ECE606: Solid State Devices
Lecture 4

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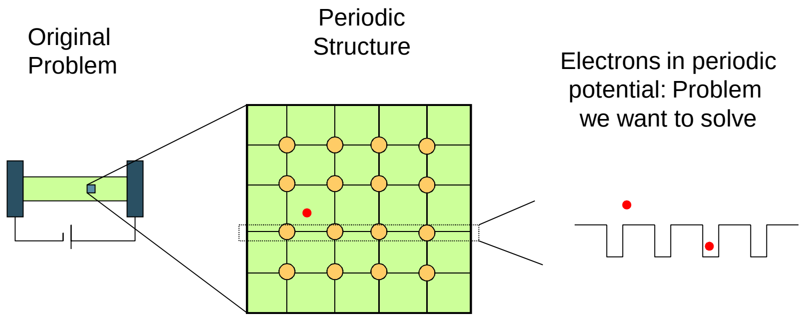
Presentation Outline

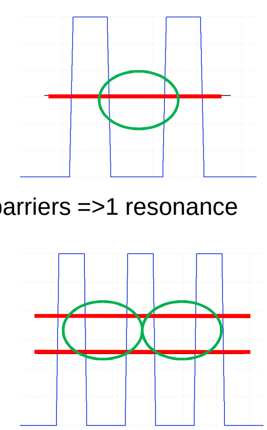
- Schrodinger equation in periodic U(x)
- Bloch theorem
- Band structure
- Properties of electronic bands
- E-k diagram and constant energy surfaces
- Conclusions

Reference: Vol. 6, Ch. 3

Getting Back to Crystals



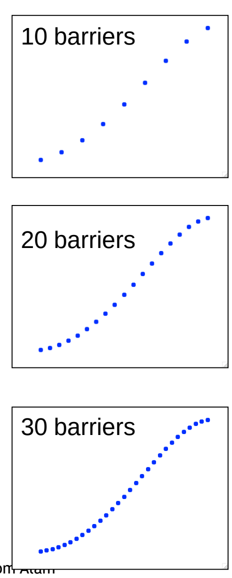
Reminder Transmission through Repeated wells



2 barriers =>1 resonance

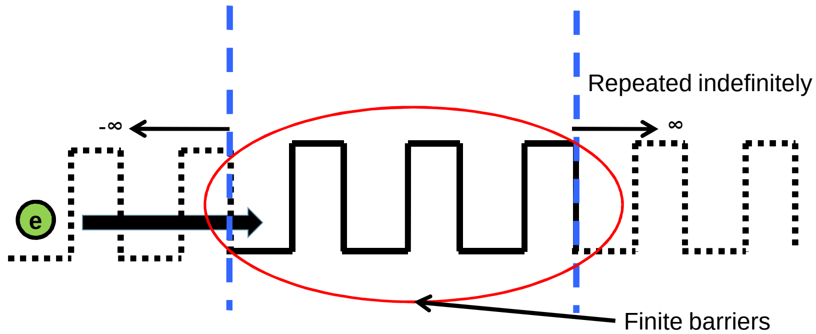
3 barriers =>2 resonance

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.

Comparison with Periodic structure

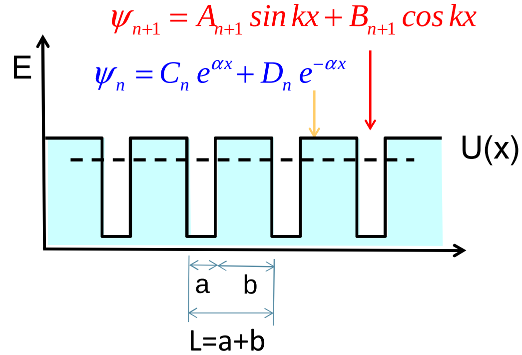


As the number of barriers is increased the electrons see no difference between the actual structure and a structure that is simply modeled as being repeated indefinitely (Periodic).

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 ?

Four Steps of Finding Energy Levels for Closed Systems

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

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

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

Imposed Boundary Conditions

4) Det(coefficient matix)=0

Set 2N-2 equations for 2N-2 unknowns

N is very large for crystal, but changing steps 2 and 3 a little bit we can still solve the problem in a few minutes

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- **Bloch theorem**
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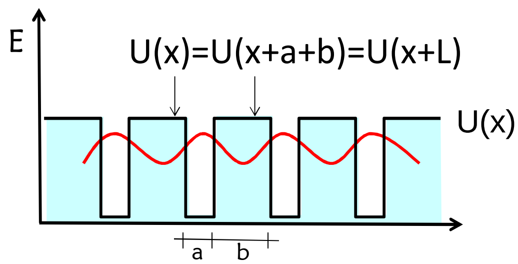
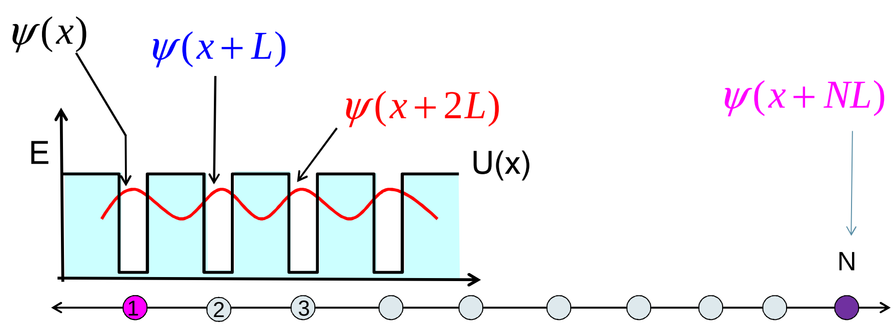
Periodic U(x) and Bloch's Theorem

not our old (k)

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



Phase-factor for N-cells



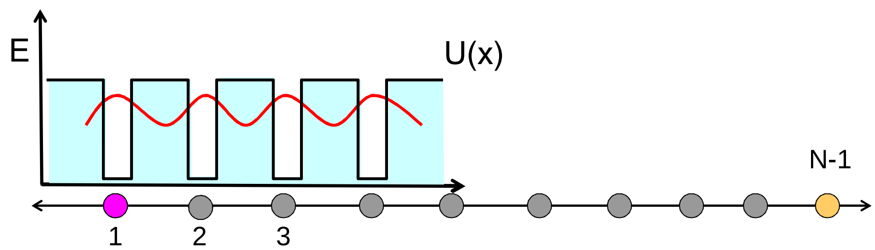
$$\psi[x+L] = \psi(x)e^{ikL}$$

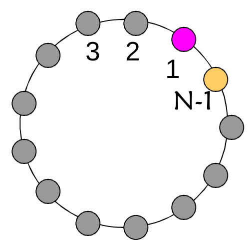
$$\psi[x+2L] = \psi(x+L)e^{ikL}$$

$$= \psi(x)e^{ikL\times 2}$$

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

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

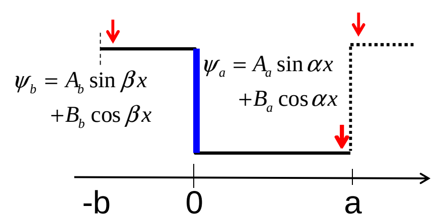
$$\psi\big|_{x=0^-} = \psi\big|_{x=0^+}$$

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

$$B_a = B_b$$

$$\alpha A_a = \beta A_b$$

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



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

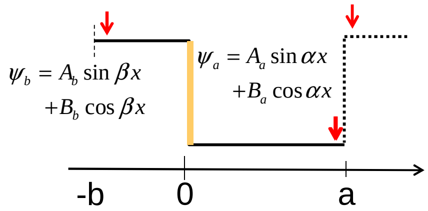
$$\left.\frac{d\psi_a}{dx}\right|_{x=a} = \left.\frac{d\psi_b}{dx}\right|_{x=-b} e^{ikL}$$

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

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

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

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



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

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

$\Rightarrow$ 4)

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

$\Downarrow$

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

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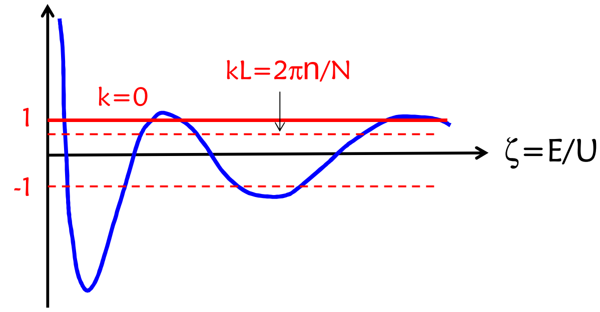
Graphical solution to Energy Levels

$$\frac{1-2\xi}{2\xi\sqrt{1-\xi}}\times\text{...........} = \cos kL$$

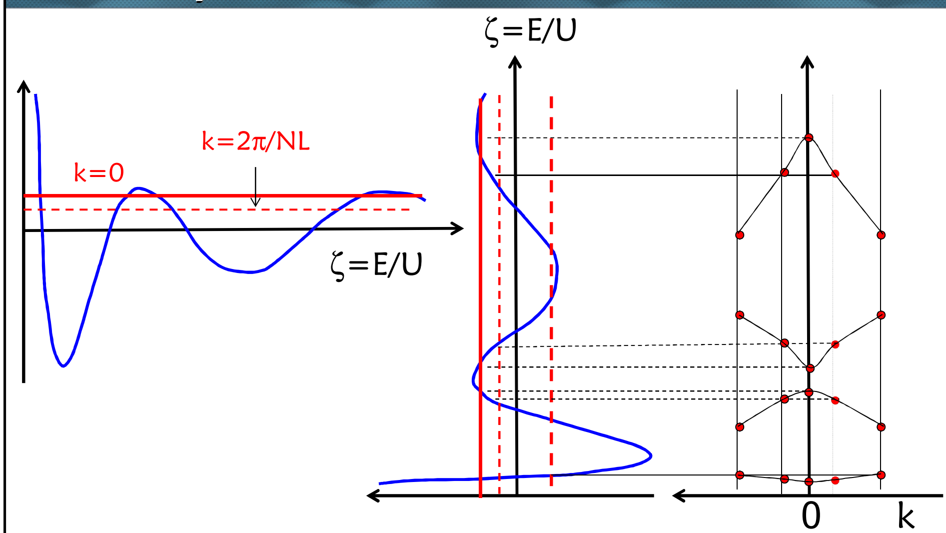
$$k = \pm\frac{2\pi n}{NL} \quad n = -\frac{N}{2}\text{.....}-1, 0, 1, \text{....}\frac{N}{2}$$

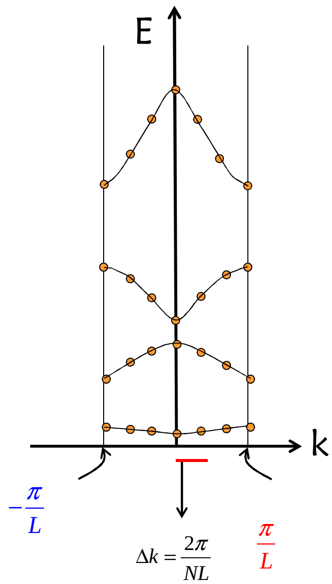


Right Hand side is a set of N flat lines between -1 and 1

Left Hand side is an ocillatory function with damping

Energy Band Diagram



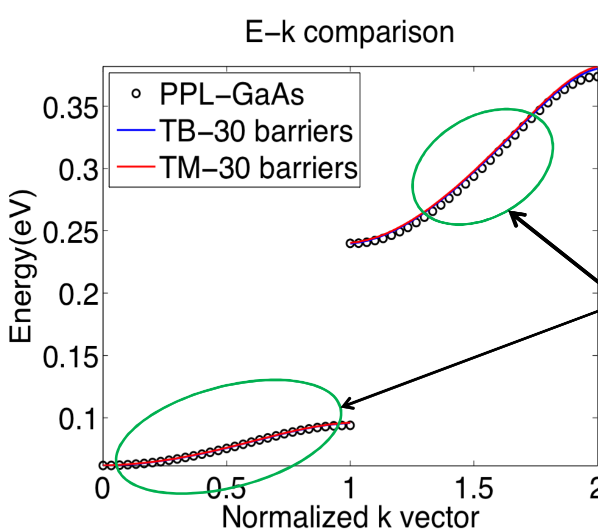


$$k = \pm\frac{2\pi n}{NL} \quad n = -\frac{N}{2} \ldots\ldots -1, 0, 1, \ldots\ldots \frac{N}{2}$$

$$\frac{States}{band} = \frac{k_{max} - k_{min}}{\Delta k} = \frac{2\pi/L}{2\pi/NL} = N$$

4 states per atom, N atoms
=> 4 bands, N states in each band

GaAs Well Comparison - 30 Barriers

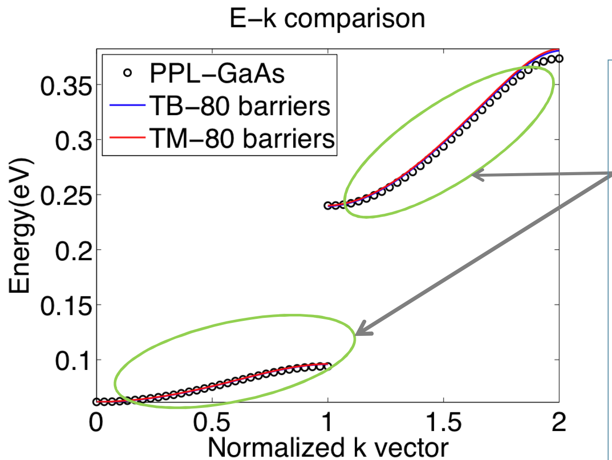


A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 30 barriers using tight-binding.
- TM: 30 barriers using transfer matrices.

It can be seen that the results of these three approaches agree well.

GaAs Well Comparison - 80 Barriers

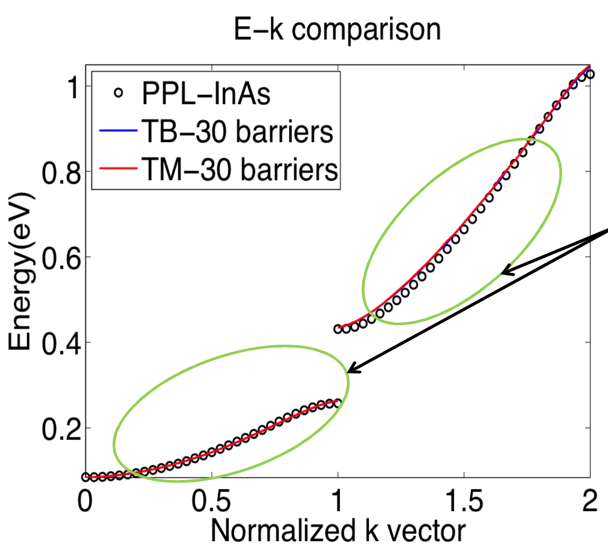


A GaAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 80 barriers using tight-binding.
- TM: 80 barriers using transfer matrices.

It can be seen that the results of these three approaches agree well.

InAs Well Comparison - 30 Barriers



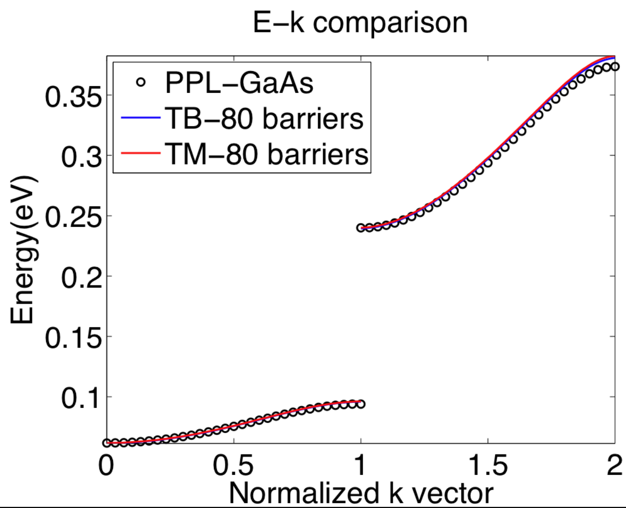
An InAs structure with 6nm wells, 2nm barriers and 0.4eV barrier height is modeled as follows,

- PPL-Periodic structure repeated indefinitely.
- TB: 30 barriers using tight-binding.
- TM: 30 barriers using transfer matrices.

It can be seen that the results of these three approaches agree well.

Key Summary

- Finite superlattice with large number of repeated cells approaches the periodic potential model



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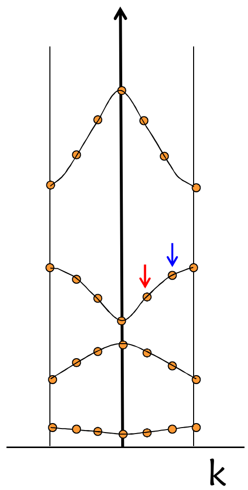
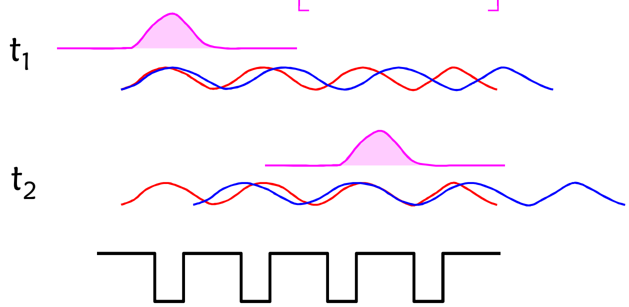
Wave Packet and Group Velocity



$$\psi(x,t) = Ae^{ikx - i\frac{E}{\hbar}t} + Ae^{i(k+\Delta k)x - i\left(\frac{E+\Delta E}{\hbar}\right)t}$$

$$= Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i(\Delta k)x - i\left(\frac{\Delta E}{\hbar}\right)t}\right]$$



Group Velocity for a Given Band

$$\psi(x,t) = Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i(\Delta k)x - i\left(\frac{\Delta E}{\hbar}\right)t}\right] = Ae^{ikx - i\frac{E}{\hbar}t}\left[1 + e^{i \times const.}\right]$$

$p = \hbar k$ momentum

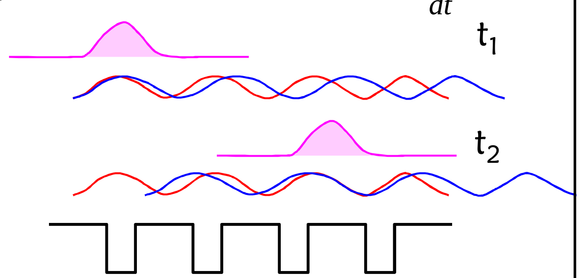
$F = ma = \dfrac{dp}{dt}$ force

$$\left[x\Delta k - t\frac{\Delta E}{\hbar}\right] = \text{constant.}$$

$$\frac{d}{dt}\left[x\Delta k - t\frac{\Delta E}{\hbar}\right] = \frac{d}{dt}(\text{constant})$$

$$\frac{dx}{dt}\Delta k - \frac{\Delta E}{\hbar} = 0 \rightarrow \frac{dx}{dt} = \frac{1}{\hbar}\frac{\Delta E}{\Delta k}$$

$$\upsilon = \frac{dx}{dt} = \frac{1}{\hbar}\frac{dE}{dk}$$

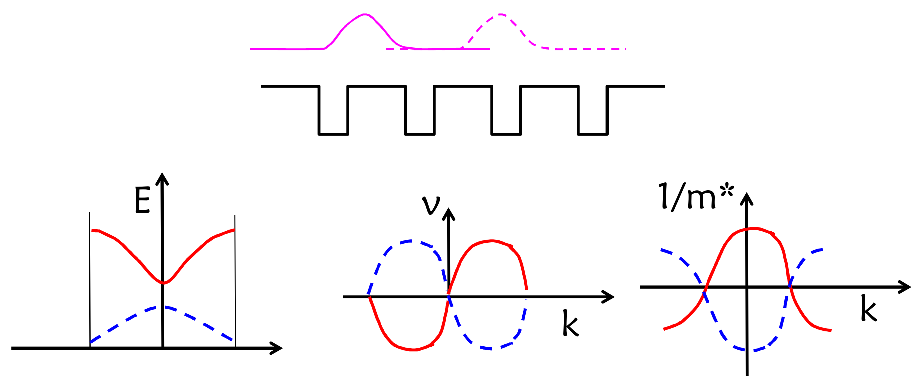


$$a = \frac{d\upsilon}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right] = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right][1] = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right]\left[\frac{1}{\hbar}\frac{d(\hbar k)}{dk}\right]$$

$$a = \frac{1}{\hbar^2}\frac{d^2E}{d^2k}\frac{d(\hbar k)}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{d^2k}\frac{dp}{dt} = \frac{1}{m^*}F$$

$$m^* = \left[\frac{1}{\hbar^2}\frac{d^2E}{d^2k}\right]^{-1}$$

Effective Mass for a Given Band

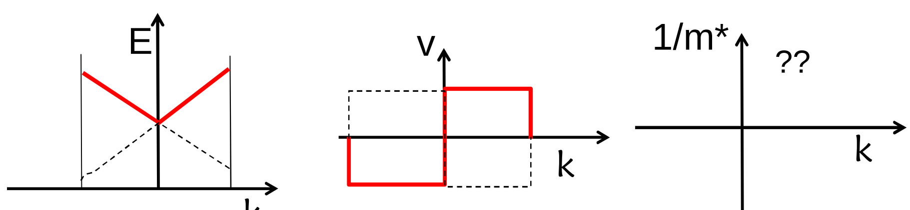


$$\upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k} \qquad \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

mass for each band

mass changes throughout the band

Effective Mass is not Essential ...



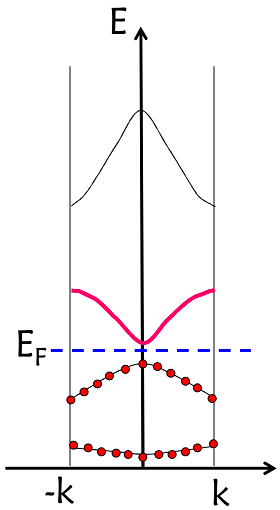
$$F = \hbar\frac{\Delta k}{\Delta t} \qquad \upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k} \qquad \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

$$k = k_0 + \int_0^t \frac{F}{\hbar}dt \qquad x = x_0 + \int_0^t \upsilon dt$$

Mass appears to be ill-defined

Integral description of the momentum and position change of wavepackets
Do not need effective mass
=> Effective mass is not a critical physical property!
=> Graphene is a material with such linear dispersion!

Electron and Hole fluxes: Filled/Empty Bands



Need
- inversion symmetry
  (number of states in +/-k identical)
- Pauli exclusion principle

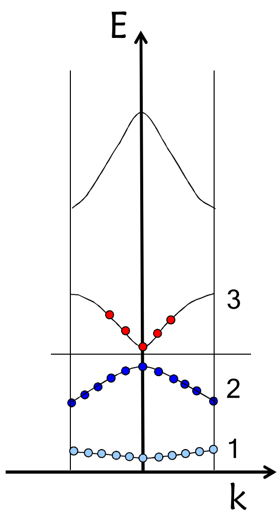
$$J_3 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i = 0$$

Empty bands carry no current

Full bands carry no current

$$J_2 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i = -\frac{q}{L}\sum_{0}^{k_{max}} \upsilon_i - \frac{q}{L}\sum_{-k_{min}}^{0} -|\upsilon_i| = 0$$

Partially filled bands



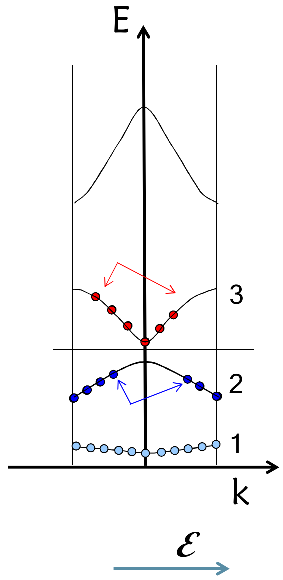
Partial filling can be achieved by:
- Optical excitation
- Thermal excitation
- Doping + a little thermal excitation

Empty bands carry no current

Full bands carry no current

Let's imagine there is a way to get some electrons from the valence band into the conduction band!

Electron and Hole Fluxes: Partially Filled Bands



$$J_3 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i \neq 0$$

$$J_2 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i = -\frac{q}{L}\sum_{all} \upsilon_i + \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

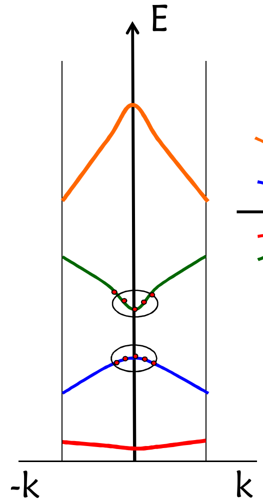
$$= \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

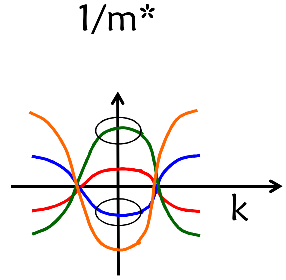
-ve charge moving with –ve mass

+ve charge moving with +ve mass

Shockley example – top view of parking lot

Interpretation of the effective mass ?





$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

- m* not free mass
- m* function of k
- negative and positive (in the same band!)

But for Transport:

- Some bands are more important than others
- Some are always full
- Some are always empty

Minimizing energy:

- Electrons “fall” to the bottom
- Holes “float” to the top

“Constant” Masses at:

- Bottom conduction band
- Top valence band

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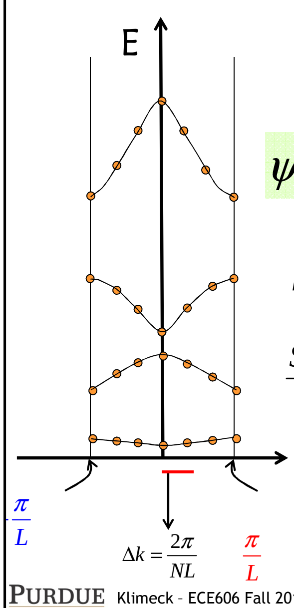
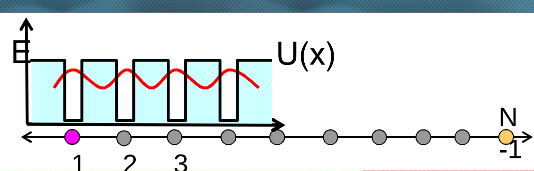
Brillouin Zone and Number of States





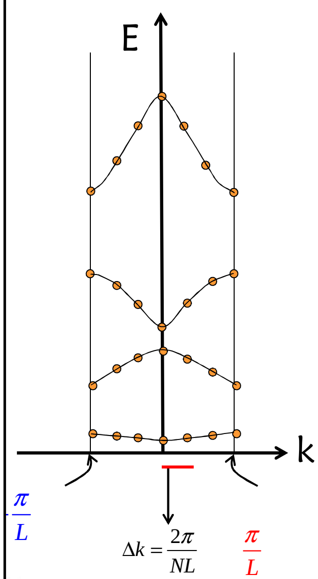
$$\psi[x+NL] = \psi(x)e^{ikLN} = \psi(x)e^{ikLN}e^{i2\pi m}$$
$$= \psi(x)e^{ikLN}e^{imkL}$$

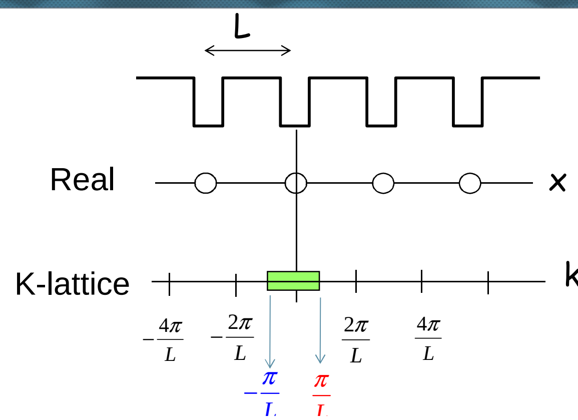
$$k = \pm\frac{2\pi n}{NL} \qquad n = -\frac{N}{2}.....-1, 0, 1, ...\frac{N}{2}$$

$$\frac{States}{band} = \frac{k_{max} - k_{min}}{\Delta k} = \frac{2\pi / L}{2\pi / NL} = N$$

4 states per atom, N atoms
=> 4 bands, N states in each band
All states are included in the first zone
Invariant to shift by $1 = e^{im2\pi} = e^{imkL}$

Solution Space: Brillouin Zone





4 states per atom, N atoms
=> 4 bands, N states in each band
All states are included in the first zone
Invariant to shift by $1 = e^{im2\pi} = e^{imkL}$
Collapse of an infinite space into a discrete space

Fourier Transform Reminders

$f(x)$	$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-i\omega x}\,dx$	**Space Mapping**
$e^{-a\|x\|}$ $e^{-\alpha x^2}$	$\sqrt{\frac{2}{\pi}}\cdot\frac{a}{a^2+\omega^2}$ $\frac{1}{\sqrt{2\alpha}}\cdot e^{-\frac{\omega^2}{4\alpha}}$	**infinite <=> infinite**
$\mathrm{rect}(ax)$ $\mathrm{tri}(ax)$	$\frac{1}{\sqrt{2\pi a^2}}\cdot\mathrm{sinc}\left(\frac{\omega}{2\pi a}\right)$ $\frac{1}{\sqrt{2\pi a^2}}\cdot\mathrm{sinc}^2\left(\frac{\omega}{2\pi a}\right)$	**finite <=> infinite**
1 e^{iax} $\cos(ax)$	$\sqrt{2\pi}\cdot\delta(\omega)$ $\sqrt{2\pi}\cdot\delta(\omega-a)$ $\sqrt{2\pi}\cdot\frac{\delta(\omega-a)+\delta(\omega+a)}{2}$	**Periodic => discrete**

Reciprocal Space

A 1D **periodic** function: $f(x) = f(x+l); \quad l = nL$

can be expanded in a Fourier series:

$$f(x) = \sum_n A_n e^{i2\pi nx/L} = \sum_g A_g e^{igx} \qquad g = \frac{2\pi n}{L}$$

The Fourier components are defined on a discrete set of periodically arranged points (analogy: frequencies) in a reciprocal space to coordinate space.

3D Generalization:

$$u_n(\mathbf{k},\mathrm{r}) = \sum_{\mathrm{G}} f_{\mathrm{G}}^n(\mathbf{k}) e^{i\mathbf{G}\cdot\mathbf{r}}; \quad \mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

$\mathbf{G} \perp \mathrm{a}$ Where *hkl* are integers. **G**=Reciprocal lattice vector

Brillouin Zone - Allowed States in a Reciprocal Lattice

$$f(\vec{r}) = \frac{1}{\sqrt{2\pi}} \int d^3\vec{k} f(\vec{k}) \exp\left(i\vec{k}\vec{r}\right)$$

Fourier transform: Represented real-space with plane waves

$$f(\vec{r}+\vec{R}) = f(\vec{r})$$

Impose periodicity in **R**

$$f(\vec{r}+\vec{R}) = \frac{1}{\sqrt{2\pi}} \int d^3\vec{k} f(\vec{k}) \exp\left(i\vec{k}\left(\vec{r}+\vec{R}\right)\right)$$

$$\exp\left(i\vec{k}\vec{R}\right) = 1 \qquad \vec{k}\vec{R} = 2\pi n$$

$$\vec{k} = \vec{G} = h\vec{k}_x + k\vec{k}_x + l\vec{k}_z$$

Reciprocal vector **G**

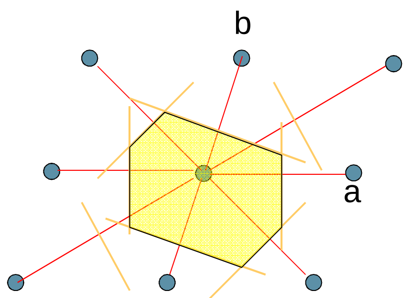
1) Define reciprocal lattice with the following vectors ….

$$k_x = 2\pi \frac{b \times c}{|a \bullet b \times c|} \quad k_y = 2\pi \frac{c \times a}{|a \bullet b \times c|} \quad k_z = 2\pi \frac{a \times b}{|a \bullet b \times c|}$$

2) Use Wigner Seitz algorithm to find the unit cell in the wave-vector (reciprocal) space.

Wigner-Seitz Method for Reciprocal Space

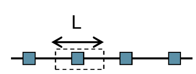
Primitive cell in real space



$$k_x = 2\pi \frac{b \times \hat{z}}{|a \bullet b \times \hat{z}|} \quad k_y = 2\pi \frac{\hat{z} \times a}{|a \bullet b \times \hat{z}|}$$

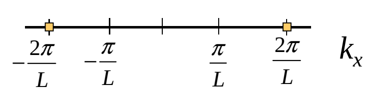
Brillouin Zone for One-dimensional Solids

Real-space

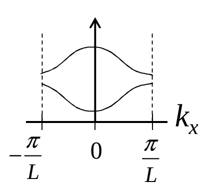


Replacing (a+b) by L …

1st B-Z



E-k diagram

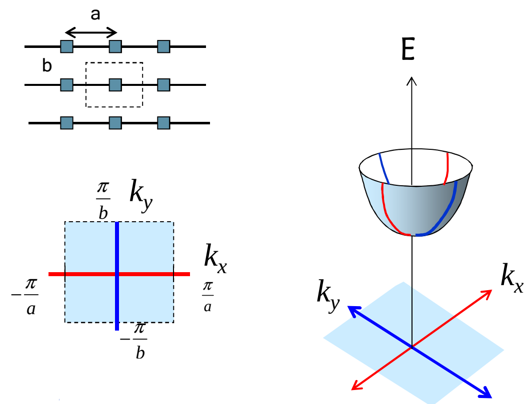


E-k diagram in 2D solids

Real-space

1st B-Z

E-k diagram

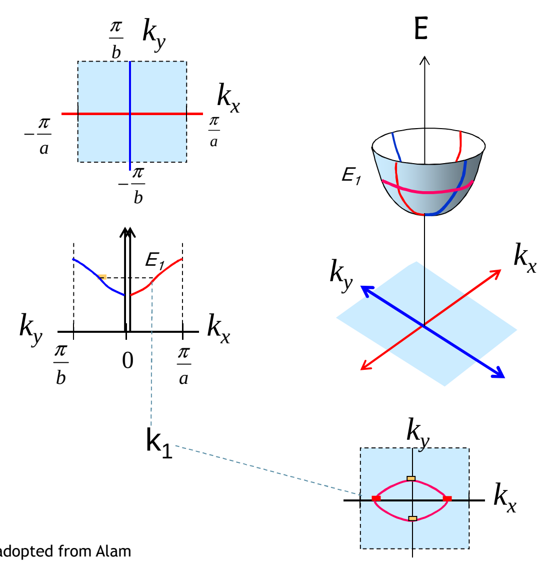


Constant Energy-surface in 2D

1st B-Z

E-k diagram

Const. Energy Surface



Conclusions

- Solution of Schrodinger equation is relatively easy for systems with well-defined periodicity.
- Electrons can only sit in-specific energy bands. Effective masses and band gaps summarize information about possible electronic states.
- Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.
- Kronig-Penney model is analytically solvable. Real band-structures are solved on computer. Such solutions are relatively easy – we will do HW problems on nanohub.org on this topic.
- Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.
- Of all the possible bands, only a few contribute to conduction. These are often called conduction and valence bands.
- For 2D/3D systems, energy-bands are often difficult to visualize. E-k diagrams along specific direction and constant energy surfaces for specific bands summarize such information.
- Most of the practical problems can only be analyzed by numerical solution.