EE-606: Solid State Devices
Lecture 4: Solution of Schrodinger Equation

Muhammad Ashraful Alam
alam@purdue.edu

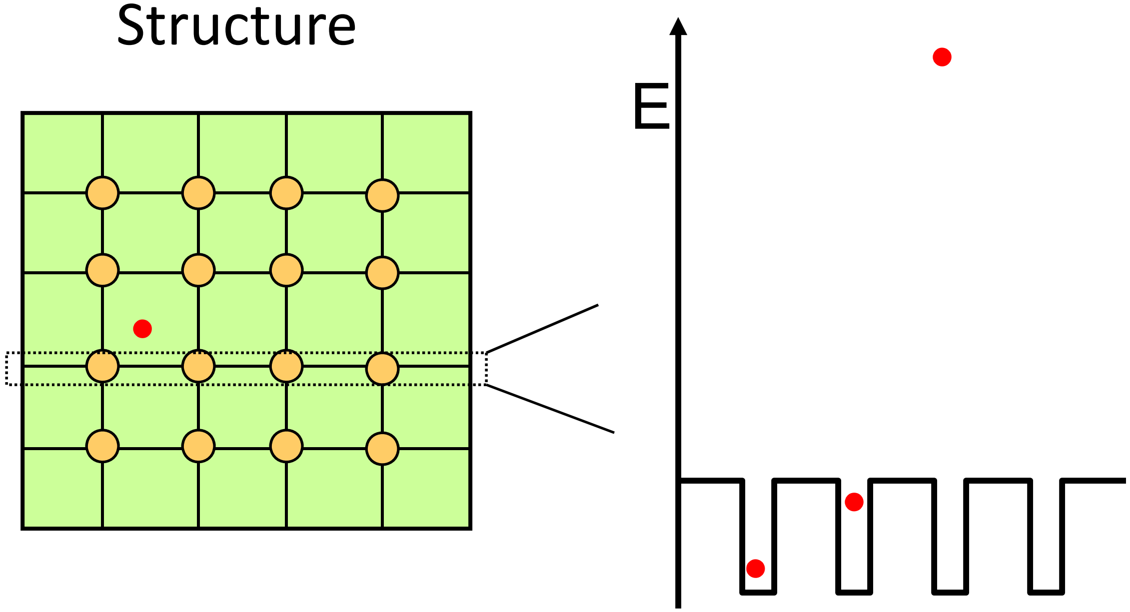
Outline

1) **Time-independent Schrodinger Equation**
2) Analytical solution of toy problems
3) Bound vs. tunneling states
4) Conclusions
5) *Additional Notes: Numerical solution of Schrodinger Equation*

Reference: Vol. 6, Ch. 2 (pages 29-45)

Motivation

Periodic Structure



Time-independent Schrodinger 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 Equation

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

If E >U, then ....

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

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

If U>E, then ....

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

A Simple Differential 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.,

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

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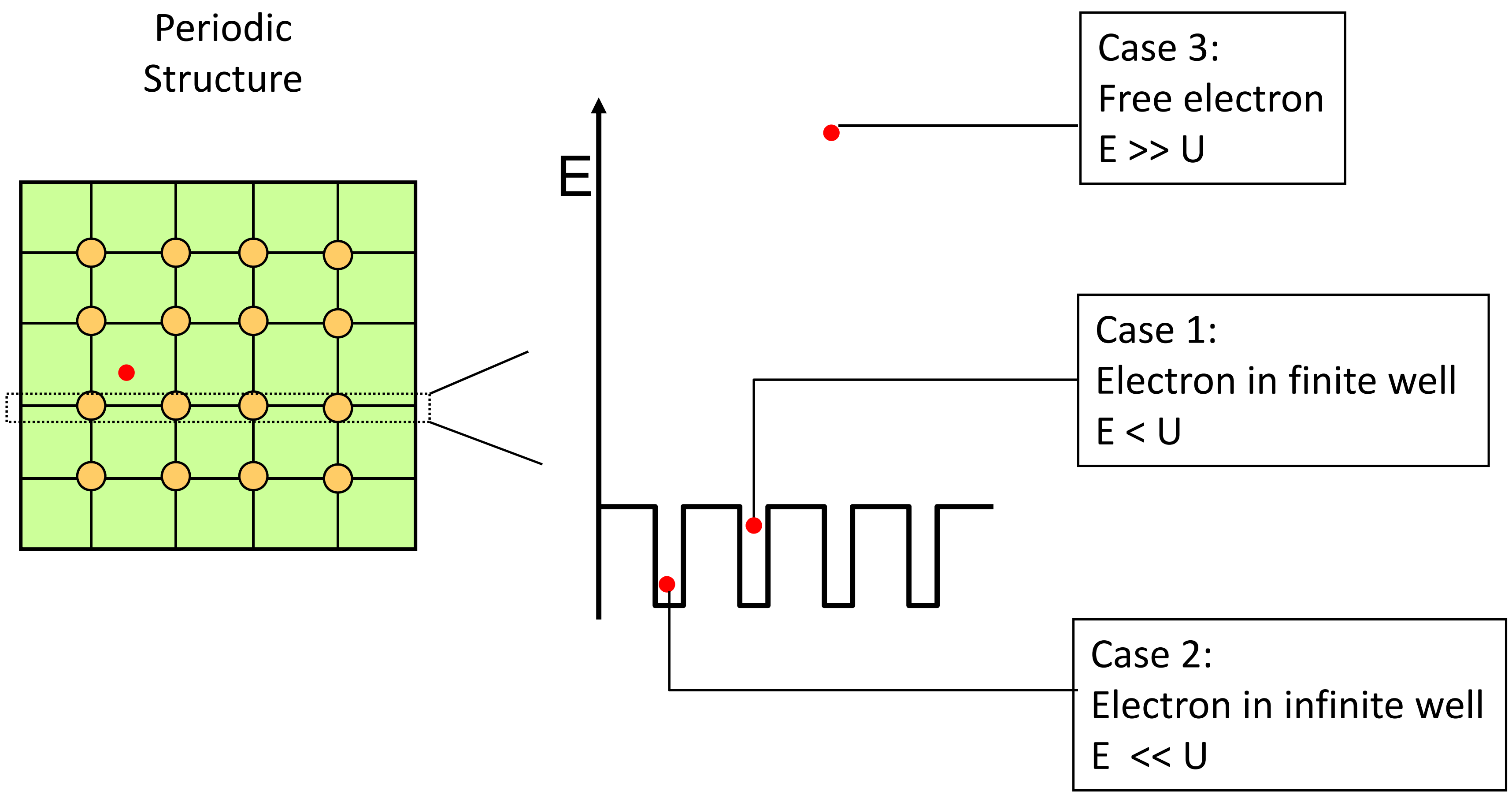
Full Problem Difficult: Toy Problems First



Five Steps for Analytical Solution

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

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

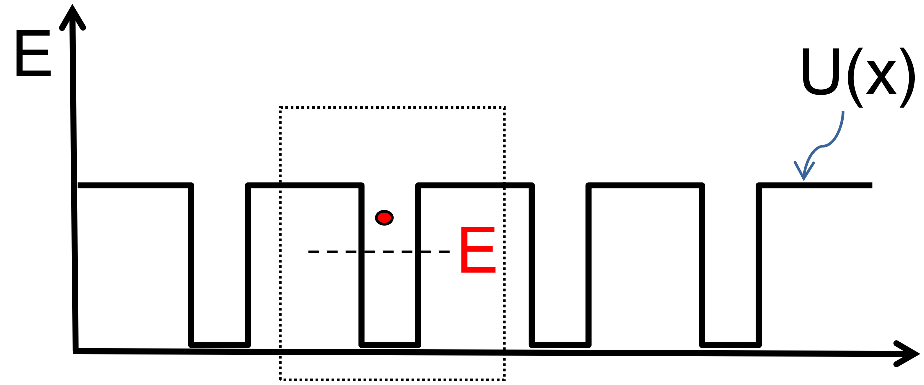
3) $$\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$$ $$\left.\frac{d\psi}{dx}\right|_{x=x_B^-} = \left.\frac{d\psi}{dx}\right|_{x=x_B^+}$$ → Set 2N-2 equations for 2N-2 unknowns (for continuous U)

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

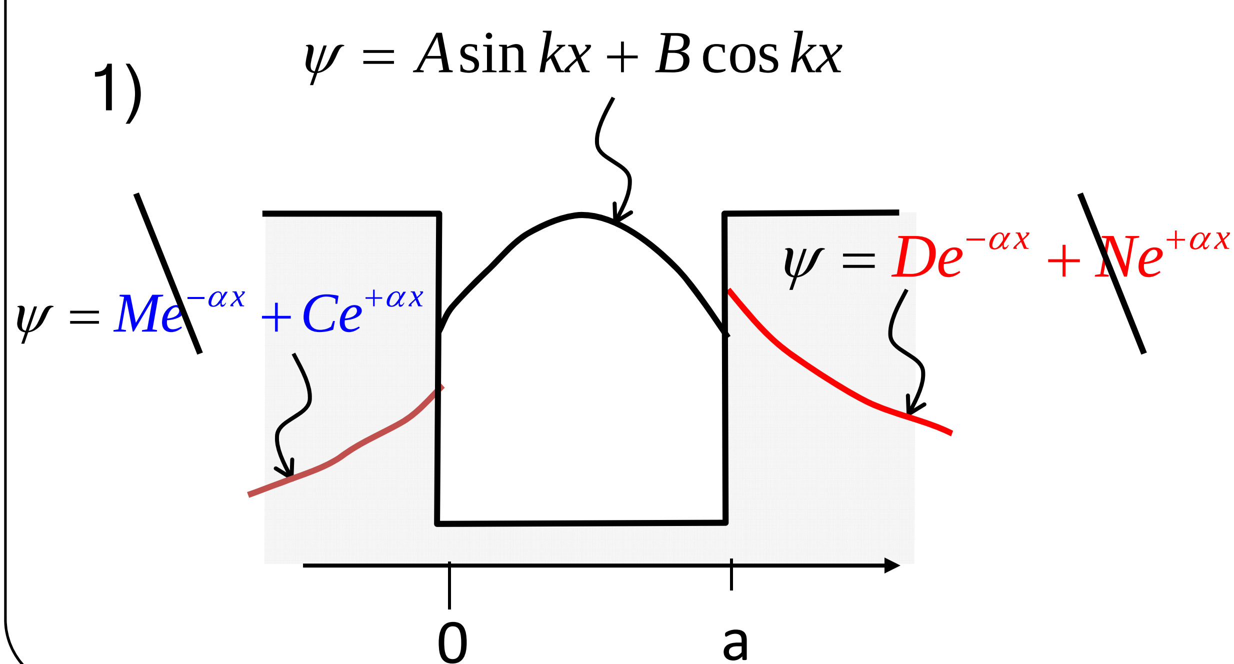
5) $$\int_{-\infty}^{\infty} |\psi(x,E)|^2 \, dx = 1$$

for wave function

Case 1: Bound-levels in Finite Well (steps 1,2)



1)



2) Boundary conditions

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

Step3: Continuity of wave-function

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

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

$\Rightarrow$

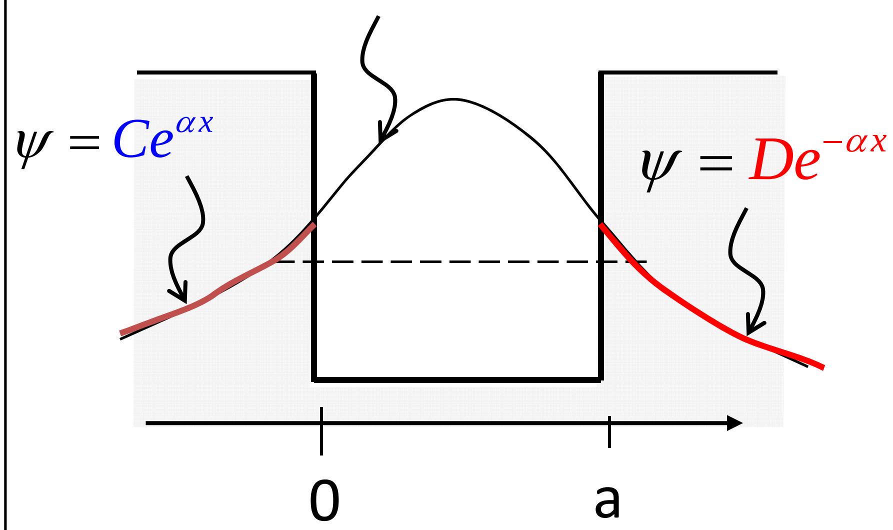
$$C = B$$

$$\alpha C = -kA$$

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

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

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



Step 3: Continuity of Wavefunction

$$C = B$$

$$\alpha C = -kA$$

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

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

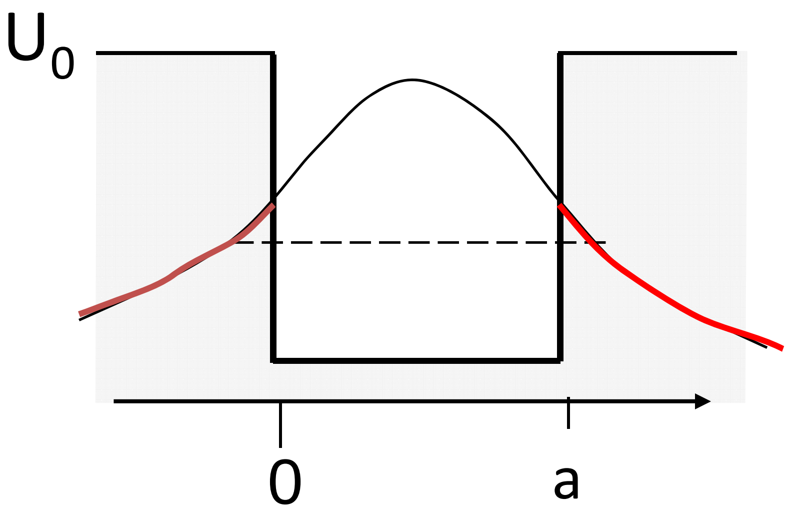
$$\Downarrow$$

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

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

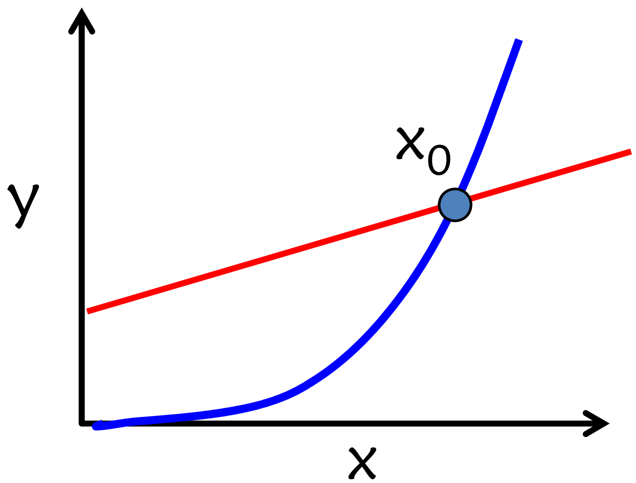
(i) Use Matlab function
(ii) Use graphical method

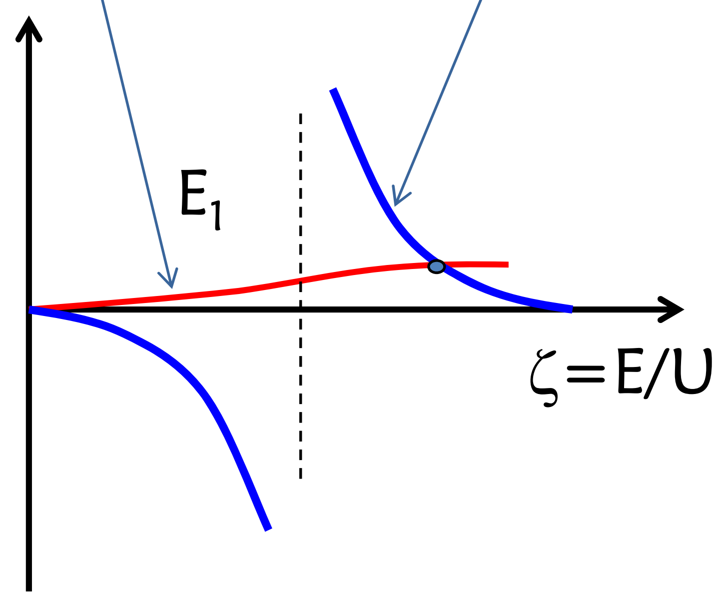
Step 4: Graphical Method for Bound Levels

$$x^2 = x + 5$$

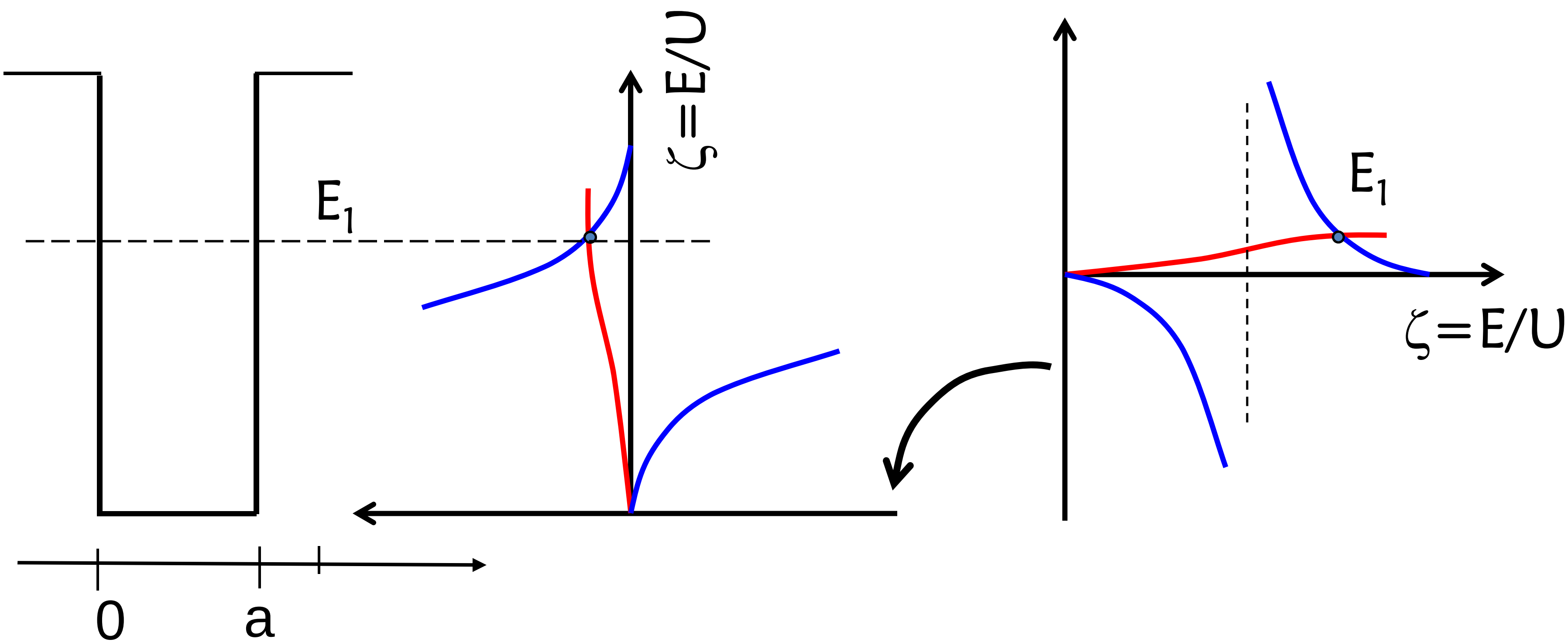
$$y_1 = x^2 \quad y_2 = x + 5$$

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

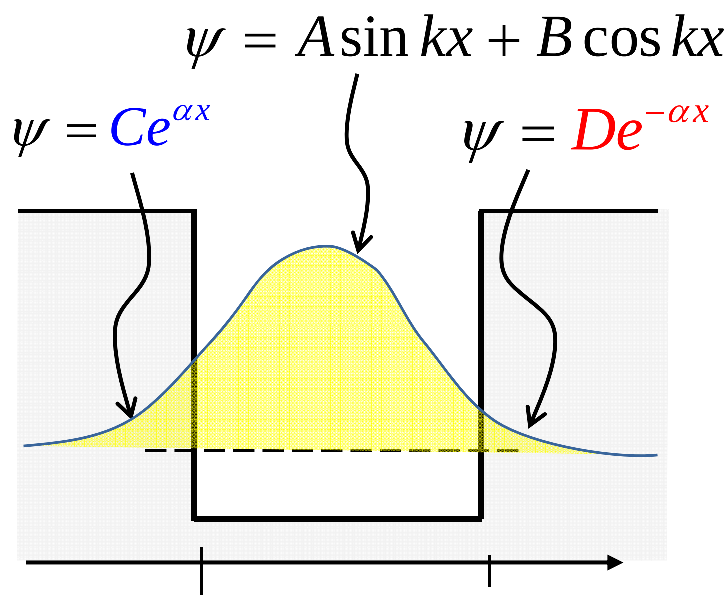




Step 4: Graphical Method for Bound Levels



Step 5: Wave-functions



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

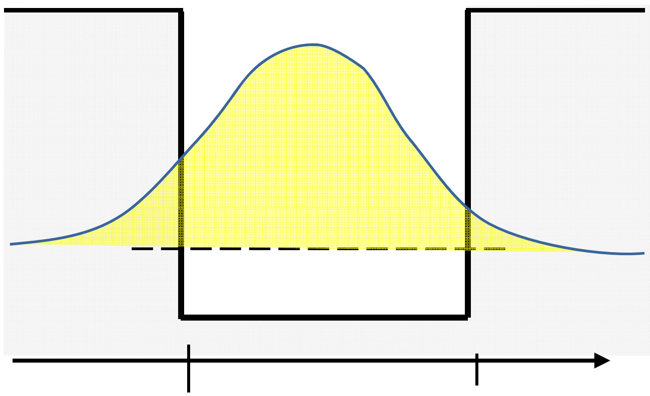
$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

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

Step 5: Calculating Wave-function

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

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



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

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow$$

$$\int_{-\infty}^{0} C^2 e^{2\alpha x} dx + \int_0^a \left[A\sin(kx) + B\sin(kx) \right]^2 dx + \int_a^{\infty} D^2 e^{-2\alpha x} dx$$

Aside: Infinite Quantum Well

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

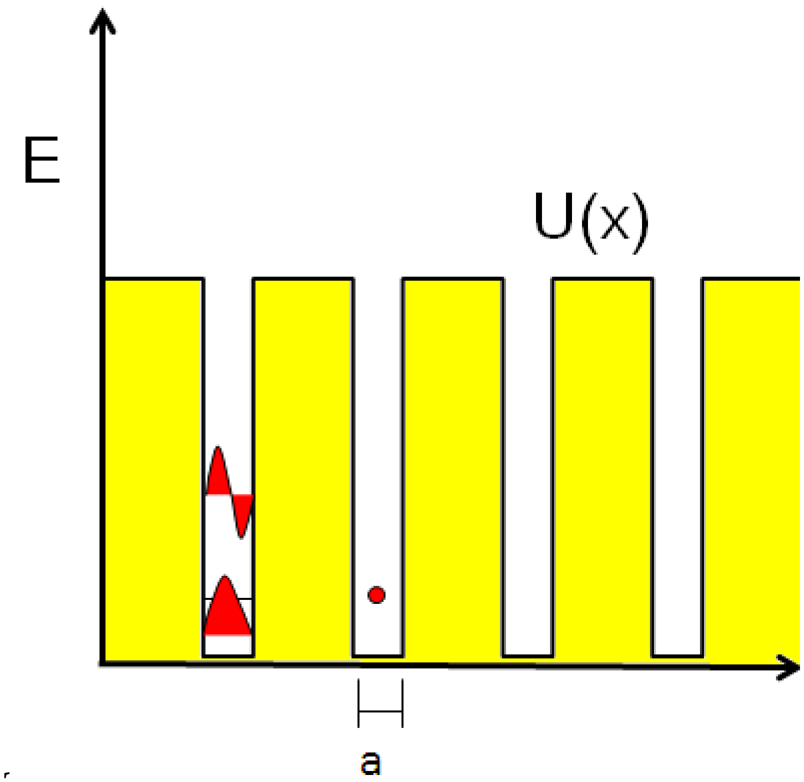
1) Solutions: $\psi = A\sin kx + B\cos(kx)$

2) Boundary conditions

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

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

$$k_n = \frac{n\pi}{a} = \frac{\sqrt{2m_0E_n}}{\hbar} \qquad E_n = \frac{\hbar^2n^2\pi^2}{2m_0a^2}$$



Five steps for Analytical Solution: Follow rules

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

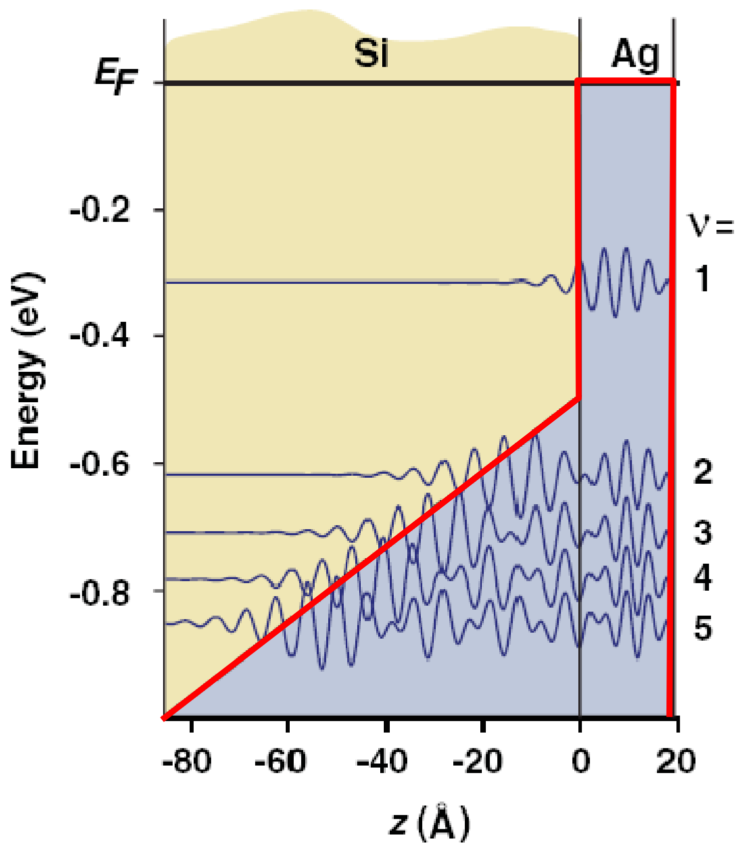
2) $$\psi(x=-\infty)=0$$ $$\psi(x=+\infty)=0$$ → Reduces 2 unknowns

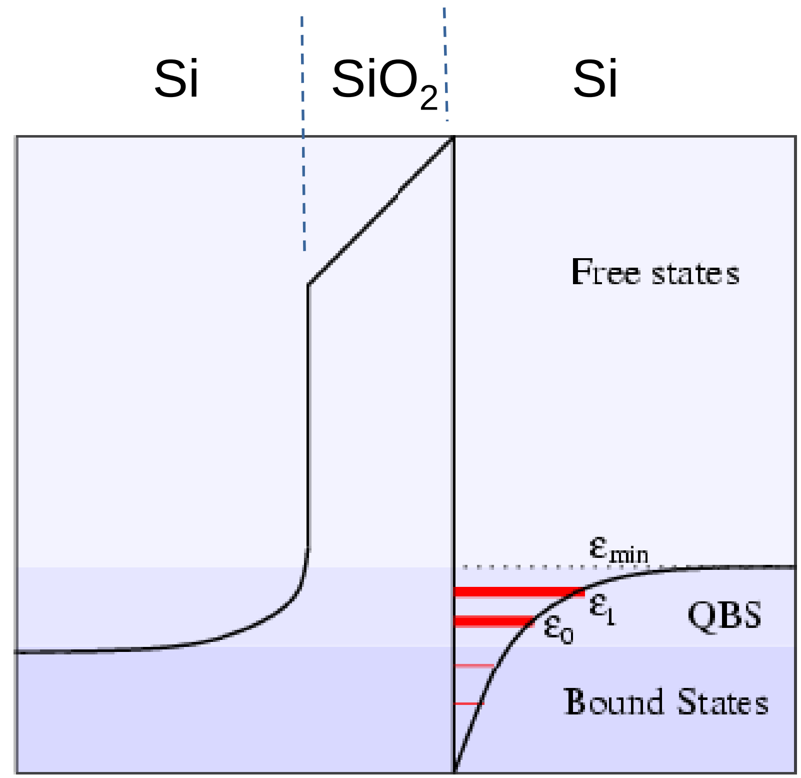
3) $$\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$$ $$\left.\frac{d\psi}{dx}\right|_{x=x_B^-} = \left.\frac{d\psi}{dx}\right|_{x=x_B^+}$$ → Set 2N-2 equations for 2N-2 unknowns (for continuous U)

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

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

Practical examples: Si/Ag and Si/SiO2





Speer et. al, Science 314, 2006.

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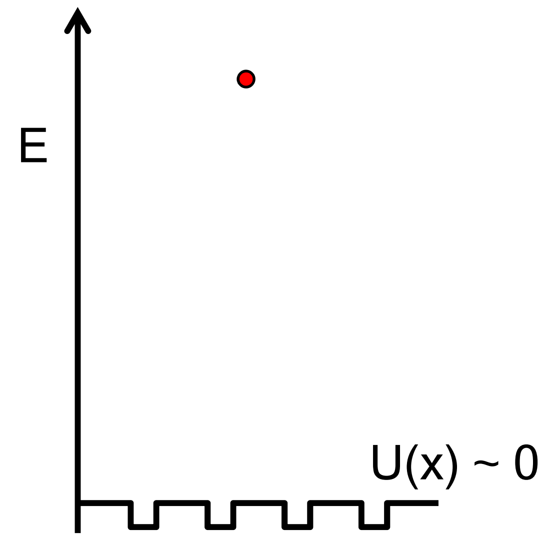
Case 2: Solution for Particles with E>>U

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



1) Solution

$$\psi(x)=A\sin(kx)+B\cos(kx)$$
$$\equiv A_+e^{ikx}+A_-e^{-ikx}$$

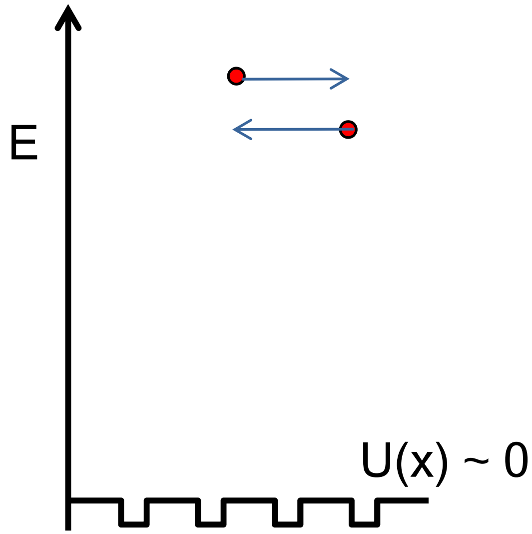
2) Boundary condition

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

Free Particle …

$$\psi(x) = A\sin(kx) + B\cos(kx)$$
$$\equiv A_+ e^{ikx} + A_- e^{-ikx}$$

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



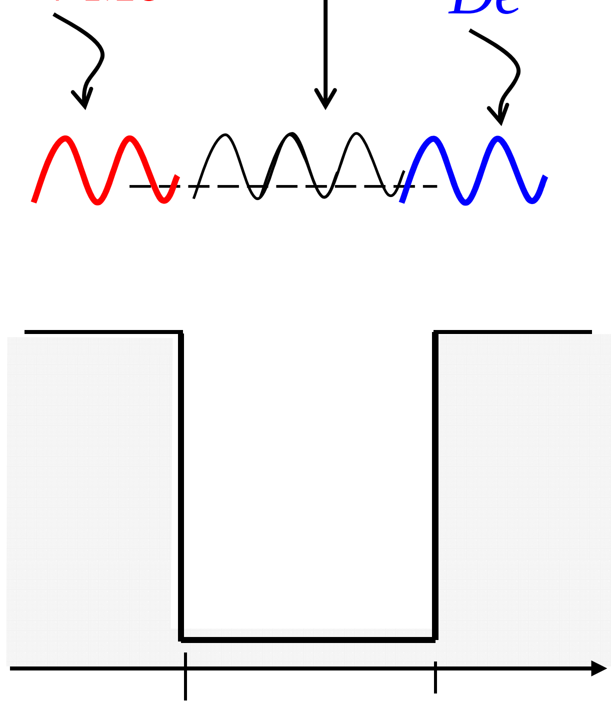
Probability: $$|\psi|^2 = \psi\psi^* = |A_+|^2 \; or \; |A_-|^2$$

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

Case 3: Bound vs. Tunneling State

$$Ae^{ik_1x} + Be^{-ik_1x}$$

$$Ce^{ik_1x} + Me^{-ik_1x} \qquad De^{ik_1x} + Ne^{-ik_1x}$$



Boundary conditions
N=0

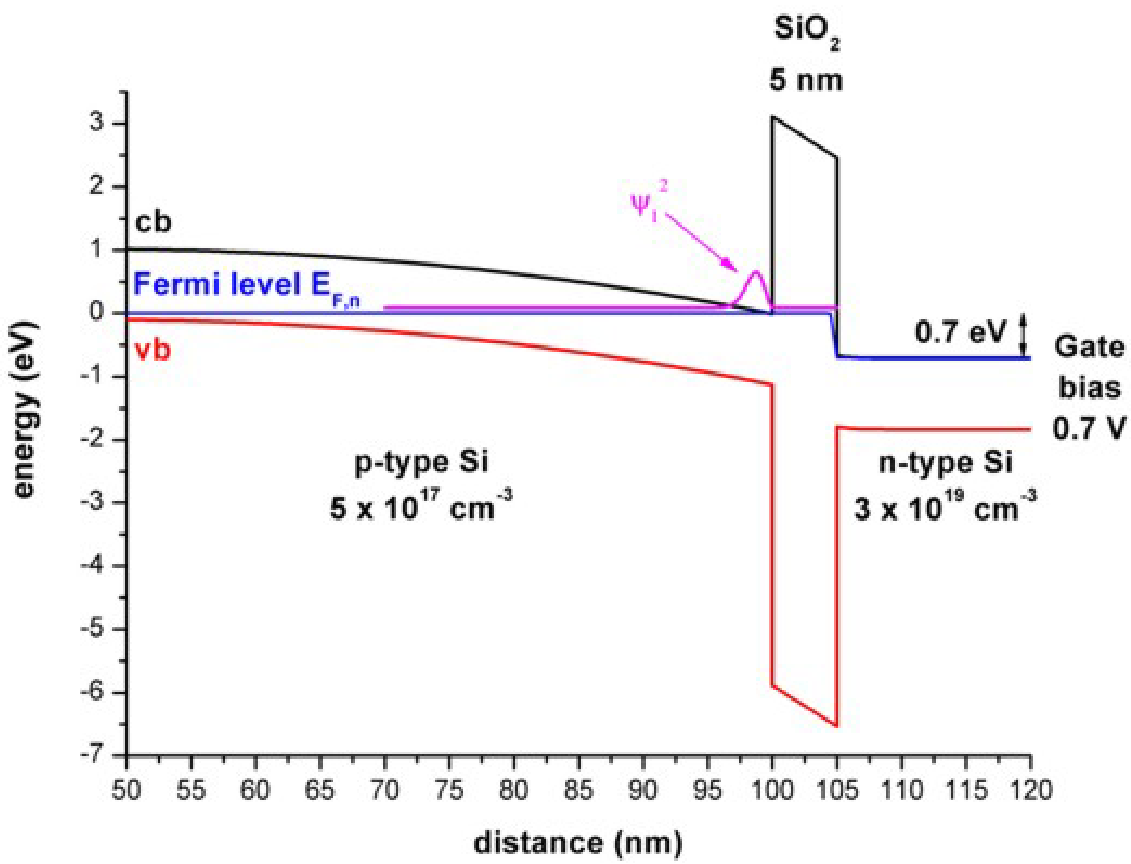
5 unknowns (C,M,A,B,D)

4 equations from
x=0 and x=a interfaces

No bound levels

Ratios of D/C is of
Interest.

Practical Example: Oxide Tunneling



Conclusions

1) We have discussed the analytical solution of Schrodinger equation for simple potentials. Such potential arises in wide variety of practical systems.

2) Numerical solution is very powerful, but it is easy to get wrong results if one is not careful.

3) Solving bound level problem is different compared to the solution of tunneling problem. The corresponding recipes should be followed carefully.

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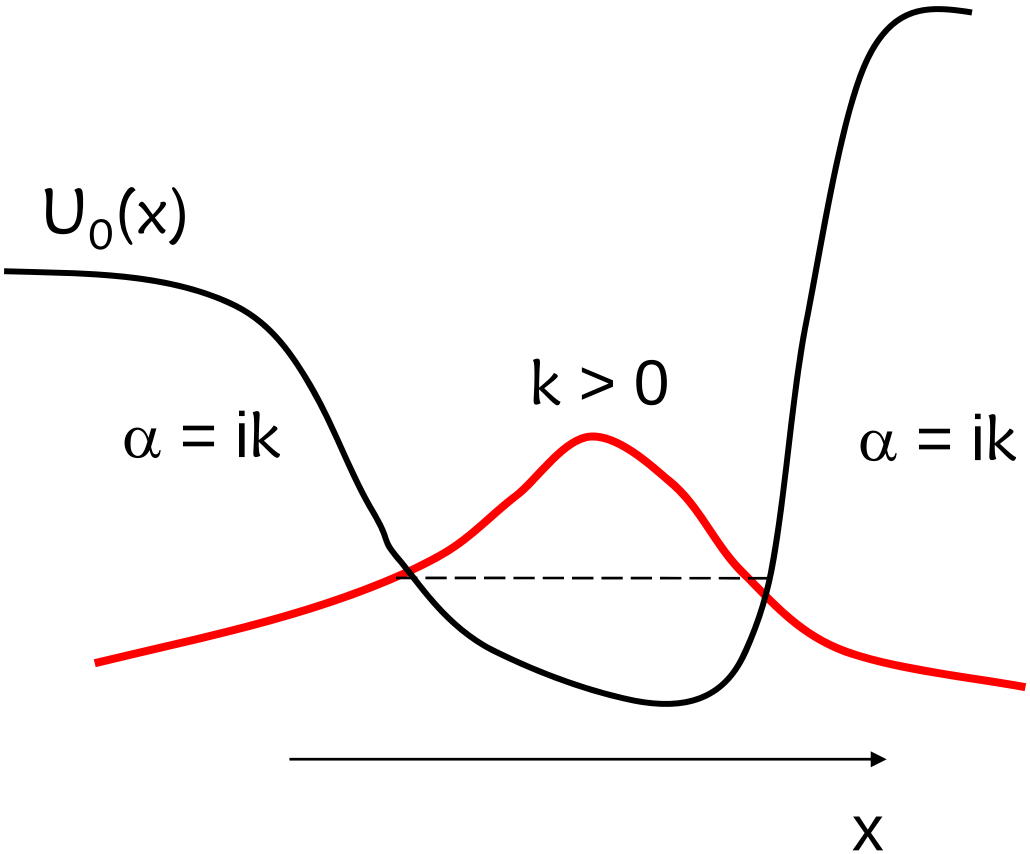
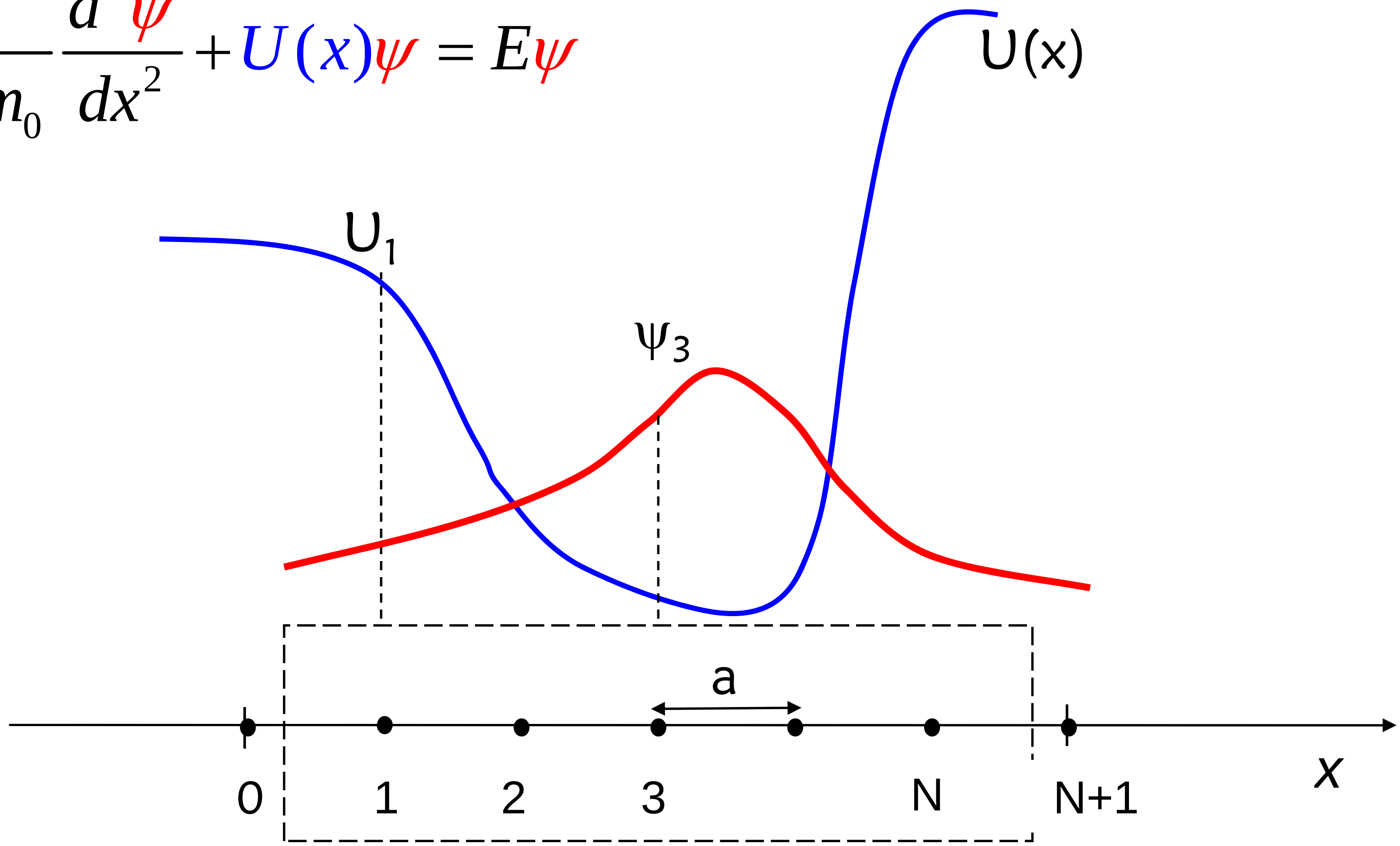
Numerical solution of Schrodinger Equation

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



(1) Define a grid …

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



Aside: Finite difference – Connecting neighbors

$$\psi(x_0+a)=\psi(x_0)+a\left.\frac{d\psi}{dx}\right|_{x_0=a}+\frac{a^2}{2}\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}+\ldots$$

$$\psi(x_0-a)=\psi(x_0)-a\left.\frac{d\psi}{dx}\right|_{x_0=a}+\frac{a^2}{2}\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}-\ldots$$

$$\psi(x_0+a)+\psi(x_0-a)-2\psi(x_0)=a^2\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}$$

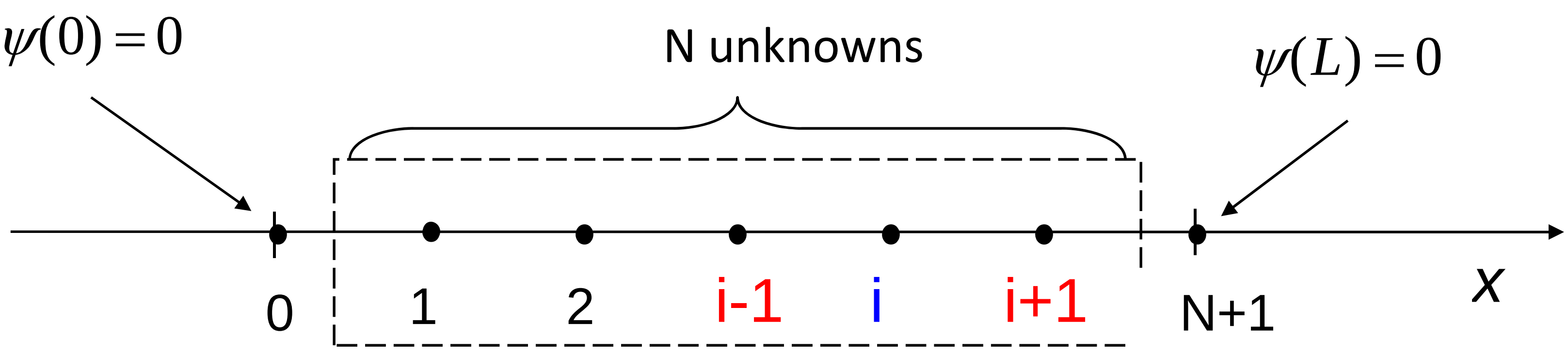
$$\left.\frac{d^2\psi}{dx^2}\right|_i=\frac{\psi_{i-1}-2\psi_i+\psi_{i+1}}{a^2}$$

(2) Express equation in Finite Difference Form

$$-\left(t_0 a^2\right)\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi \qquad t_0 \equiv \frac{\hbar^2}{2m_0 a^2}$$

$$\left.\frac{d^2\psi}{dx^2}\right|_i = \frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{a^2}$$

$$\left[-t_0\psi_{i-1} + \left(2t_0 + U_i\right)\psi_i - t_0\psi_{i+1}\right] = E\psi_i$$



(3) Define the matrix …

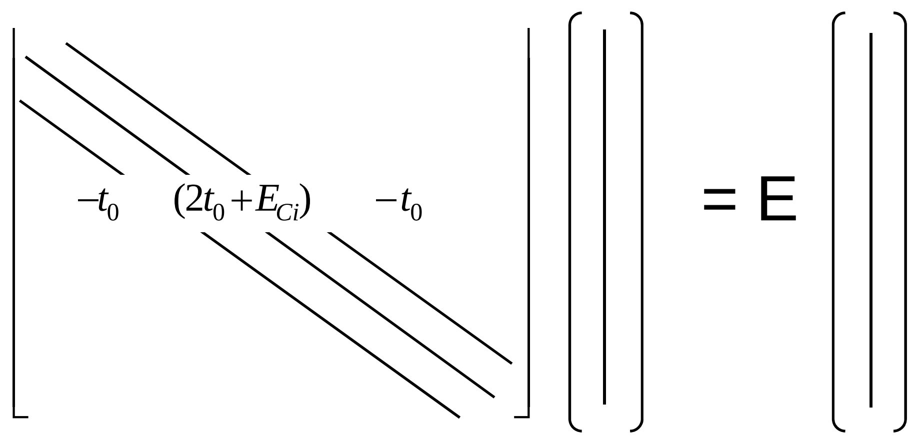
$$\left[-t_0\psi_{i-1}+(2t_0+E_{Ci})\psi_i-t_0\psi_{i+1}\right]=E\,\psi_i$$ (i = 2, 3…N-1)

$$\left[-t_0\cancel{\psi_0}+(2t_0+E_{Ci})\psi_1-t_0\psi_2\right]=E\psi_i$$ (i = 1)

$$\left[-t_0\psi_{N-1}+(2t_0+E_{Ci})\psi_N-t_0\cancel{\psi_{N+1}}\right]=E\psi_i$$ (i = N)

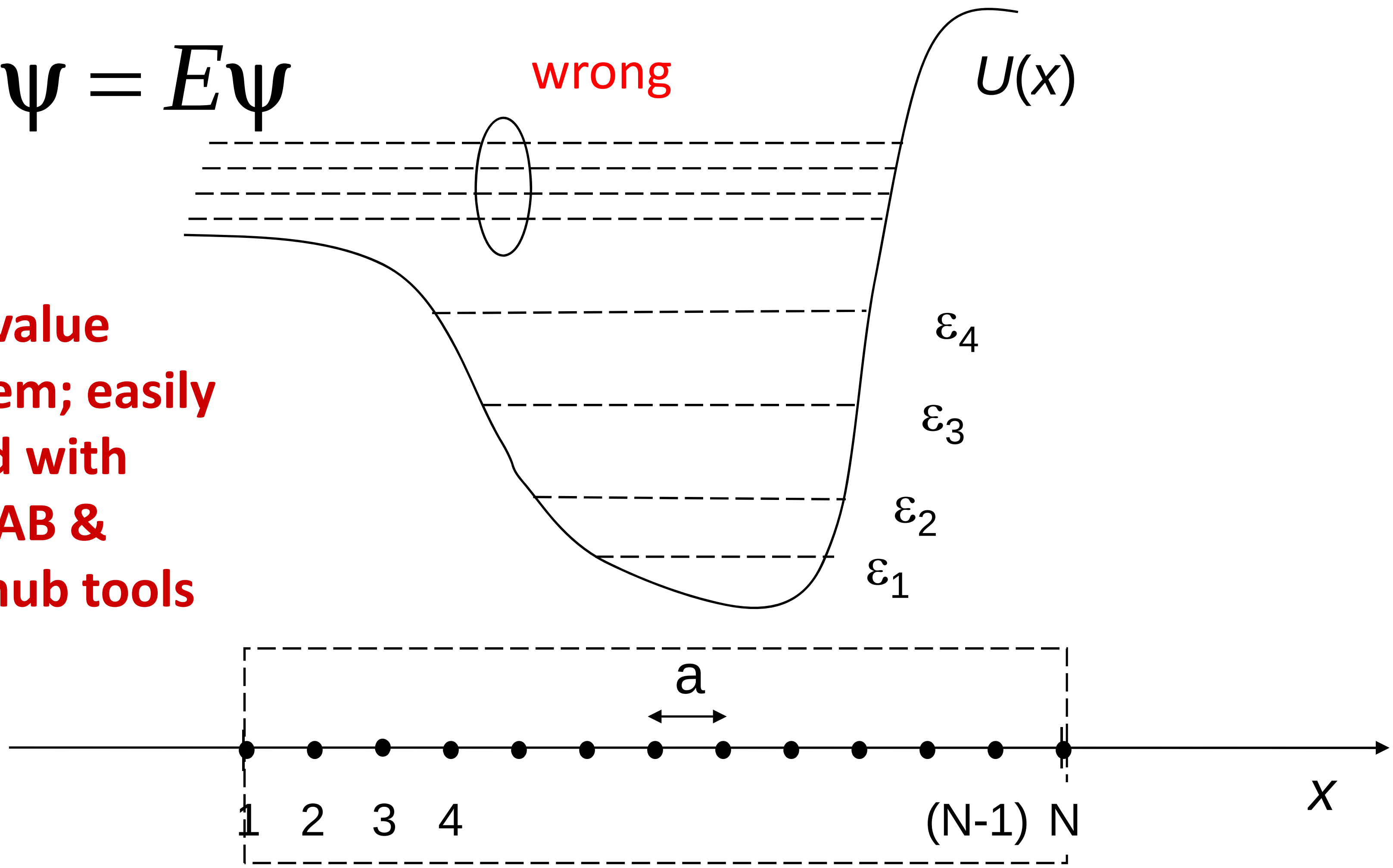
$$\mathbf{H}\psi = E\psi$$

N x N　　N x 1



(4) Solve the Eigen-value Problem

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



Eigenvalue problem; easily solved with MATLAB & nanohub tools