Section 6
Electron Tunneling -
Emergence of Bandstructure

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School of Electrical and Computer Engineering

Section 6
Electron Tunneling - Emergence of Bandstructure

Video

Video Segment

Video Segment

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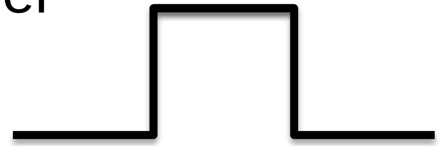
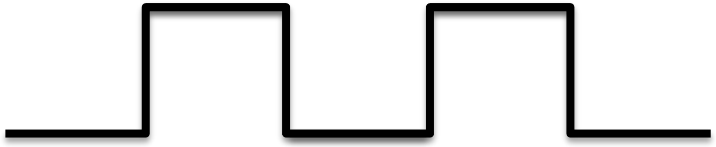
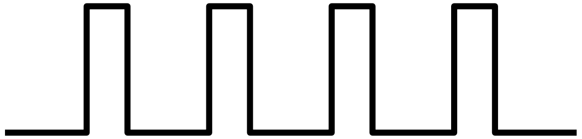
- 6.1 Transfer Matrix Method
- 6.2 Tunneling through a single barrier



- 6.3 Tunneling through a double barrier structure



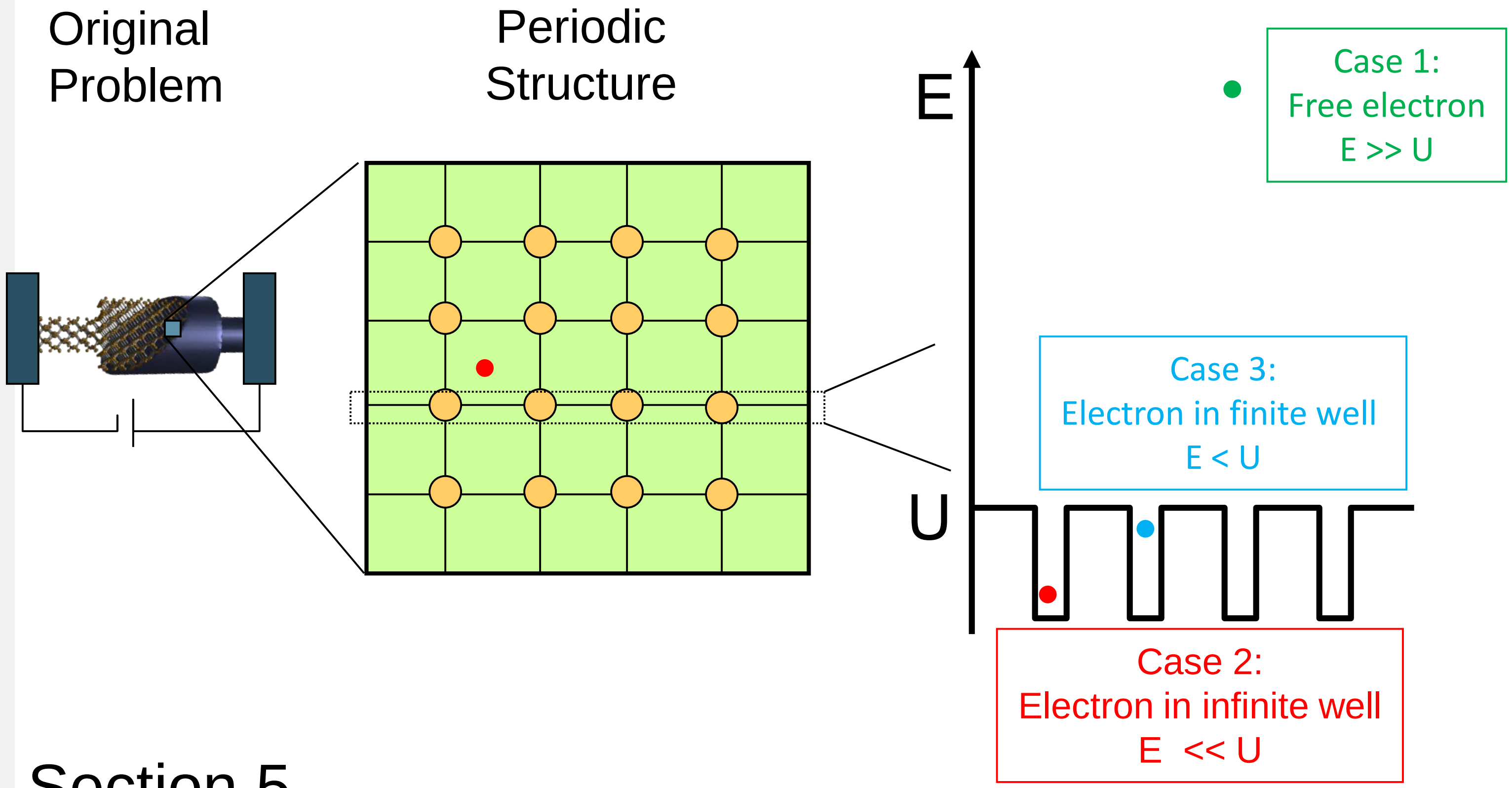
- 6.4 Tunneling through N barriers - Formation of bandstructure



- 6.5 Analytical and Numerical Solution Strategies

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

Reminder of Section 5
Analytical Solutions to Free and Bound Electrons



1) $$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

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

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

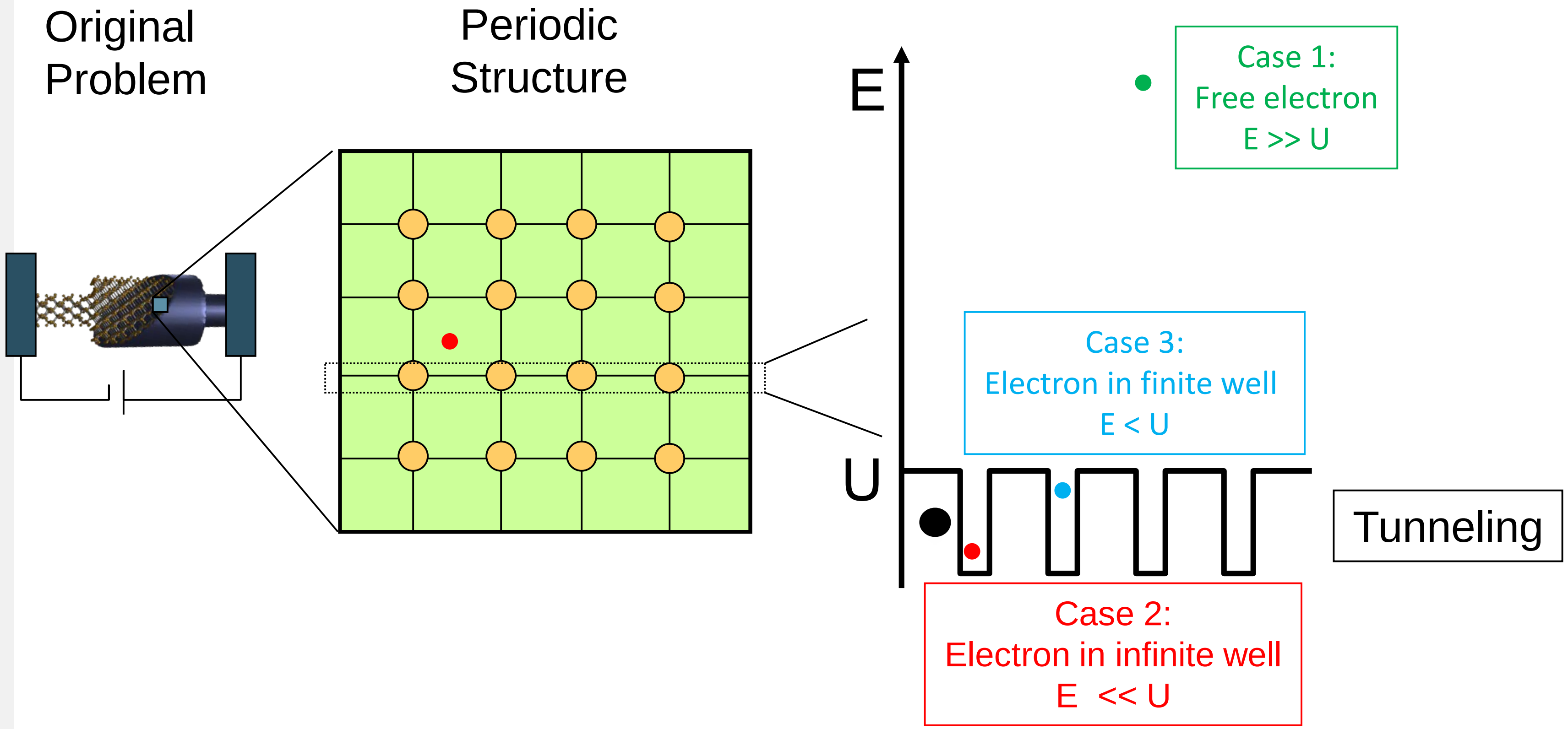
4) Det (coefficient matrix)=0
And find E by graphical or numerical solution

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

Section 5

- Section 5.1 – Free and Tightly Bound Electrons
  - »Time Independent Schrödinger Equation
  - »(Almost) Free Electrons
  - »Tightly bound electrons – infinite potential well
- Section 5.2 - Electrons in a finite potential well

Reminder of Section 5
Analytical Solutions to Free and Bound Electrons



1) $$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

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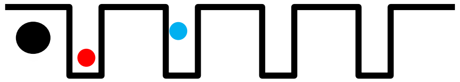
Section 5
Bound and free states
Not tunneling

Section 6
Electron Tunneling – Emergence of Bandstructure

Reminder of Section 5: Five Steps for ~~Closed~~ Open System Analytical Solution



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

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

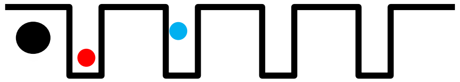
2) ~~$\psi(x=-\infty)=0$~~ ~~$\psi(x=+\infty)=0$~~ → Boundary Conditions at the **Open** edge Reduces 2 unknowns

3) $$\psi\big|_{x=x_B^-}=\psi\big|_{x=x_B^+}$$
$$\left.\frac{d\psi}{dx}\right|_{x=x_B^-}=\left.\frac{d\psi}{dx}\right|_{x=x_B^+}$$
→ 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) ~~$$\int_{-\infty}^{\infty}\left|\psi(x,E)\right|^2dx=1$$~~
~~Normalization of unity probability for wave function~~

Reminder:
Five Steps for ~~Closed~~ Open System Analytical Solution



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

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

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

2) ~~$\psi(x=-\infty)=0$~~ ~~$\psi(x=+\infty)=0$~~ $\longrightarrow$

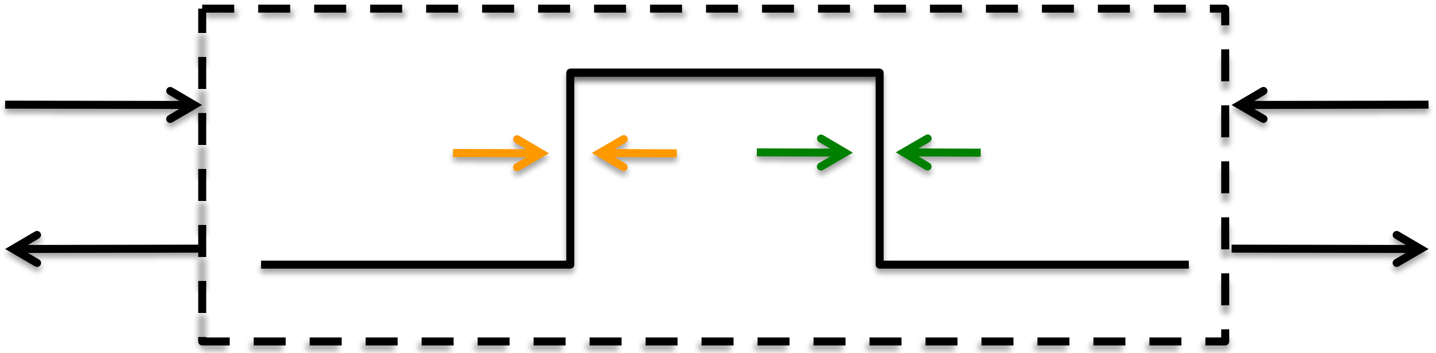
3) $$\psi\big|_{x=x_B^-}=\psi\big|_{x=x_B^+}$$

$$\left.\frac{d\psi}{dx}\right|_{x=x_B^-}=\left.\frac{d\psi}{dx}\right|_{x=x_B^+} \longrightarrow$$

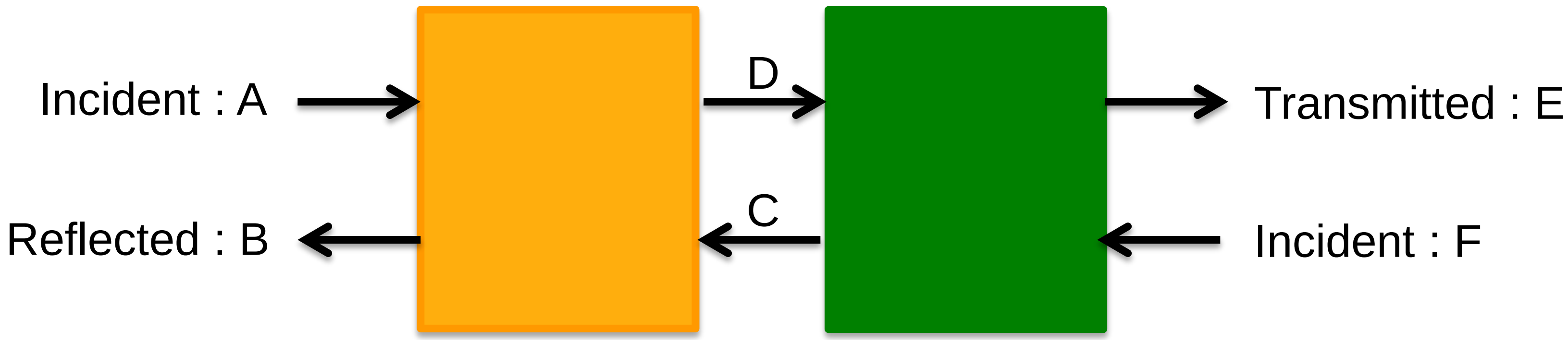
4) Det (coefficient matrix)=0
~~And find E by graphical or numerical solution~~

Transmission through a single barrier
Scattering Matrix approach

Define our system : Single barrier



One matrix each for each interface: 2 S-matrices



No particles lost! Typically A=1 and F=0.

Transmission through a single barrier
Scattering Matrix approach

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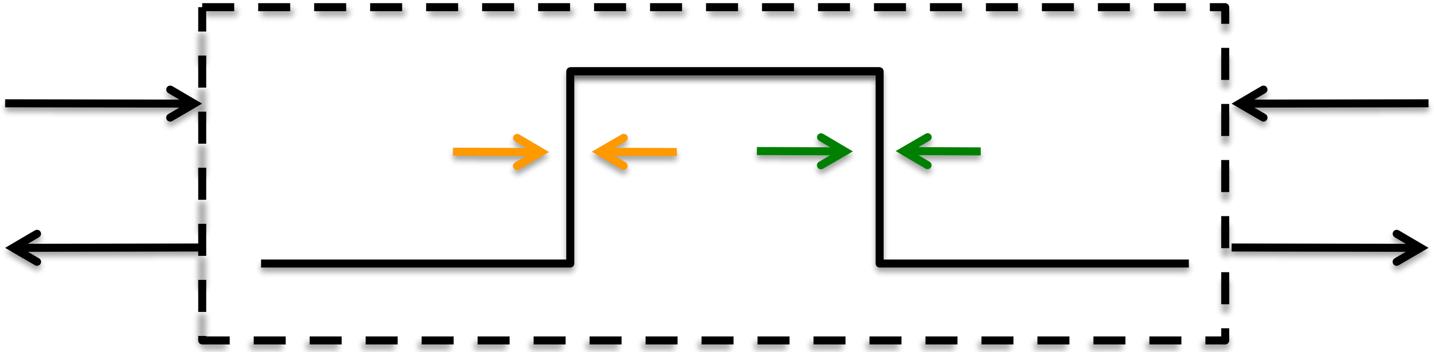

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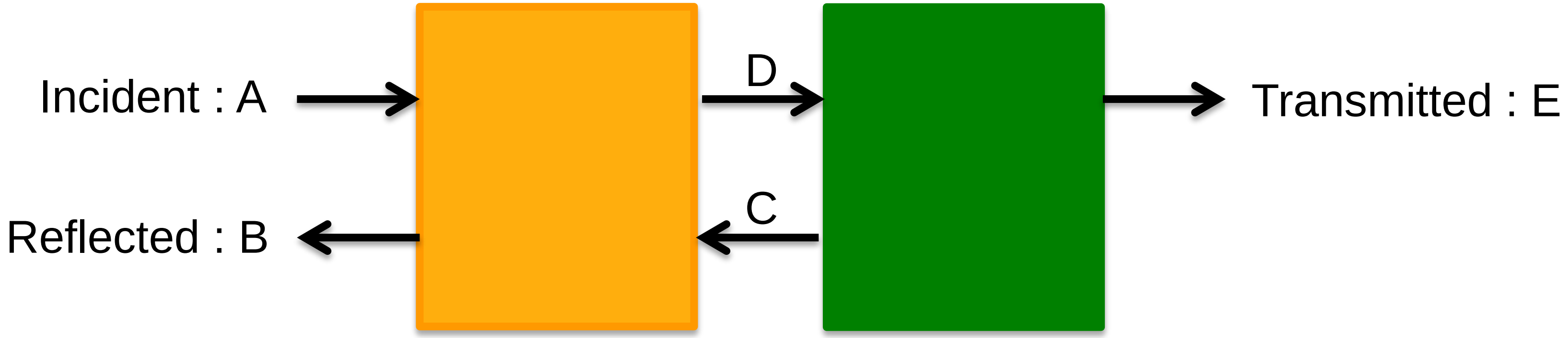
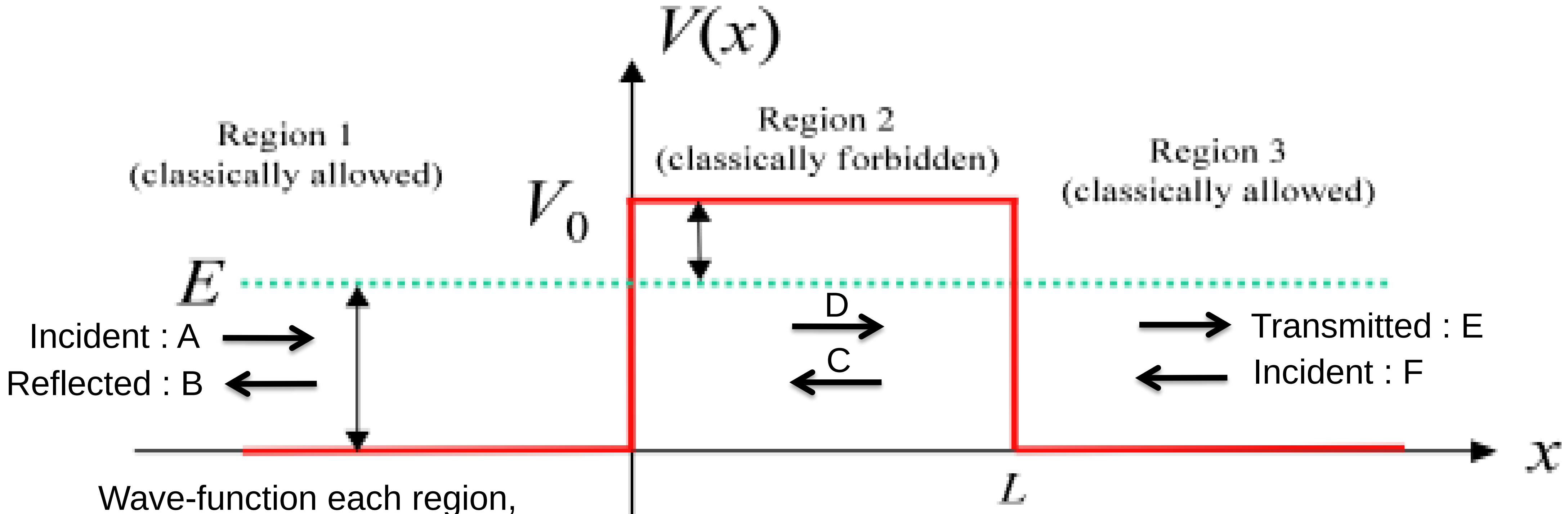


No particles lost! Typically A=1 and F=0.

Boundary Conditions at the **Open** edge
Reduces 2 unknowns

Tunneling through a single barrier



Wave-function each region,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

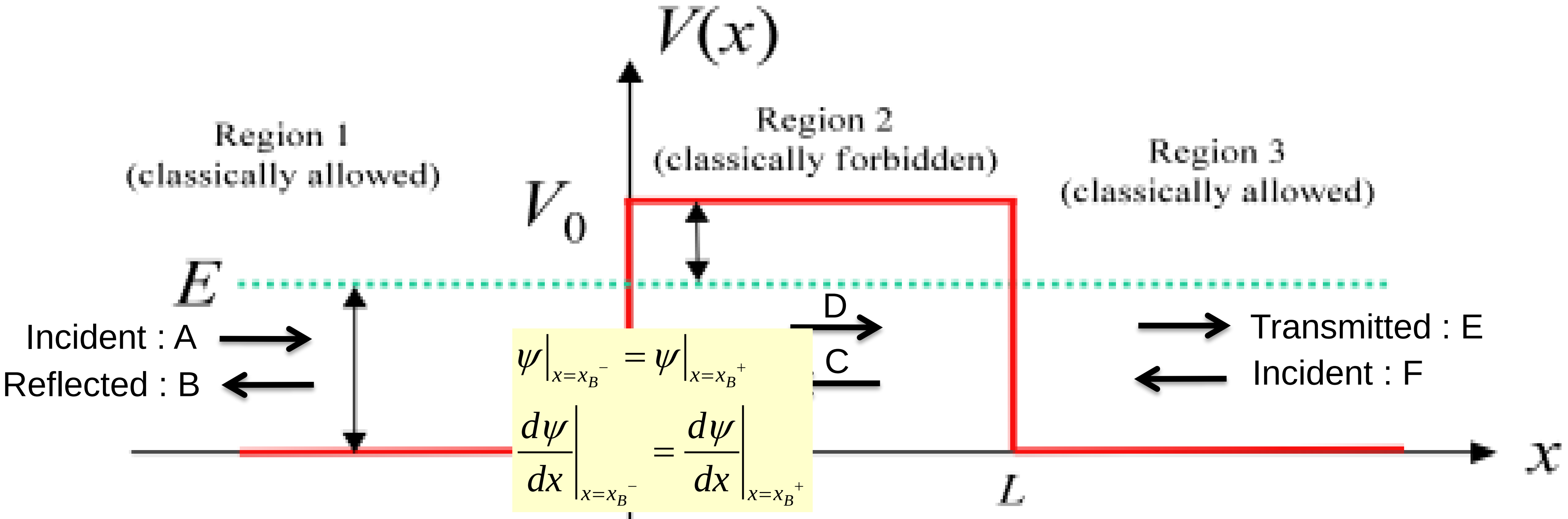
$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}$$

$$\gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

Tunneling through a single barrier



$$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$

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

Wave-function each region,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}$$

$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

Applying boundary conditions at each interface (x=0 and x=L) gives,

$$\psi_1(0) = \psi_2(0) \rightarrow A + B = C + D$$

$$\psi_1'(0) = \psi_2'(0) \rightarrow ik(A - B) = -\gamma(C - D)$$

$$\psi_2(L) = \psi_3(L) \rightarrow Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL}$$

$$\psi_2'(L) = \psi_3'(L) \rightarrow -\gamma\left(Ce^{-\gamma L} - De^{\gamma L}\right) = ik\left(Ee^{ikL} - Fe^{-ikL}\right)$$

Interface Boundary Conditions

Applying boundary conditions at each interface (x=0 and x=L) gives,

$$\psi_1(0) = \psi_2(0) \quad \rightarrow \quad A + B = C + D$$

$$\psi_1'(0) = \psi_2'(0) \quad \rightarrow ik(A - B) = -\gamma(C - D)$$

Which in matrix can be written as,

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) \\ \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\psi_2(L) = \psi_3(L) \quad \rightarrow \quad Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL}$$

$$\psi_2'(L) = \psi_3'(L) \quad \rightarrow \quad -\gamma\left(Ce^{-\gamma L} - De^{\gamma L}\right) = ik\left(Ee^{ikL} - Fe^{-ikL}\right)$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{(ik+\gamma)L} & \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{-(ik-\gamma)L} \\ \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{(ik-\gamma)L} & \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{-(ik+\gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

Generalization to Transfer Matrix Method

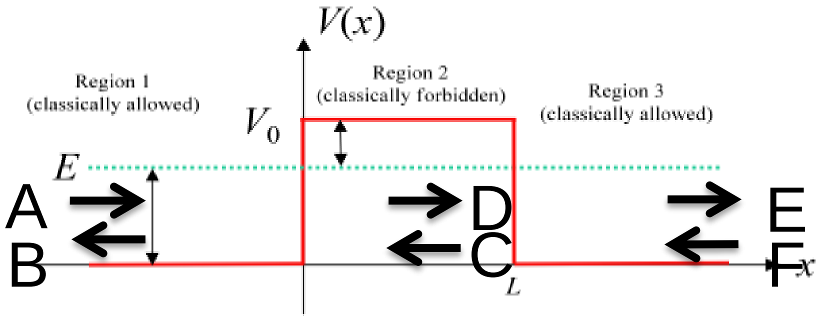
Which in matrix can be written as,

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) \\ \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right) e^{(ik+\gamma)L} & \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right) e^{-(ik-\gamma)L} \\ \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right) e^{(ik-\gamma)L} & \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right) e^{-(ik+\gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

- The complete transfer matrix

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



Generalization to Transfer Matrix Method

- The complete transfer matrix

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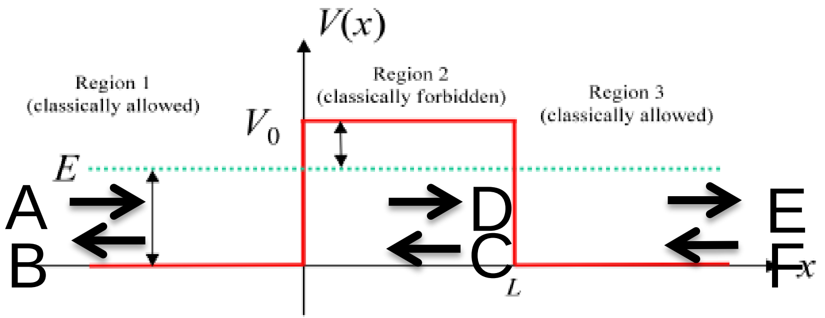

- In general for any intermediate set of layers, the TMM is expressed as:

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

- 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!

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status

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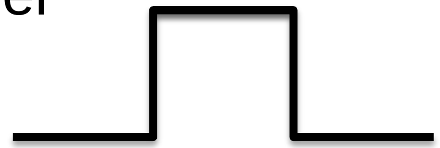

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix}$$

- 6.3 Tunneling through a double barrier structure
- 6.4 Tunneling through N barriers - Formation of bandstructure
- 6.5 Analytical and Numerical Solution Strategies

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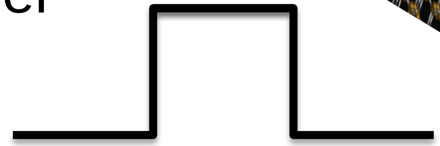
- 6.1 Transfer Matrix Method
- 6.2 Tunneling through a single barrier
  - » Analytical Solution
  - » Numerical observations



status

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