) = 0$$

Step 3b: $\quad x > a \qquad V(x) = +\infty$

$$\Longrightarrow \quad \psi(x) = 0$$

Step 3c: $\quad 0 < x < \infty \qquad V(x) = 0$

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

general solution

$$\psi(x) = B \sin\left(\sqrt{\frac{2mE}{\hbar^2}}\, x\right) + C \cos\left(\sqrt{\frac{2mE}{\hbar^2}}\, x\right)$$

where B, C are complex constant

Step 3d: match solution at $x = 0$

$$\psi(0^-) = 0$$

$$\psi(0^+) = B \cdot 0 + C \cdot 1$$

continuity $\Longrightarrow$ $C = 0$

Step 3e: match solutions at $x = a$

$$\psi(a^+) = 0$$

$$\psi(a^-) = B \sin\left(\sqrt{\frac{2mE}{\hbar^2}}\, a\right)$$

continuity $\Longrightarrow$ $\sin\left(\sqrt{\frac{2mE}{\hbar^2}}\, a\right) = 0$

$$\Longrightarrow \sqrt{\frac{2mE}{\hbar^2}}\, a = n\pi, \quad n = 0, \pm 1, \pm 2, \ldots$$

discrete solutions labelled
by quantum number n

nonzero, distinct solutions $\Longrightarrow$ $n = 1, 2, 3, \ldots$

wavefunction: $\psi_n(x) = B_n \sin\left(\frac{n\pi x}{a}\right)$

separation constants: $E_n = n^2 \frac{\pi^2 \hbar^2}{2ma^2}$

Step 3F: normalize $\psi(x)$

choose B_n so $\int_{-\infty}^{\infty} dx\, |\psi_n(x)|^2 = 1$

$$\int_{-\infty}^{\infty} dx\, |\psi_n(x)|^2 = \int_0^a dx\, |\psi_n(x)|^2$$

$$= \int_0^a dx\, |B_n|^2 \sin^2 \frac{n\pi x}{a}$$

$$= |B_n|^2 \int_0^a dx\, \sin^2 \frac{n\pi x}{a}$$

$$= |B_n|^2 \cdot \frac{1}{2} a$$

choose $B_n = \sqrt{\frac{2}{a}}$

$$\psi_n(x) = 0 \qquad x < 0$$

$$= \sqrt{\frac{2}{\pi}} \sin\left(\frac{n\pi x}{a}\right) \qquad 0 < x < a$$

$$= 0 \qquad x > a$$

most general solution

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \cdot \psi_n(x)\, \chi_{E_n}(t)$$

$$= \sum_{n=1}^{\infty} c_n \sqrt{\tfrac{2}{a}} \sin\left(\tfrac{n\pi x}{a}\right) e^{iE_n t/\hbar}$$

where $c_1, c_2, c_3, \ldots$
are complex constants

Step 5 Normalize the wavefunction

$$\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = 1$$

$$\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = \int_0^a dx\, |\psi(x,t)|^2$$

$$= \int_0^a dx\, \psi(x,t)^* \psi(x,t)$$

$$= \int_0^a dx \left(\sum_{m=1}^{\infty} c_m^* \sqrt{\tfrac{2}{a}} \sin \tfrac{m\pi x}{a}) e^{+iE_m t/\hbar} \right)$$

$$\times \left(\sum_{n=1}^{\infty} c_n \sqrt{\tfrac{2}{a}} \sin \tfrac{n\pi x}{a}\, e^{-iE_n t/\hbar} \right)$$

$$= \frac{2}{a} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n^* e^{+iE_m t/\hbar} e^{-iE_n t/\hbar}$$

$$\times \int_0^a dx \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a}$$

$$\int_0^a dx \sin\frac{m\pi x}{a} \sin\frac{n\pi x}{a} = 0 \qquad m \neq n$$

$$= \tfrac{1}{2}a \qquad m = n$$

collapses double sum over m, n
to single sum over n

$$\int_{-\infty}^{\infty} dx \, |\Psi(x,t)|^2$$

$$= \frac{2}{a} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n e^{+iE_m t/\hbar} e^{-iE_n t/\hbar} \left(\tfrac{1}{2} a \, \delta_{mn}\right)$$

$$= \frac{2}{a} \sum_{n=1}^{\infty} c_n^* c_n e^{+iE_n t/\hbar} e^{-iE_n t/\hbar} \, \tfrac{1}{2} a$$

$$= \sum_{n=1}^{\infty} |c_n|^2$$

most general normalized solution
to Schroedinger equation

$$\Psi(x,t) = 0 \qquad x < 0$$

$$= \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \, e^{-iE_n t/\hbar} \qquad 0 < x < a$$

$$= 0 \qquad x > a$$

where $E_n = n^2 \dfrac{\pi^2 \hbar^2}{2 m a^2}$

c_n are complex constants satisfying $\sum_{n=1}^{\infty} |c_n|^2 = 1$