Section 7
Bandstructure in 1D Periodic Potentials

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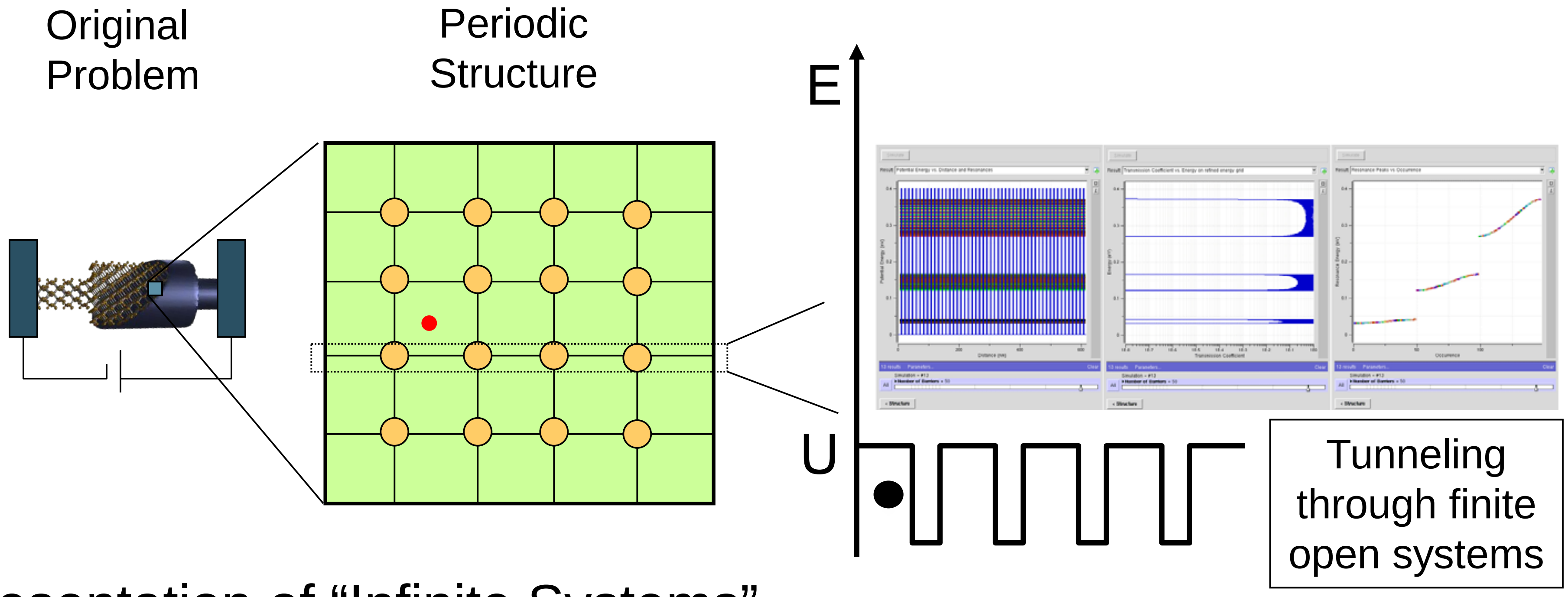
Section 7
Bandstructure - in 1D Periodic Potentials



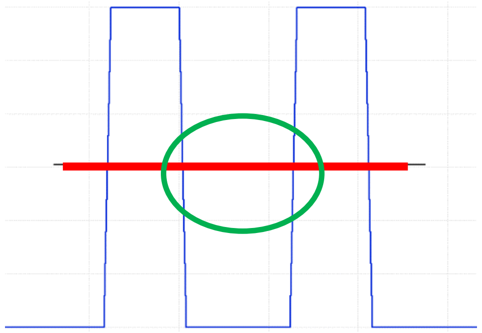
Goal: Representation of “Infinite Systems”

- 7.1 Bandstructure - Problem Formulation
- 7.2 Bandstructure - Solutions
- 7.3 Band Properties

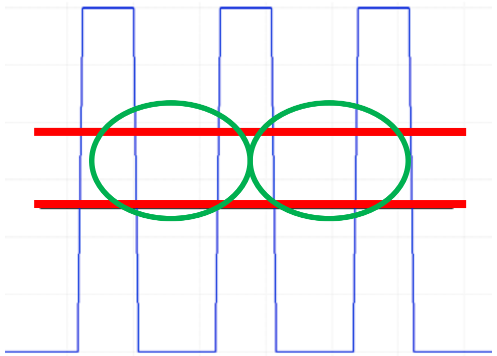
Reference: Vol. 6, Ch. 3

Daniel Mejia, Gerhard Klimeck (2019), "Periodic Potential Lab - Kronig Penney Model, " https://nanohub.org/resources/kronigpenneylab. (DOI: 10.21981/TT2Y-A185).

Reminder
Transmission through Repeated Wells

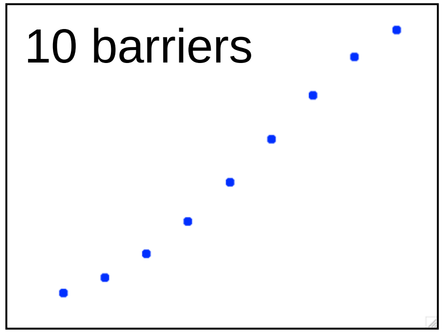


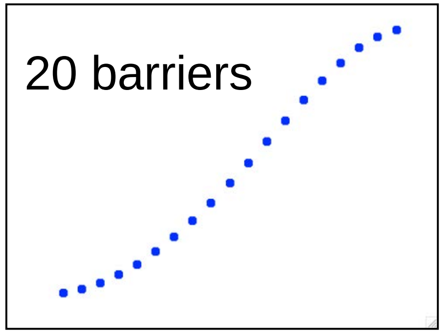
2 barriers =>1 resonance

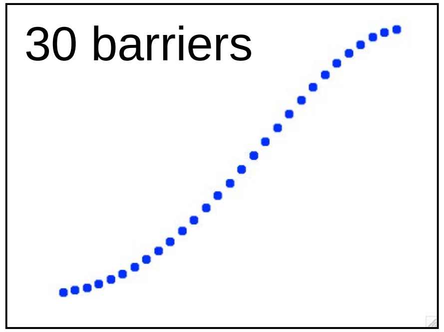


3 barriers =>2 resonance

n barriers =>n-1 resonance



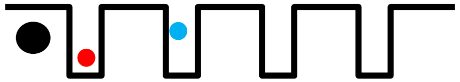




As the number of barriers are increased more and more energy resonances begin to appear and energy bands are formed.

What if the number of wells is infinite?

Reminder:
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

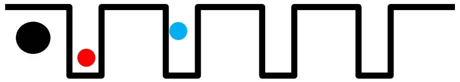
3) $$\psi\big|_{x=x_B^-}=\psi\big|_{x=x_B^+}$$
$$\frac{d\psi}{dx}\bigg|_{x=x_B^-}=\frac{d\psi}{dx}\bigg|_{x=x_B^+}$$
→ Boundary Condition at each interface: Set 2N-2 equations for 2N-2 unknowns (for continuous U)

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~~

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

~~Open~~ Periodic



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

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

Bloch Theorem

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

Edge => huge number of cells

Boundary Conditions at the ~~Open~~ Periodic edge
Reduces 2 unknowns

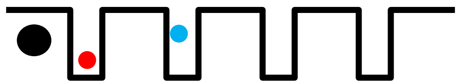
3) $$\psi\big|_{x=x_B^-}=\psi\big|_{x=x_B^+}$$
$$\frac{d\psi}{dx}\bigg|_{x=x_B^-}=\frac{d\psi}{dx}\bigg|_{x=x_B^+}$$ →
Boundary Condition at each interface:
Set 2N-2 equations for
2N-2 unknowns (for continuous U)

Interface => interfaces in periodic cell

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~~ System Analytical Solution



~~Open~~ **Periodic**

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

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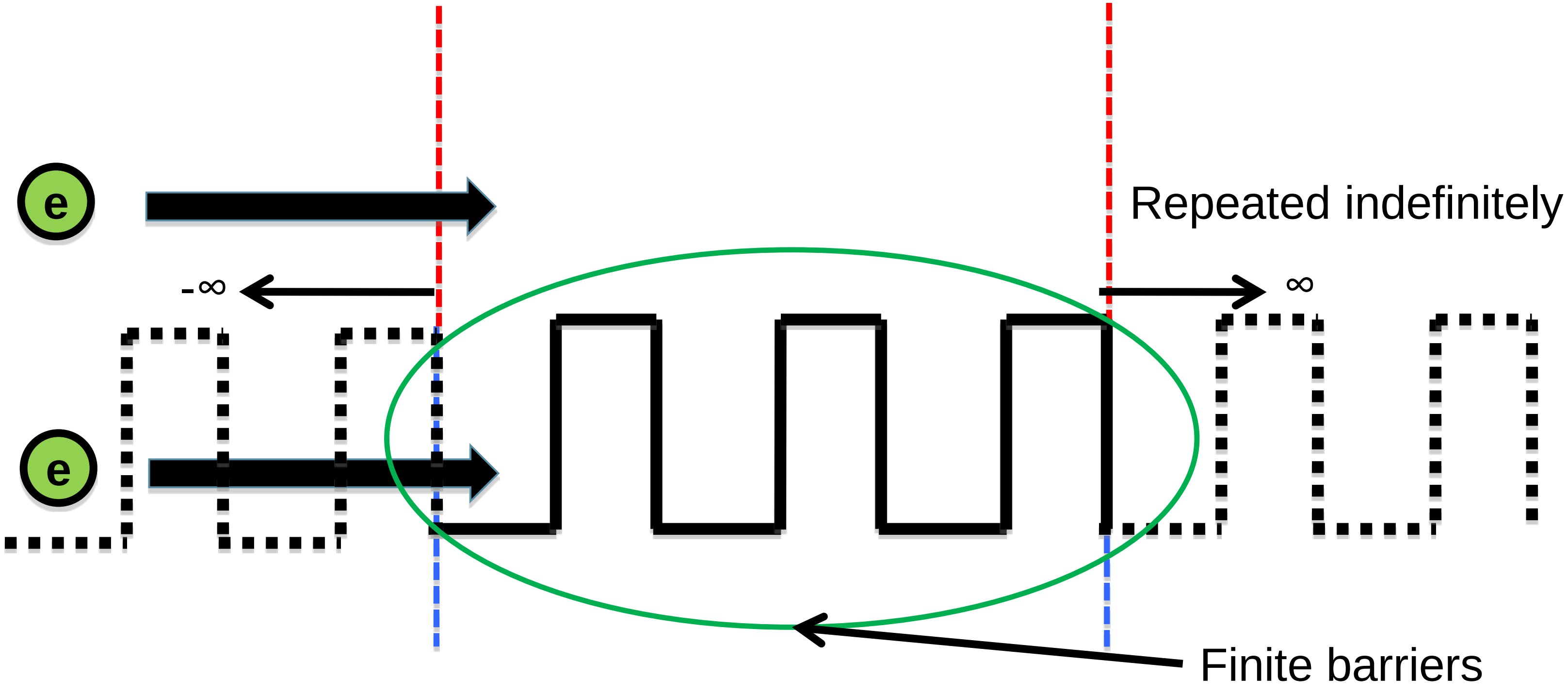
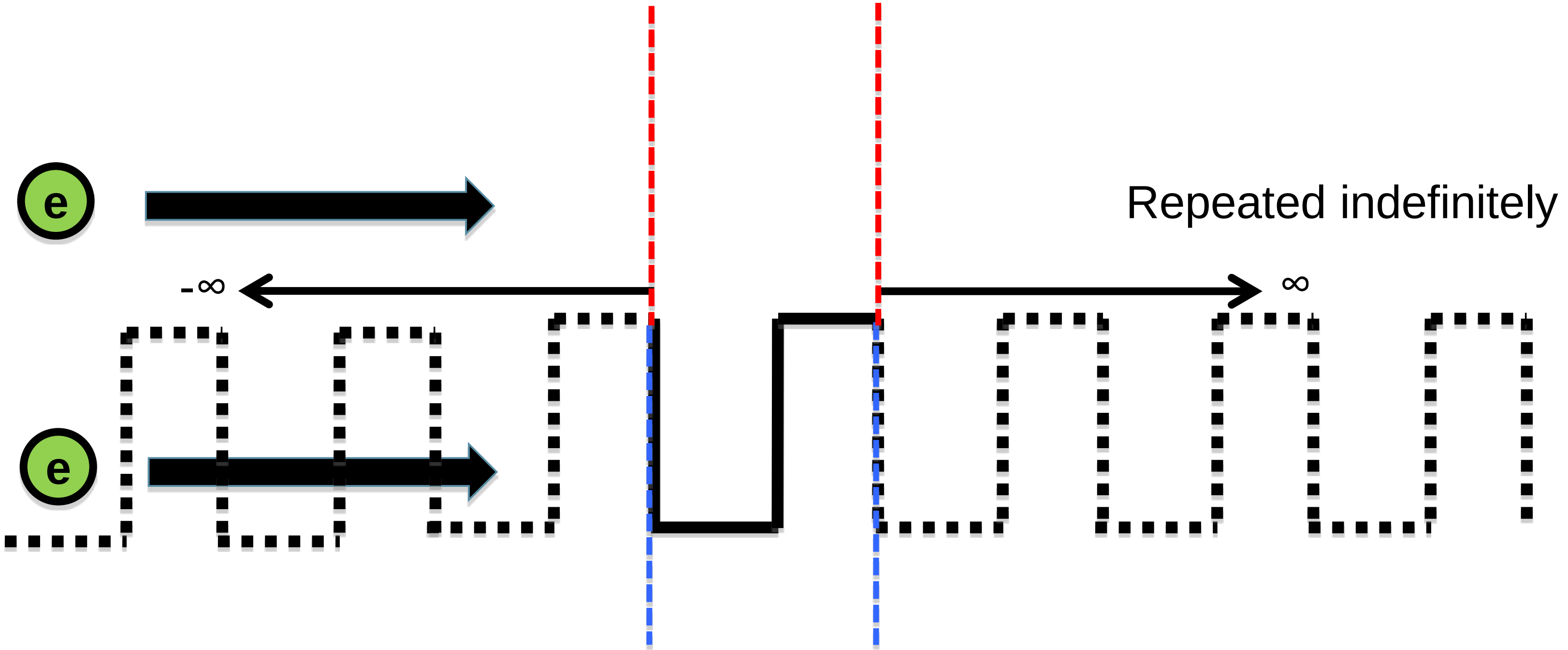
Periodic Potential Concept



As the number of barriers is increased the electrons see no difference between the actual structure and a structure that is simply modeled as being repeated indefinitely (Periodic).

Choosing the Smallest Unit Cell

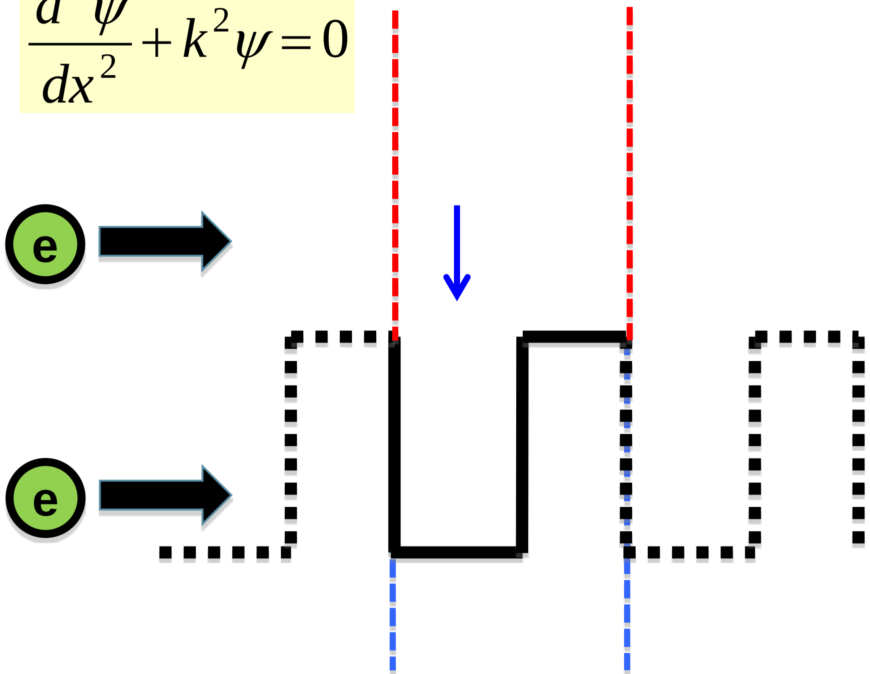


As the number of barriers is increased the electrons see no difference between the actual structure and a structure that is simply modeled as being repeated indefinitely (Periodic).

Choose the smallest cell to reduce computational work load

Solution Ansatz
Choose the Simplest Basis Set

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



Propagation above barriers

$$\psi_{n+1} = A_{n+1}\sin kx + B_{n+1}\cos kx$$

Decays in barriers

$$\psi_n = C_n e^{\alpha x} + D_n e^{-\alpha x}$$

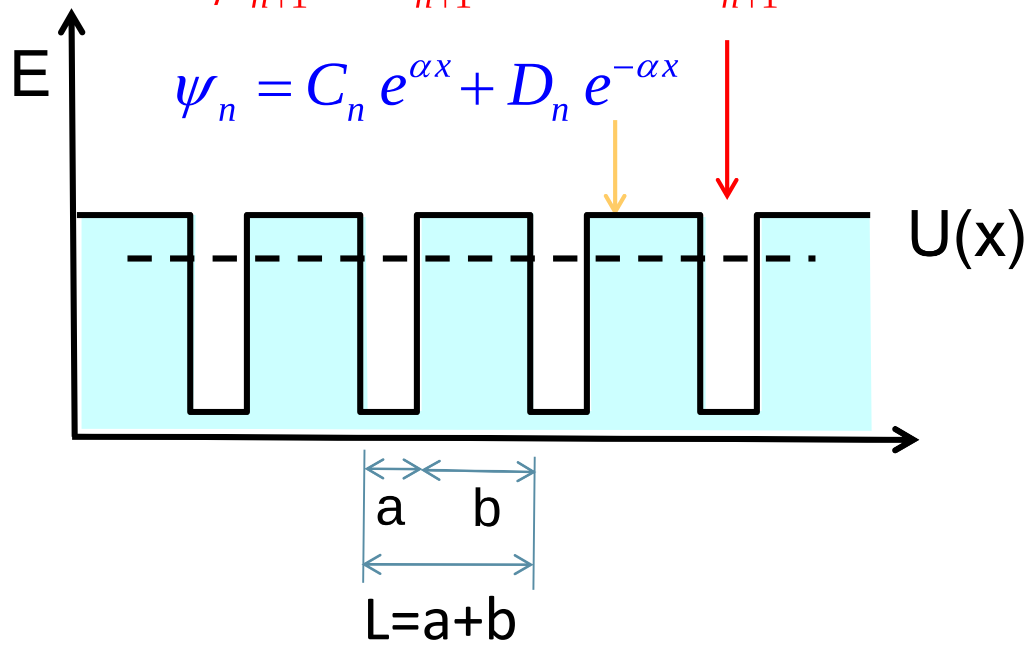
As the number of barriers is increased the electrons see no difference between the actual structure and a structure that is simply modeled as being repeated indefinitely (Periodic).

Choose the smallest cell to reduce computational work load

Finally an (almost) Real Problem …

$$\psi_{n+1} = A_{n+1} \sin kx + B_{n+1} \cos kx$$

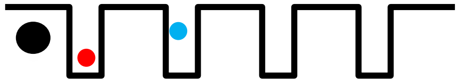
$$\psi_n = C_n e^{\alpha x} + D_n e^{-\alpha x}$$



But N atoms have two 2N unknown constants to find ….
For large N, isn't there a better way ?

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

Periodic



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

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

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

Edge => huge number of cells

Bloch Theorem

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

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

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

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

⟶ Boundary Condition at each interface:
Set 2N-2 equations for
2N-2 unknowns (for continuous U)

Interface => interfaces in periodic cell

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

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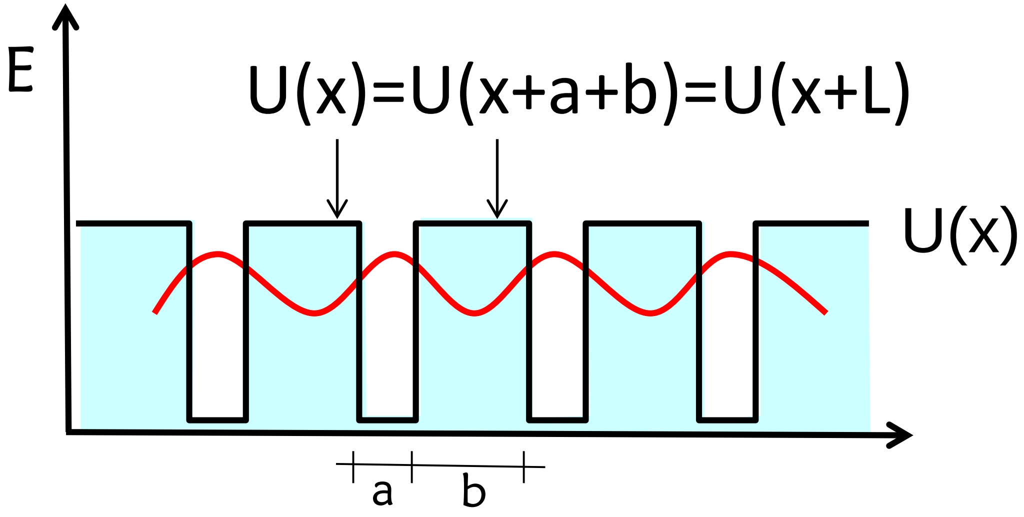
~~Normalization of unity probability
for wave function~~

 Periodic U(x) and Bloch's Theorem

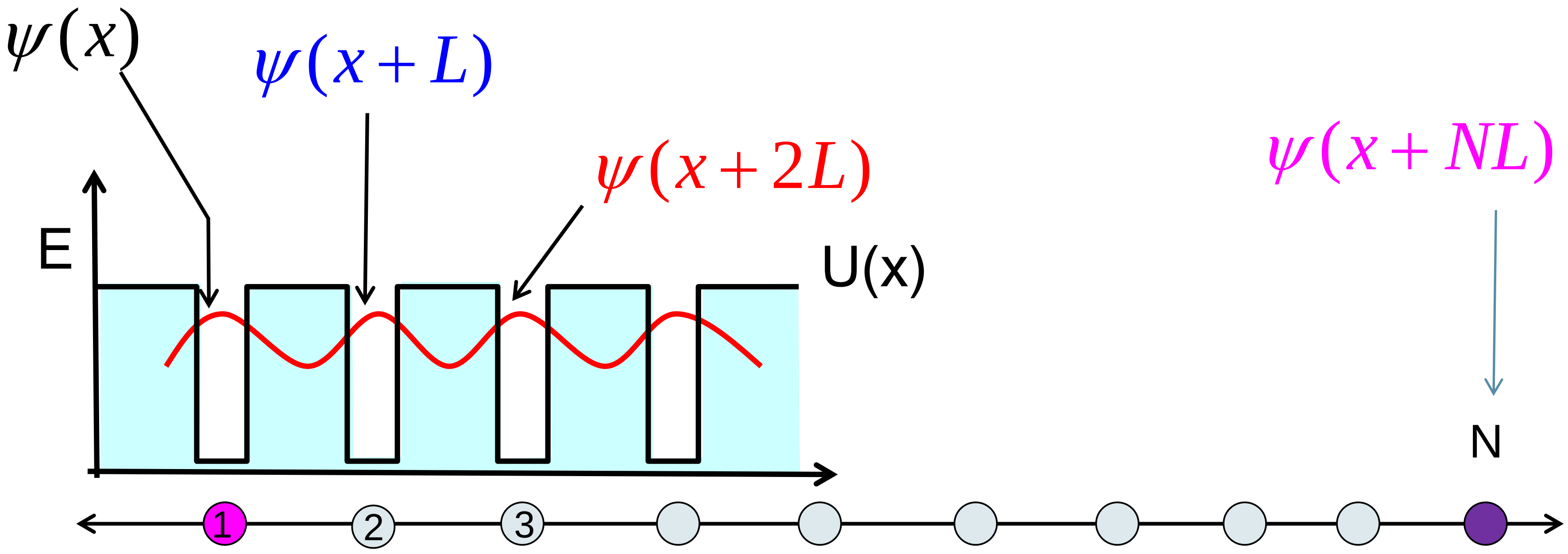


$$|\psi(x)|^2 = |\psi(x+p)|^2 \Longrightarrow \psi(x+p) = \psi(x)\,\mathrm{e}^{ikL}$$

p =some period length

not our old (k)

Phase-factor for N-cells

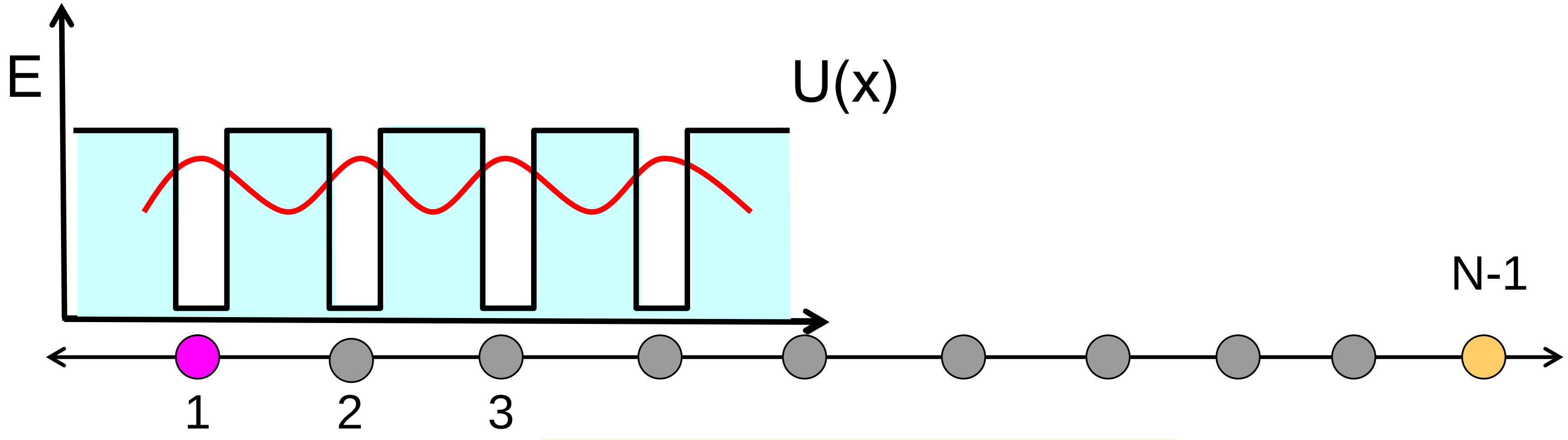


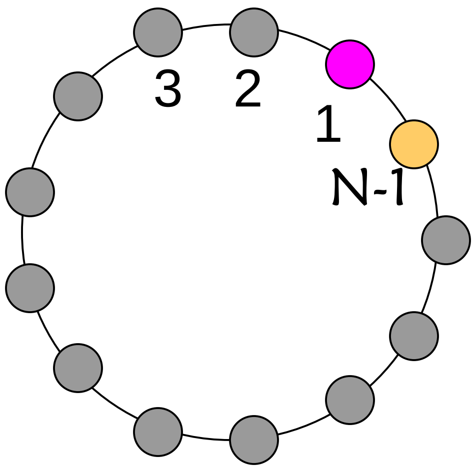
$$\psi[x+L] = \psi(x)e^{ikL}$$

$$\psi[x+2L] = \psi(x+L)e^{ikL}$$
$$= \psi(x)e^{ikL\times 2}$$

$$\psi[x+NL] = \psi(x)e^{ikLN}$$

Step 2: Periodic Boundary Condition





$$\psi[x+NL] = \psi(x)e^{ikLN}$$

$$e^{ikLN} = 1 \equiv e^{\pm i2\pi n}$$

$$k = \pm\frac{2\pi n}{NL} \quad n = -\frac{N}{2}.....-1,0,1,....\frac{N}{2}$$

$$k_{\max} = \frac{\pi}{L}, \quad k_{\min} = -\frac{\pi}{L}$$

Step 3: Boundary Conditions

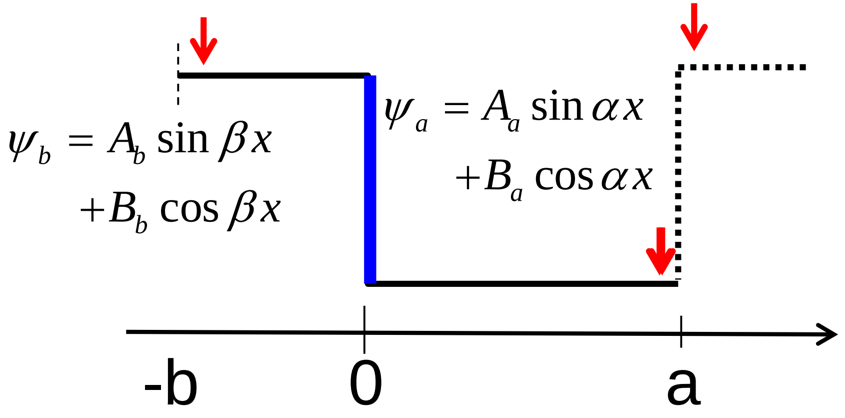
$$\psi\big|_{x=0^-} = \psi\big|_{x=0^+}$$

$$\left.\frac{d\psi}{dx}\right|_{x=0^-} = \left.\frac{d\psi}{dx}\right|_{x=0^+}$$

$$B_a = B_b$$

$$\alpha A_a = \beta A_b$$

$$\beta \equiv i\sqrt{2m(U_0 - E)/\hbar^2} \qquad \alpha \equiv \sqrt{2mE/\hbar^2}$$



$$\psi_a\big|_{x=a} = \psi_b\big|_{x=-b}\, e^{ikL}$$

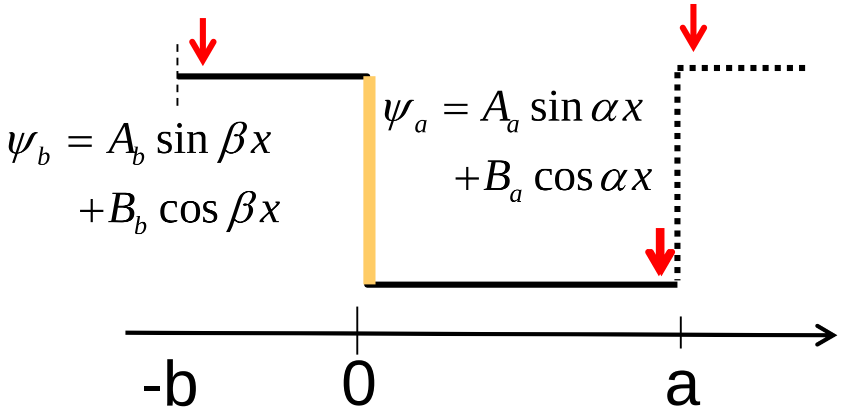
$$\left.\frac{d\psi_a}{dx}\right|_{x=a} = \left.\frac{d\psi_b}{dx}\right|_{x=-b} e^{ikL}$$

$$A_a \sin\alpha a + B_a \cos\alpha a = e^{ik(a+b)}[-A_b \sin\beta b + B_b \cos\beta b]$$

$$\alpha A_a \sin\alpha a - \alpha B_a \cos\alpha a = e^{ik(a+b)}[\beta A_b \sin\beta b + \beta B_b \cos\beta b]$$

Step 4: Det(matrix)=0 for Energy-levels

$$B_a = B_b$$
$$\alpha A_a = \beta A_b$$



$$A_a \sin \alpha a + B_a \cos \alpha a = e^{ik(a+b)}[-A_b \sin \beta b + B_b \cos \beta b]$$

$$\alpha A_a \sin \alpha a - \alpha B_a \cos \alpha a = e^{ik(a+b)}[\beta A_b \sin \beta b + \beta B_b \cos \beta b]$$

⇒

4) $$\begin{pmatrix} 0 & 1 & 0 & -1 \\ \alpha & 0 & \beta & 0 \\ * & * & & \\ * & & & \end{pmatrix} \begin{bmatrix} A_a \\ B_a \\ A_b \\ B_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

⇓

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}} \times \ldots\ldots\ldots\ldots = \cos kL \qquad \xi \equiv \frac{E}{U_0} \qquad \alpha_0 \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$

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

1) $$\frac{d^2\psi}{dx^2}+k^2\psi=0$$ → Solution Ansatz
2N unknowns
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Edge => huge number of cells

Bloch Theorem

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

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Boundary Condition at each interface:

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~~Normalization of unity probability~~
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Five Steps for Periodic System Analytical Solution

Bloch Theorem

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

Solution Ansatz
4 unknowns
for 1 periodic cell

$$\psi_a = A_a \sin\alpha x + B_a \cos\alpha x$$
$$\psi_b = A_b \sin\beta x + B_b \cos\beta x$$

2) $$\psi[x+NL] = \psi(x)e^{ikLN}$$ ←

Periodic Boundary Conditions
Imposes symmetry

3) $$\psi_a\big|_{x=a} = \psi_b\big|_{x=-b}\, e^{ikL}$$
$$\frac{d\psi_a}{dx}\bigg|_{x=a} = \frac{d\psi_b}{dx}\bigg|_{x=-b} e^{ikL}$$ ←

Boundary Condition in periodic cell:
Set 4 equations for 4 unknowns

4) Det (coefficient matrix)=0
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$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}}\times............ = \cos kL \qquad \xi\equiv\frac{E}{U_0} \qquad \alpha_0\equiv\sqrt{\frac{2mU_0}{\hbar^2}}$$

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One Video Segment

- 7.1 Bandstructure - Problem Formulation
  - » Kronig-Penney Model setup
  - » Bloch theorem
  - » Analytical solution process

status

$$\psi[x+NL] = \psi(x)e^{ikLN}$$

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}} \times \text{...........} = \cos kL \qquad \xi \equiv \frac{E}{U_0} \qquad \alpha_0 \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$

One Video Segment

- 7.2 Bandstructure - Solutions

One Video Segment

- 7.3 Band Properties

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One Video Segment

- 7.2 Bandstructure - Solutions
  - » Bandgaps
  - » Comparison to finite system model

status

One Video Segment

- 7.3 Band Properties

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