Section 6

Electron Tunneling – Emergence of Bandstructure

6.5 Analytical and Numerical Solution Strategies

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School of Electrical and Computer Engineering

Video

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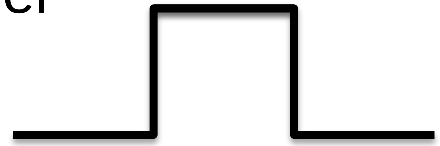
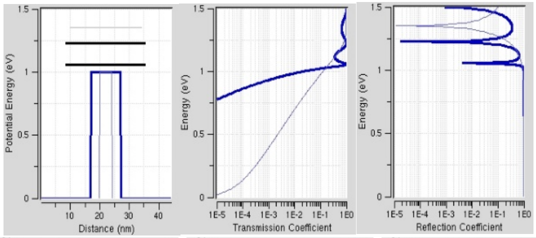
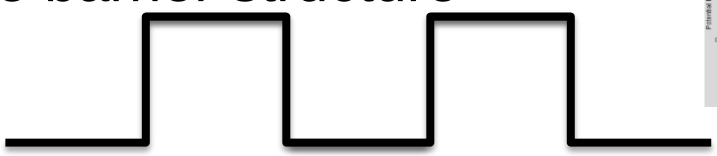
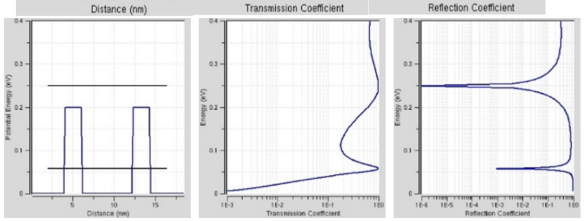
- 6.1 Transfer Matrix Method
- 6.2 Tunneling through a single barrier
  - » Analytical Solution
  - » Numerical observations



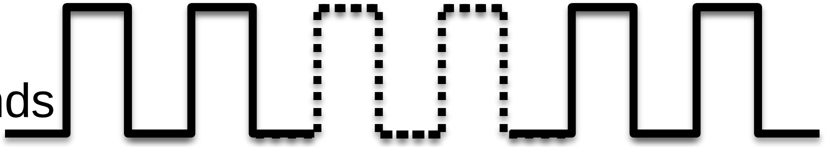


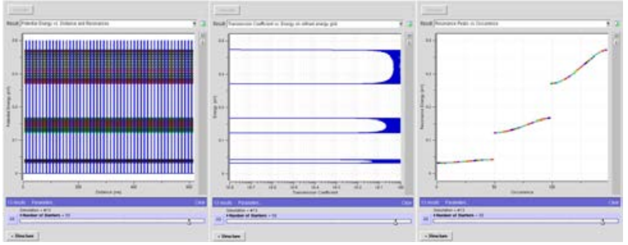
- 6.3 Tunneling through a double barrier structure
  - » Resonant Transmission
  - » Transmission Peak Width



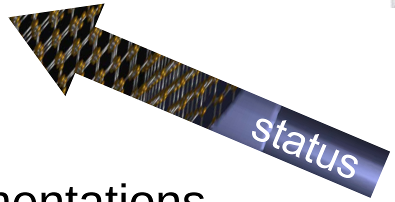


- 6.4 Tunneling through N barriers - Formation of bandstructure
  - » N wells – N Peaks
  - » S states per well – S Bands





- 6.5 Analytical and Numerical Solution Strategies
  - » Analytical segmentation
  - » Transfer Matrix Method
  - » Discretizing Schrödinger’s equation for numerical implementations



Reference:

piece-wise-constant-potential-barrier tool http://nanohub.org/tools/pcpbt

Five Steps for Closed System Analytical Solution

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

$$\psi(x)=A_+e^{ikx}+A_-e^{-ikx}$$
$$\psi(x)=De^{-\alpha x}+Ee^{+\alpha x}$$

2) $\psi(x=-\infty)=0$, $\psi(x=+\infty)=0$ → Boundary Conditions at the edge
Reduces 2 unknowns

3) $\psi\big|_{x=x_B^-}=\psi\big|_{x=x_B^+}$, $\frac{d\psi}{dx}\Big|_{x=x_B^-}=\frac{d\psi}{dx}\Big|_{x=x_B^+}$ → Boundary Condition at each interface:
Set 2N-2 equations for
2N-2 unknowns (for continuous U)

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

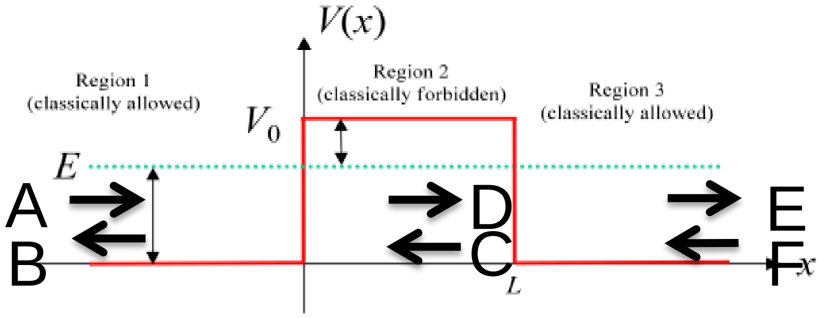
5) $\int_{-\infty}^{\infty}|\psi(x,E)|^2\,dx=1$

Normalization of unity probability
for wave function

Open System: Generalization to Transfer Matrix Method

- The complete transfer matrix

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix}$$



- In general for any intermediate set of layers, the TMM is expressed as:

$$\begin{pmatrix} A_{n-1}^{+} \\ A_{n-1}^{-} \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_{n}^{+} \\ A_{n}^{-} \end{pmatrix}$$

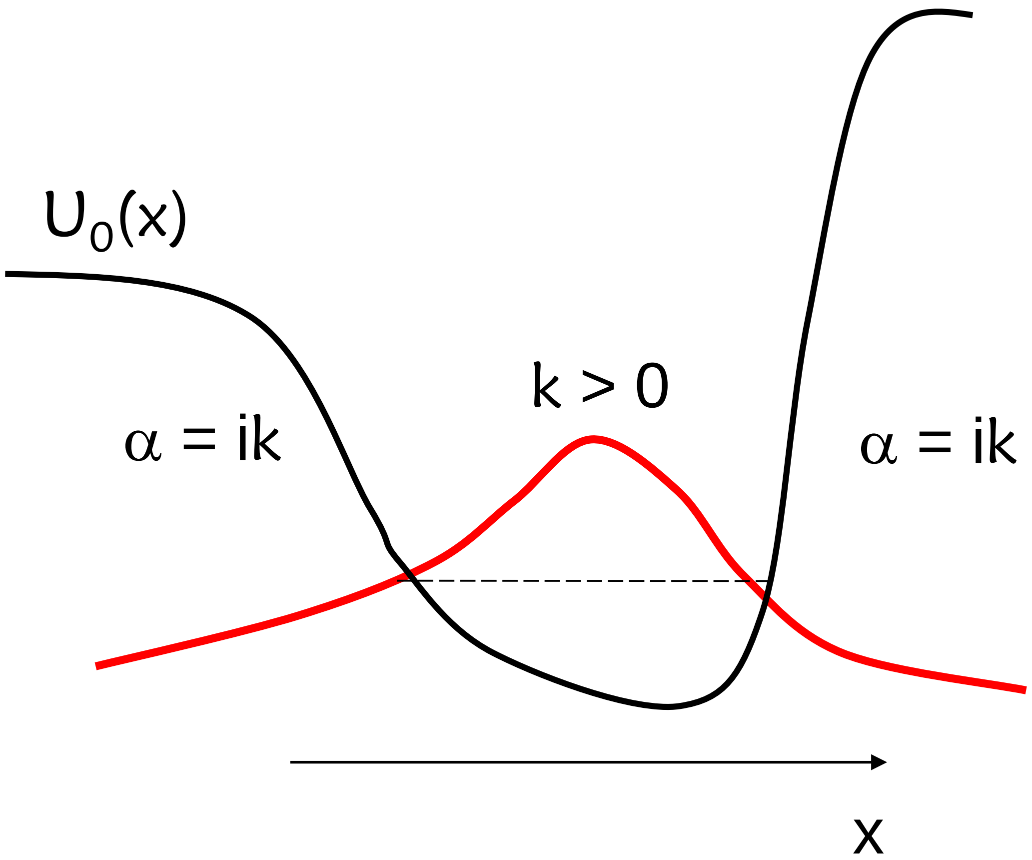
- For multiple layers the overall transfer matrix will be

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = \prod_{j=2..N} \underline{T}_j \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} .$$

- Looks conceptually very simple and analytically pleasing
- Use it for your homework assignment for a double barrier structure!

Numerical solution of Schrodinger Equation

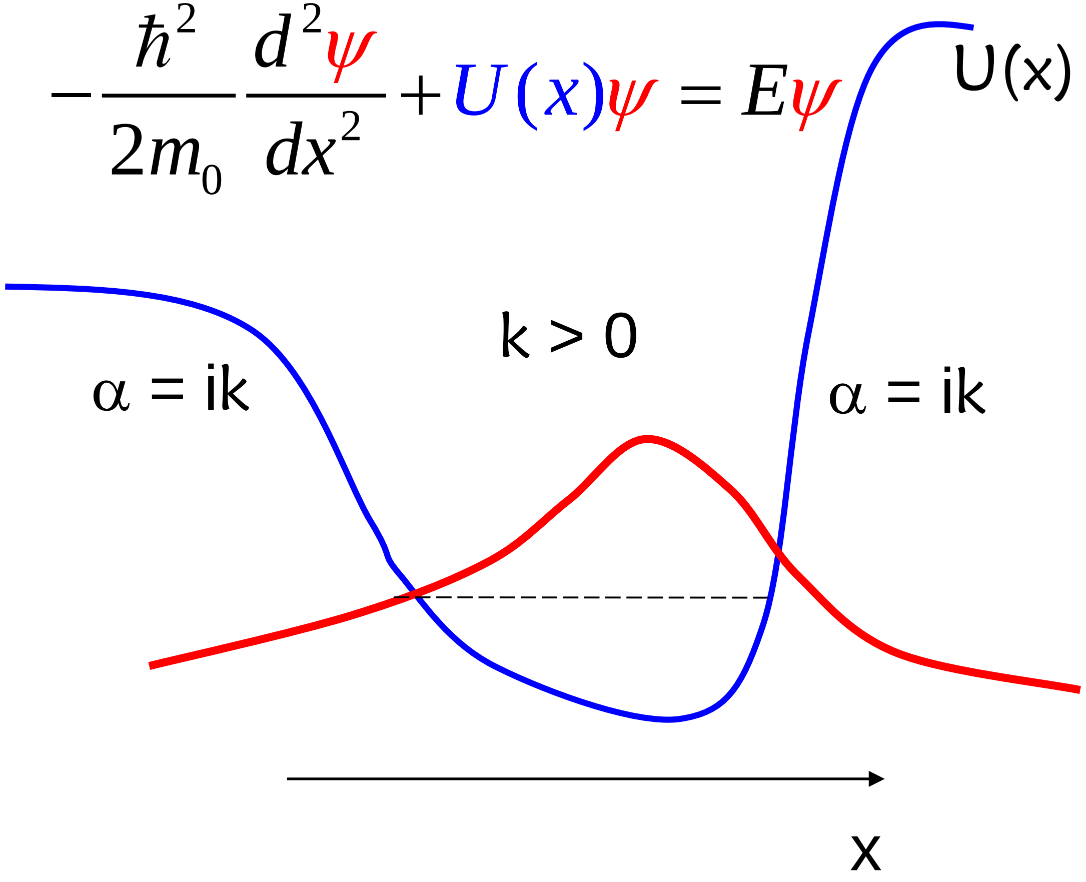
$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k \equiv \sqrt{2m_0\left[E - U(x)\right]}/\hbar$$



Numerical solution of Schrodinger Equation

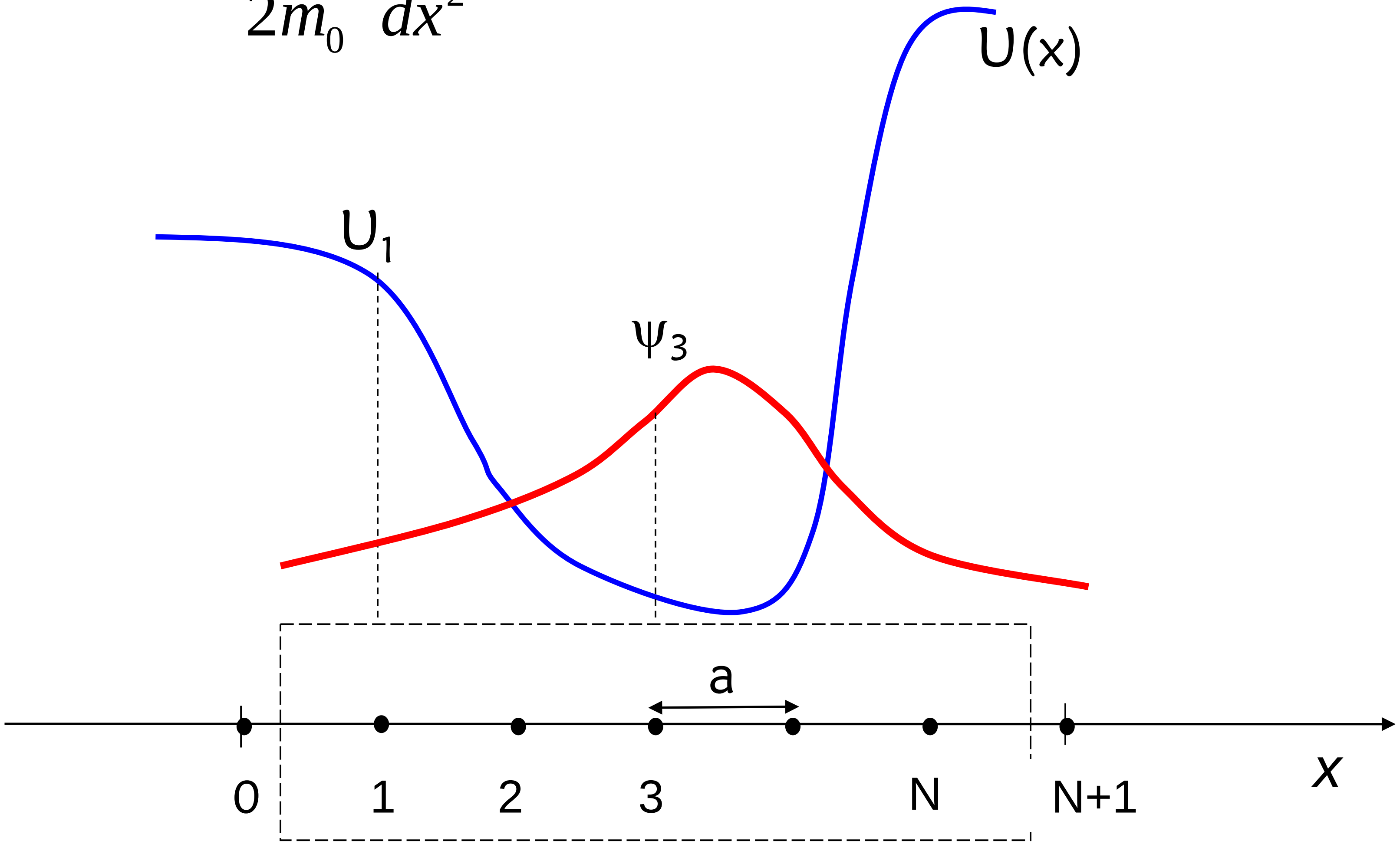
$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k \equiv \sqrt{2m_0\left[E - U(x)\right]}/\hbar$$

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



(1) Define a grid …

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



Second Derivative on a Finite Mesh

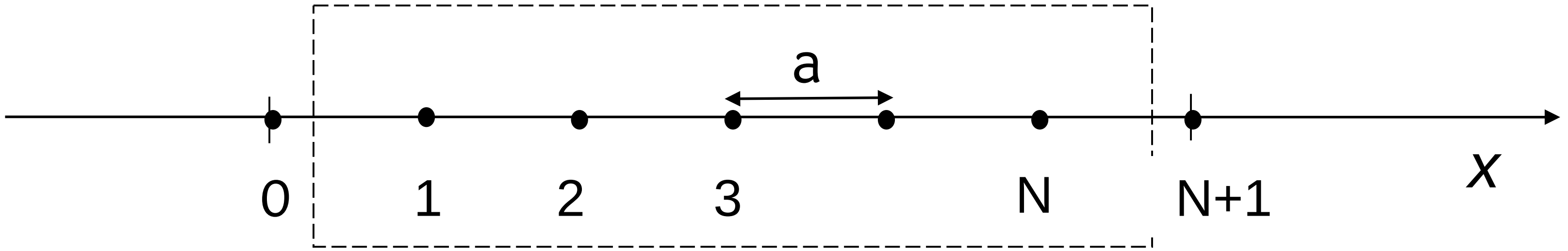
$$\psi(x_0+a)=\psi(x_0)+a\left.\frac{d\psi}{dx}\right|_{x_0=a}+\frac{a^2}{2}\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}+\dots$$

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

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

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

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

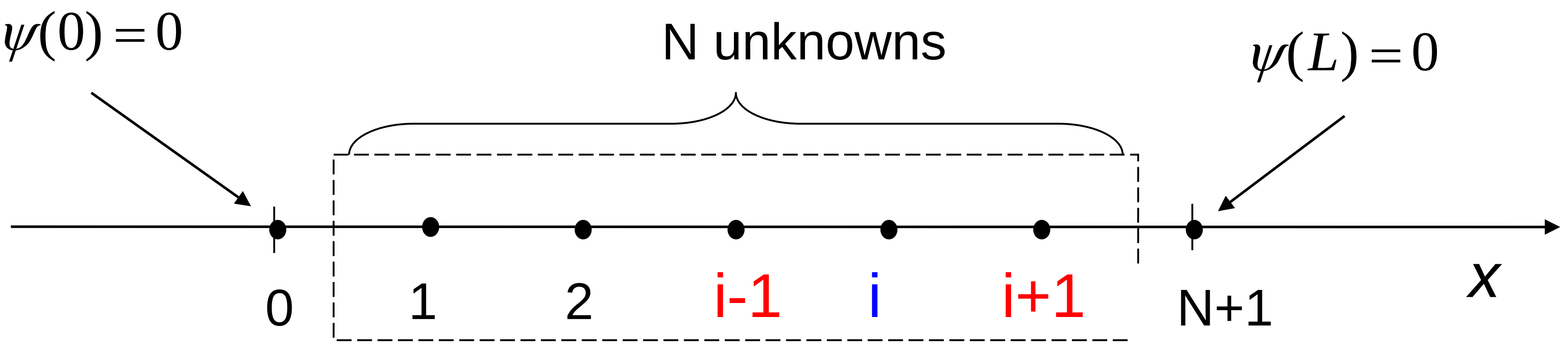


(2) Express equation in Finite Difference Form

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

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

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



(3) Define the matrix …

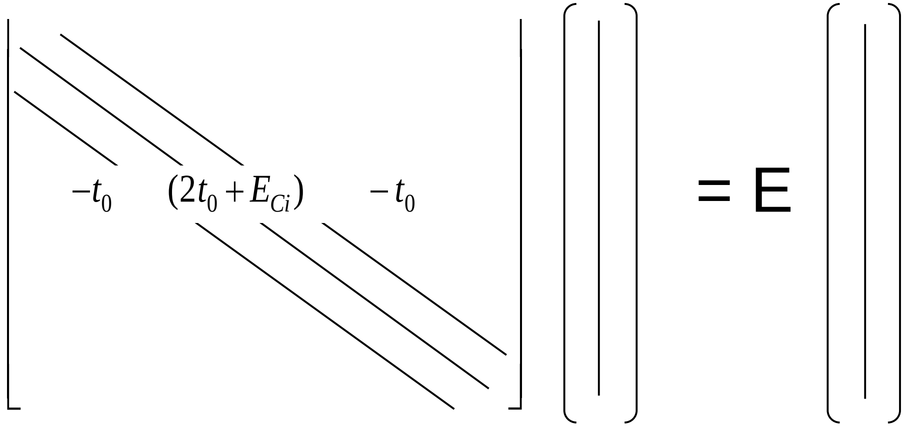
$$\left[-t_0\psi_{i-1} + \left(2t_0 + E_{Ci}\right)\psi_i - t_0\psi_{i+1}\right] = E\,\psi_i \qquad \text{(i = 2, 3…N-1)}$$

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

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

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

N x N (H) N x 1 (ψ)

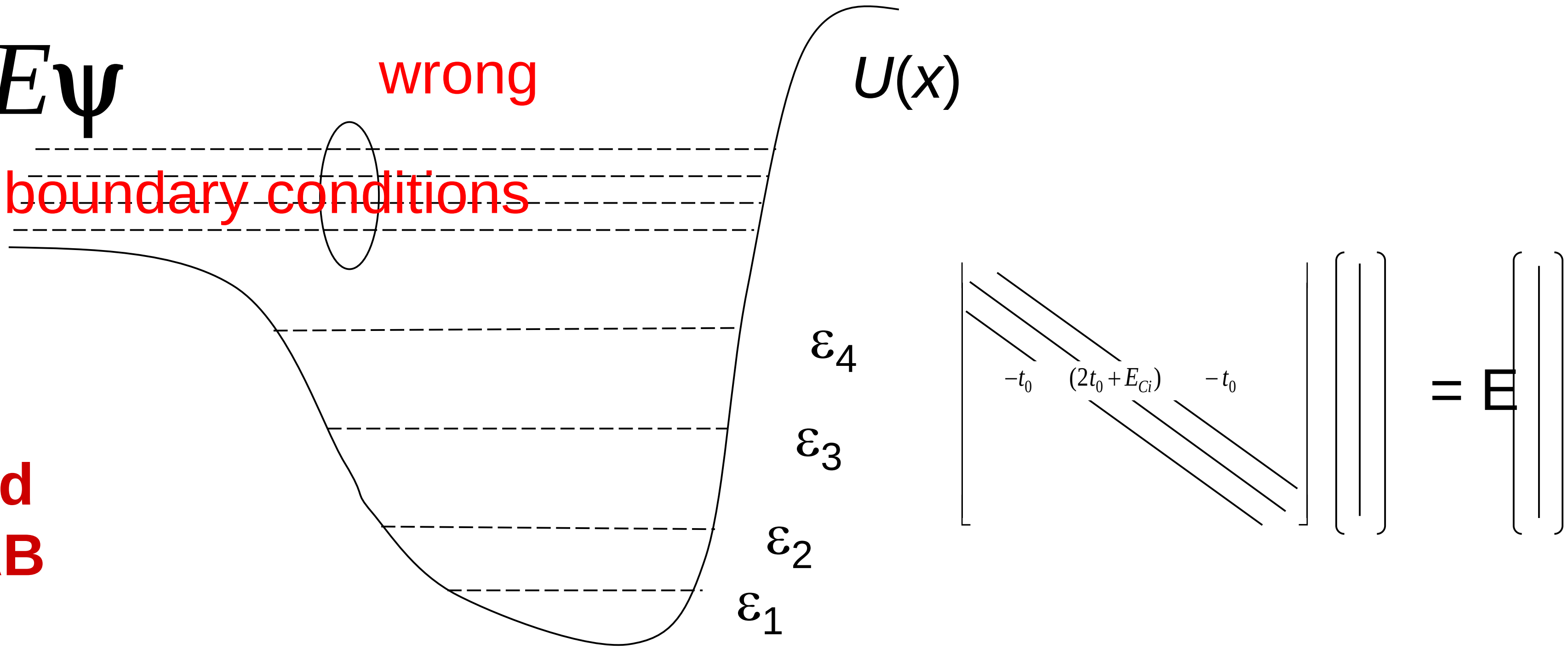


(4) Solve the Eigen-value Problem

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

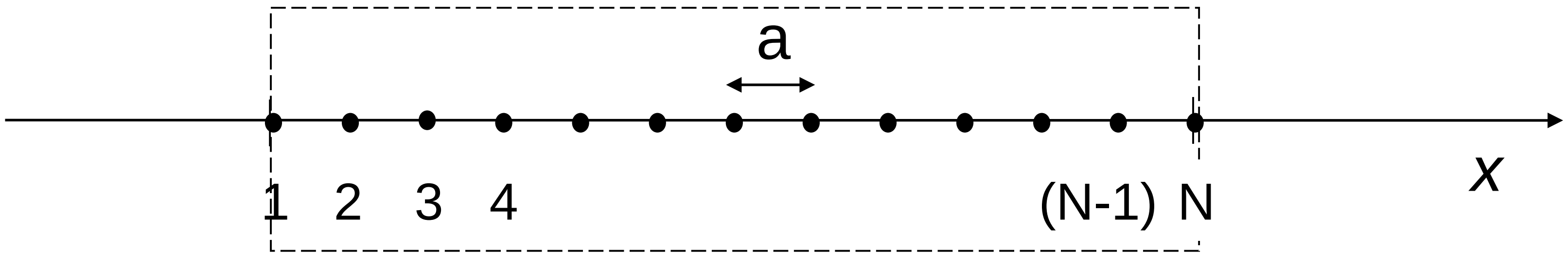
wrong

Need open boundary conditions



Eigenvalue problem; easily solved with MATLAB & nanohub tools

$$\begin{bmatrix} \ddots & & \\ -t_0 & (2t_0 + E_{Ci}) & -t_0 \\ & & \ddots \end{bmatrix} \{\psi\} = E \{\psi\}$$



Gerhard Klimeck (2010), "Nanoelectronic Modeling: From Quantum Mechanics and Atoms to Realistic Devices," https://nanohub.org/resources/8086.

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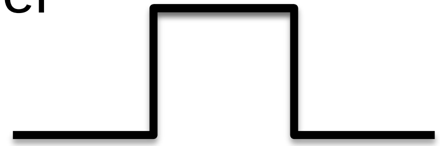

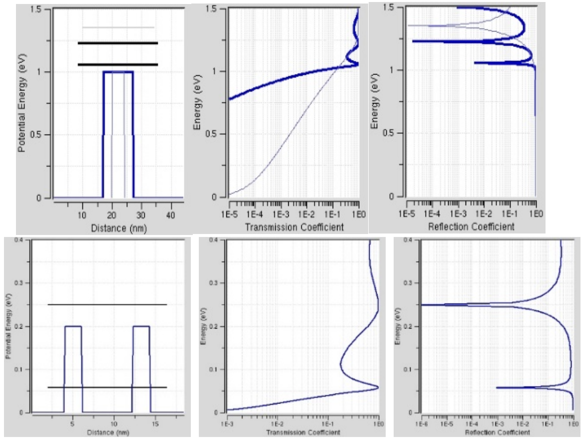

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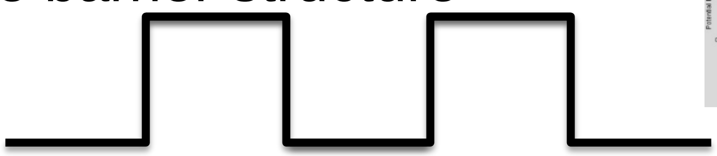

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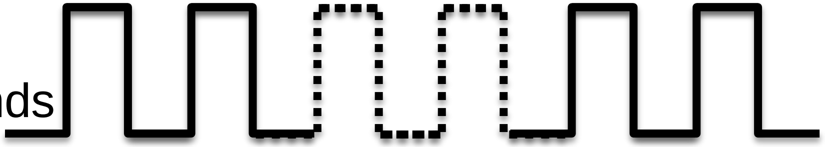

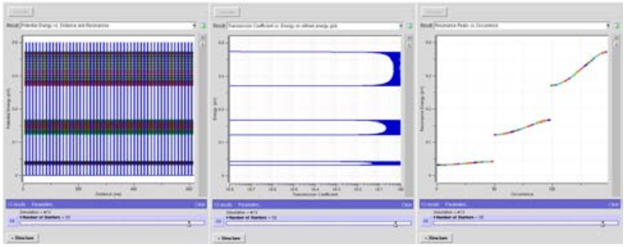

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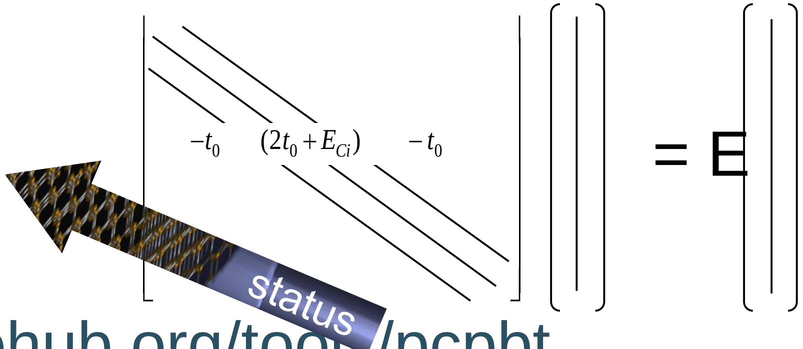

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