Wavefunction

Probability of Finding the Particle between (a,b)

$$P_{a<x<b} = \int_a^b |\Psi(x,t)|^2 dx$$

Time-independent Shrodinger's Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\Psi}{dx^2}+U(x)\Psi = i\hbar\frac{d\Psi}{dt}$$

Assume

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

$$-e^{-\frac{iEt}{\hbar}}\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+e^{-\frac{iEt}{\hbar}}U(x)\psi(x)=i\hbar\frac{-iE}{\hbar}\psi(x)e^{-\frac{iEt}{\hbar}}$$

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi = E\psi$$

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi = 0$$

Time-independent Schrodinger's Equation

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

If E >U, then ....

$$k\equiv\frac{\sqrt{2m_0[E-U]}}{\hbar} \qquad \frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad \psi(x)=A\,sin(kx)+B\,cos(kx) \equiv A_+e^{ikx}+A_-e^{-ikx}$$

If U>E, then ....

$$\alpha\equiv\frac{\sqrt{2m_0[U-E]}}{\hbar} \qquad \frac{d^2\psi}{dx^2}-\alpha^2\psi=0 \qquad \psi(x)=De^{-\alpha x}+Ee^{+\alpha x}$$

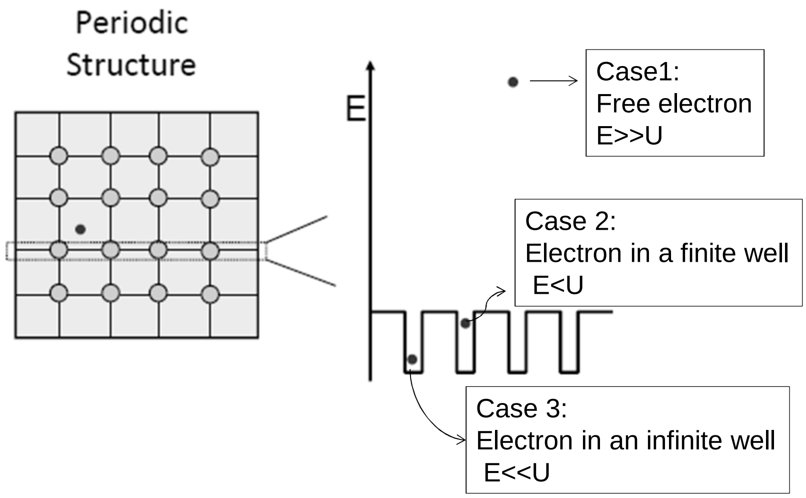
Basic Steps to Solve the Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

- Obtain U(x) and the boundary conditions for a given problem.
- Solve the 2nd order equation – pretty basic
- Interpret $|\psi|^2=\psi^*\psi$ as the probability of finding an electron at x
- Compute anything else you need, e.g.,

$$p=\int_0^\infty \Psi^*\left[\frac{\hbar}{i}\frac{d}{dx}\right]\Psi\,dx \qquad E=\int_0^\infty \Psi^*\left[-\frac{\hbar}{i}\frac{d}{dt}\right]\Psi\,dx$$

Solution of Schrodinger's Equation



Five Steps to Solve this Problem

1) $\dfrac{d^2\psi}{dx^2} + k^2\psi = 0$ $\longrightarrow$ 2N unknowns for N regions

2) $\psi(x = -\infty) = 0$, $\psi(x = +\infty) = 0$ $\longrightarrow$ Reduces 2 unknowns

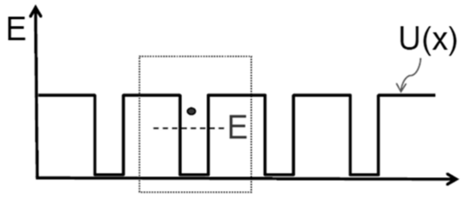
3) $\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$, $\left.\dfrac{d\psi}{dx}\right|_{x=x_B^-} = \left.\dfrac{d\psi}{dx}\right|_{x=x_B^+}$ $\longrightarrow$ Set 2N-2 equations for 2N-2 unknowns (for continuous U)

4) Det (coefficient matrix)=0
And find E by graphical or numerical solution

5) $\int_{-\infty}^{\infty} |\psi(x,E)|^2 \, dx = 1$

for wave function

Case 1: Bounded Levels in a Finite Well

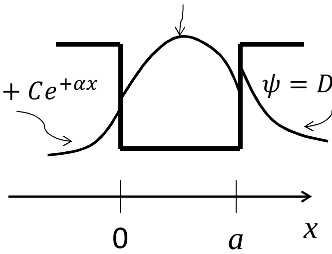


$\psi = A\sin kx + B\cos kx$

Step 1:

$\psi = \cancel{M}e^{-\alpha x} + Ce^{+\alpha x}$

$\psi = De^{-\alpha x} + \cancel{N}e^{+\alpha x}$



Step 2:
Boundary Condition

$$\psi(x = -\infty) = 0$$
$$\psi(x = +\infty) = 0$$

Continuity of Wavefunction

3) $$\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$$
$$\frac{d\psi}{dx}\bigg|_{x=x_B^-} = \frac{d\psi}{dx}\bigg|_{x=x_B^+}$$

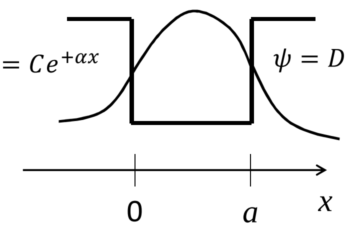
$\Rightarrow$

$$C = B$$
$$\alpha C = -kA$$
$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$
$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$

$\psi = A\sin kx + B\cos kx$

$\psi = Ce^{+\alpha x}$

$\psi = De^{-\alpha x}$



Continuity of Wavefunction

$$C = B$$
$$\alpha C = -kA$$

$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$
$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$

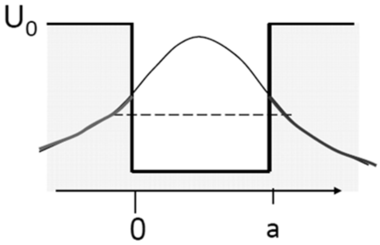
$$\Downarrow$$

$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Step 4: Bound-level in Finite Well

det (Matrix)=0

$$\tan(\alpha a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1} \qquad \xi \equiv \frac{E}{U_0} \quad \alpha \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$



Only unknown is E

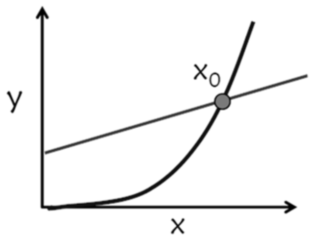
(i) Use Matlab function
(ii) Use graphical method

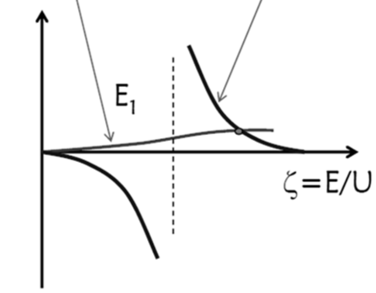
Graphical Method for Bound Levels

$$x^2 = x + 5$$

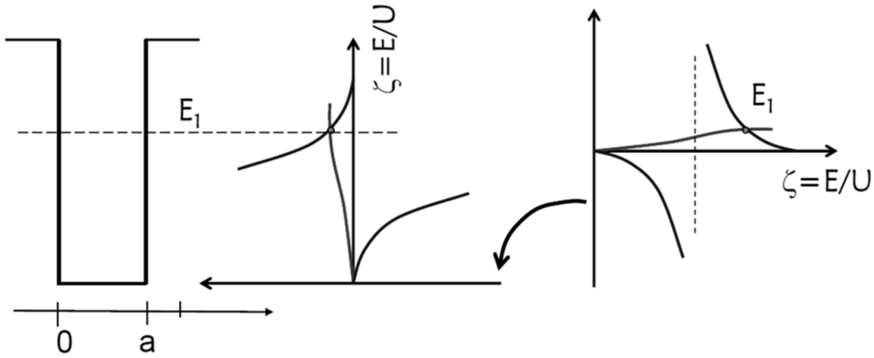
$$y_1 = x^2 \quad y_2 = x + 5$$

$$\tan(\alpha_0 a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$



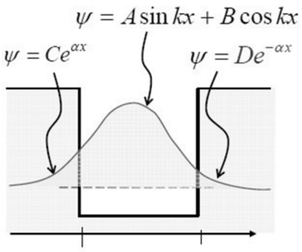


Graphical Method for Bound Levels



Wave Function

Step 5:



$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & -\alpha De^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

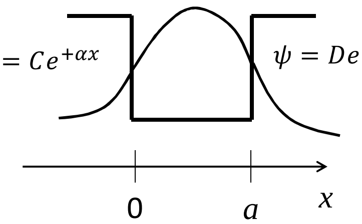
$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

$$\begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

Calculation of Wave Function

$\psi = A\sin kx + B\cos kx$

$\psi = Ce^{+\alpha x}$



$\psi = De^{-\alpha x}$

$$\begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

$$\boxed{\begin{aligned} &\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow \\ &\int_{-\infty}^{0} C^2 e^{2\alpha x} dx + \int_0^a \left[A\,sin(kx) + B\,sin(kx)\right]^2 dx + \int_a^{\infty} D^2 e^{-2\alpha x} dx \end{aligned}}$$

Case 2: Infinite Quantum Well

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k \equiv \frac{\sqrt{2m_0[E-U]}}{\hbar}$$

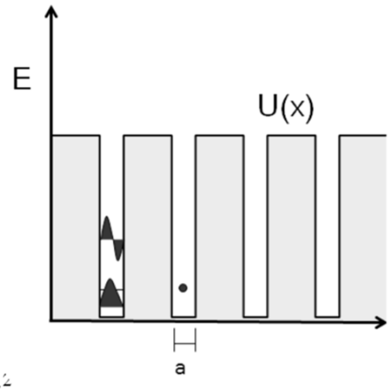
1) Solutions: $\psi = A\sin kx + B\cos(kx)$

2) Boundary conditions

$$\psi(x=0) = 0 = A\,sin\,k(0) + B\,cos\,k(0)$$

$$\psi(x=a) = 0 = A\,sin(ka) = A\,sin(n\pi)$$

$$k_n = \frac{n\pi}{a} = \frac{\sqrt{2m_0E_n}}{\hbar} \qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2m_0 a^2}$$



Five Steps to Solve this Problem

1) $\frac{d^2\psi}{dx^2} + k^2\psi = 0$ $\longrightarrow$ 2N unknowns for N regions

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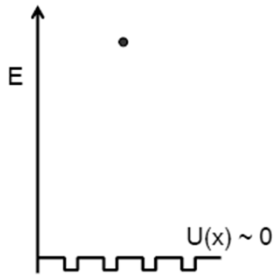
4) Det (coefficient matrix)=0
And find E by graphical or numerical solution

5) $\int_{-\infty}^{\infty} |\psi(x,E)|^2\,dx = 1$

for wave function

Case 3: E >> U

$$\frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad k\equiv\frac{\sqrt{2m_0[E-U]}}{\hbar}$$



1) Solution $\psi(x)=A\,sin(kx)+B\,cos(kx)$

$$\equiv A_+e^{ikx}+A\_e^{-ikx}$$

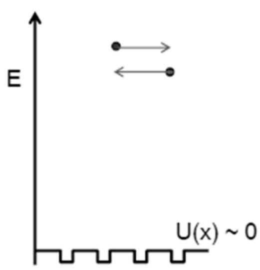
2) Boundary condition $\psi(x)=A_+e^{ikx}$ positive going wave

$=A\_e^{-ikx}$ negative going wave

Free Particle

$$\psi(x)=A\,sin(kx)+B\,cos(kx)$$

$$\equiv A_+e^{ikx}+A\_e^{-ikx}$$



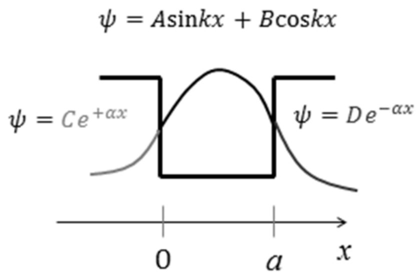
$\psi(x)=A_+e^{ikx}$ positive going wave

$=A\_e^{-ikx}$ negative going wave

Probability: $|\psi|^2-\psi\psi^*-|A_+|^2\ or\ |A\_|^2$

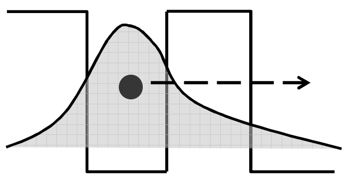
Momentum: $p=\int_0^\infty \Psi^*\left[\frac{\hbar}{i}\frac{d}{dx}\right]\Psi\ dx=\hbar k$ or $-\hbar k$

Tunneling



Electron can stay in the potential barrier. Even if the electron energy is smaller than the potential barrier. It has a chance to go through the barrier!

This is different from classical particles!



Summary

- We have solved the Schrodinger's equation for finite well, infinite potential well, and free particle.

Next Week

- Solution of Schrodinger's equation in periodic potential
- E-k diagram, band structure
- Electrons and holes