Section 7
Bandstructure in 1D Periodic Potentials
7.3 Band Properties

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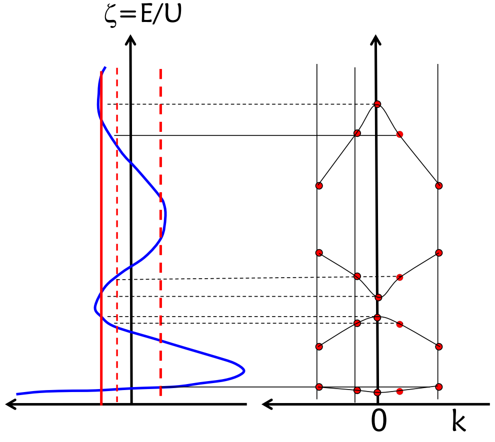
Section 7
Bandstructure - in 1D Periodic Potentials

One Video Segment

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

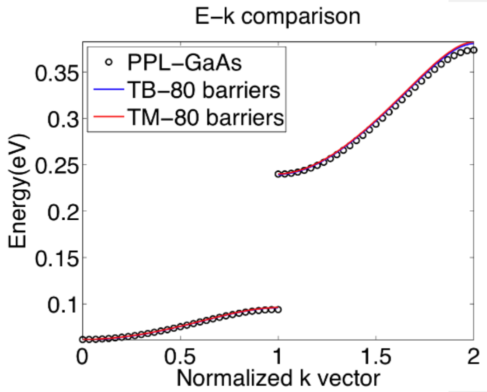
$$\psi[x+NL] = \psi(x)e^{ikLN}$$

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



One Video Segment

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



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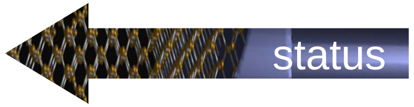
- 7.3 Band Properties

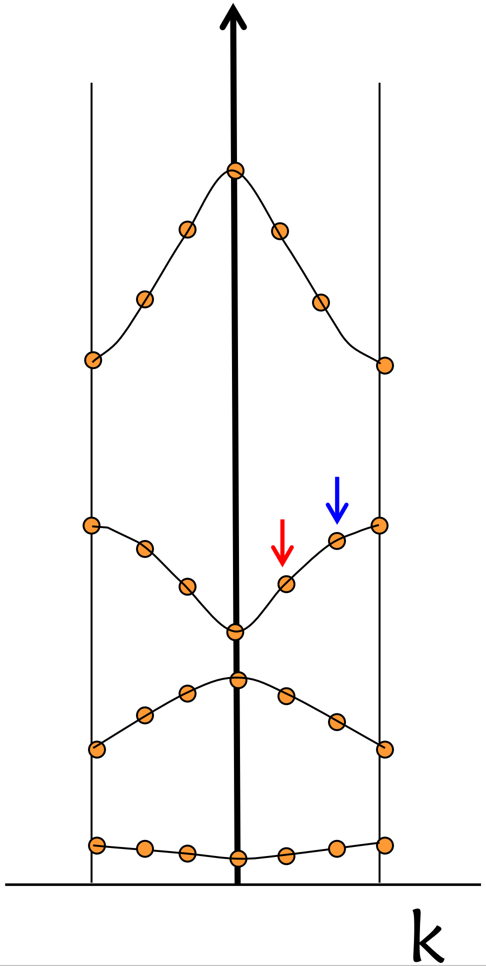


  - » Wave packets
  - » Effective mass
  - » Electrons and Holes

Reference: Vol. 6, Ch. 3

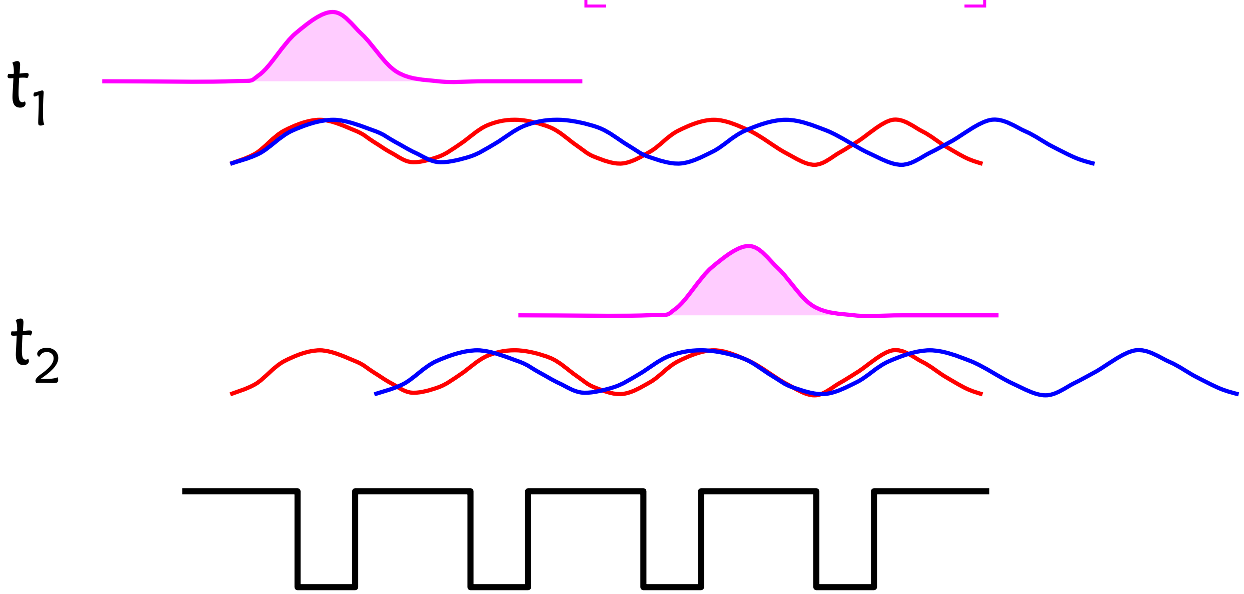
Daniel Mejia, Gerhard Klimeck (2019), "Periodic Potential Lab - Kronig Penney Model, " https://nanohub.org/resources/kronigpenneylab. (DOI: 10.21981/TT2Y-A185).

Wave Packet and Group Velocity



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

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



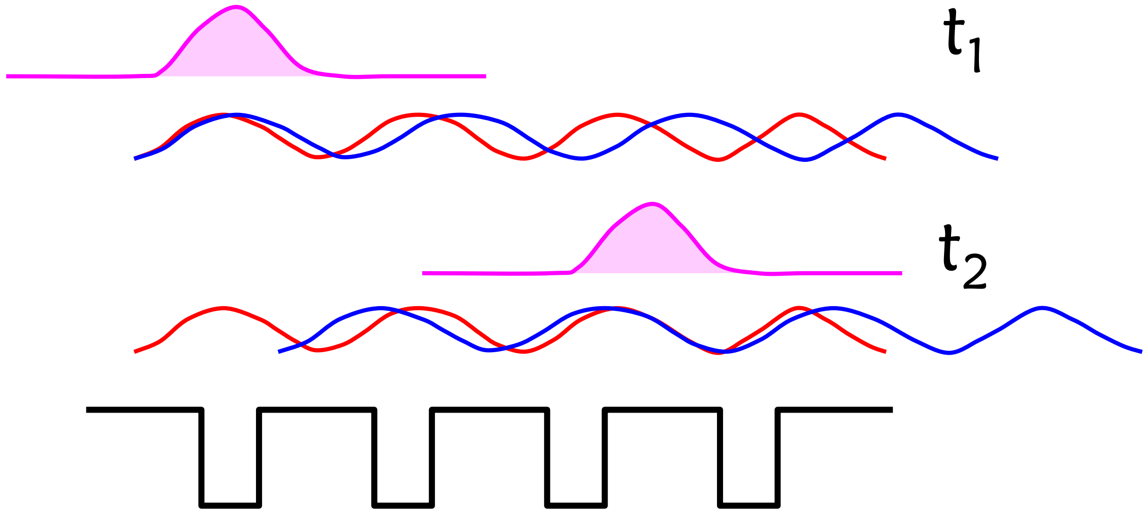
Group Velocity for a Given Band

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

$p = \hbar k$ momentum

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

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



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

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

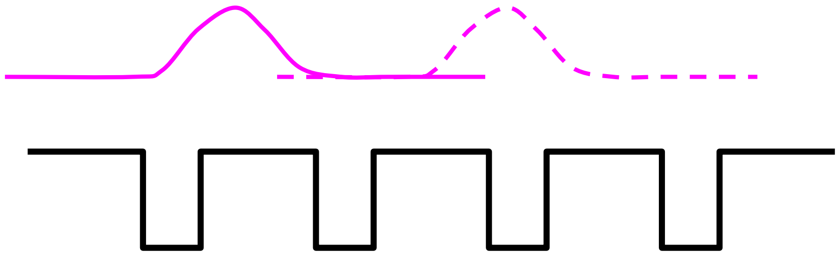
$$\upsilon = \frac{dx}{dt} = \frac{1}{\hbar}\frac{dE}{dk}$$

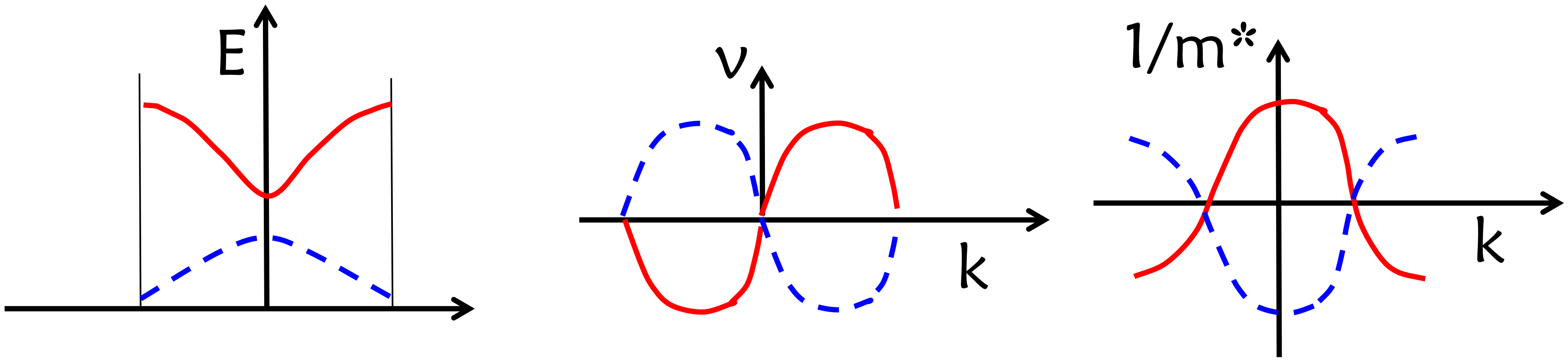
$$a = \frac{d\upsilon}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right] = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right][1] = \frac{1}{\hbar}\frac{d}{dt}\left[\frac{dE}{dk}\right]\left[\frac{1}{\hbar}\frac{d(\hbar k)}{dk}\right]$$

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

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

Effective Mass for a Given Band





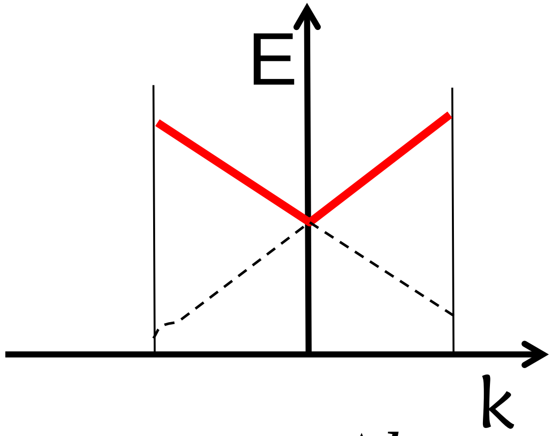
$$\upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k}$$

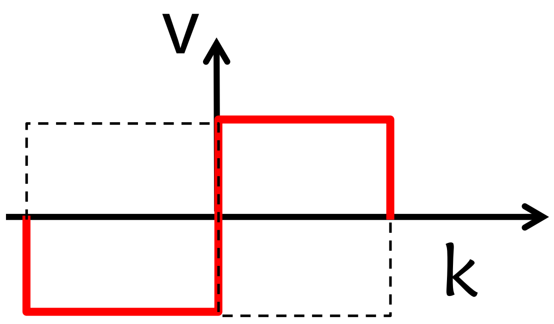
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

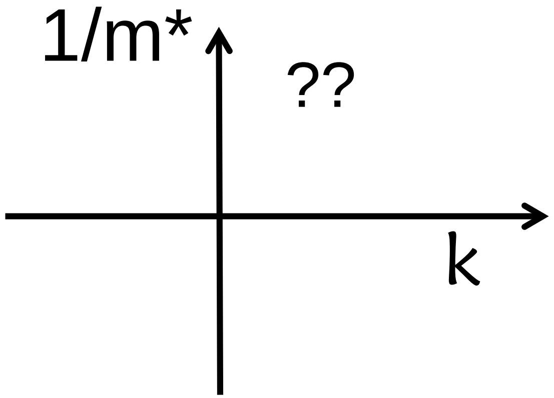
mass for each band

mass changes throughout the band

Effective Mass is not Essential …







$$F = \hbar \frac{\Delta k}{\Delta t}$$

$$\upsilon = \frac{1}{\hbar}\frac{\Delta E}{\Delta k}$$

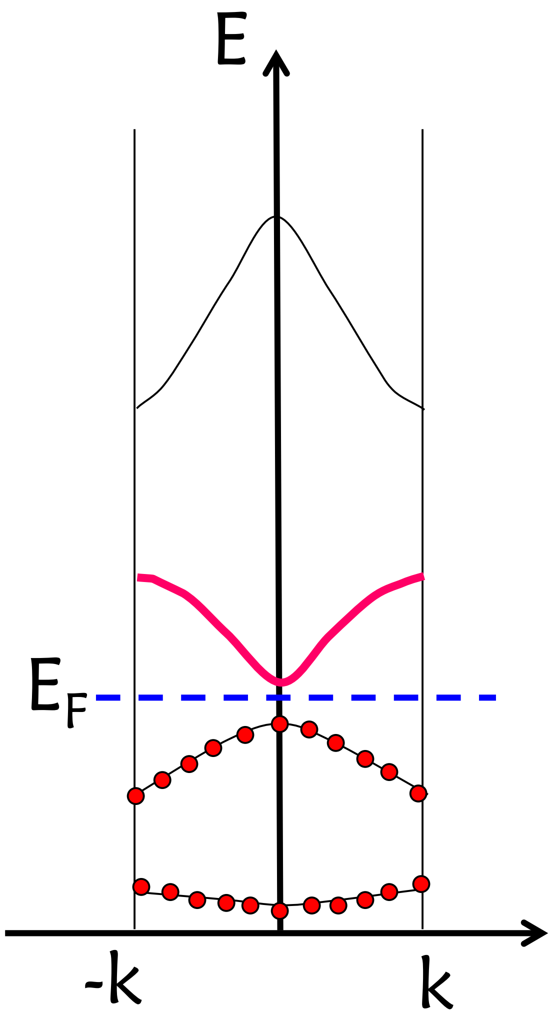
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

$$k = k_0 + \int_0^t \frac{F}{\hbar} dt$$

$$x = x_0 + \int_0^t \upsilon dt$$

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!



Need

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

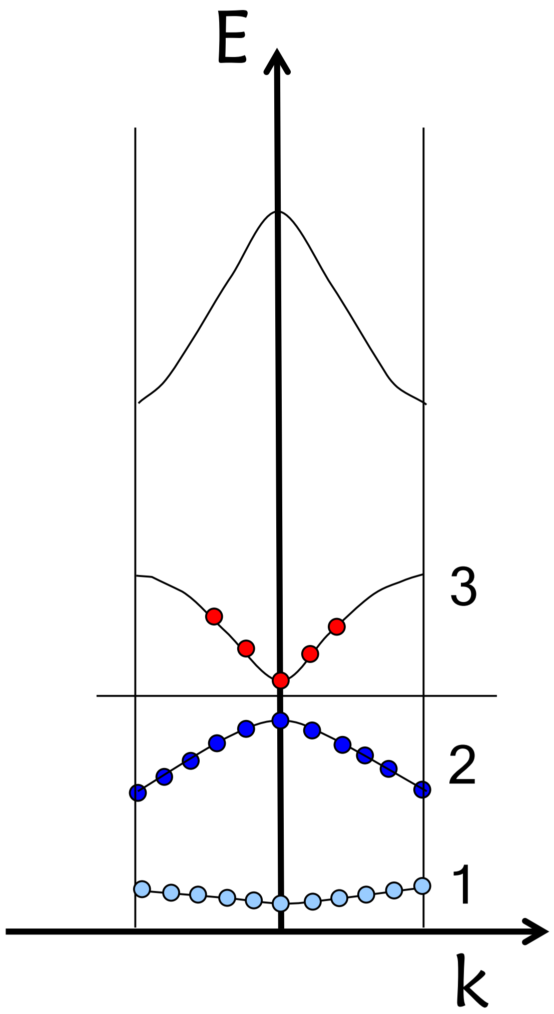
$$J_3 = -\frac{q}{L} \sum_{i(filled)} \upsilon_i = 0$$

Empty bands carry no current

Full bands carry no current

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

Partially filled bands



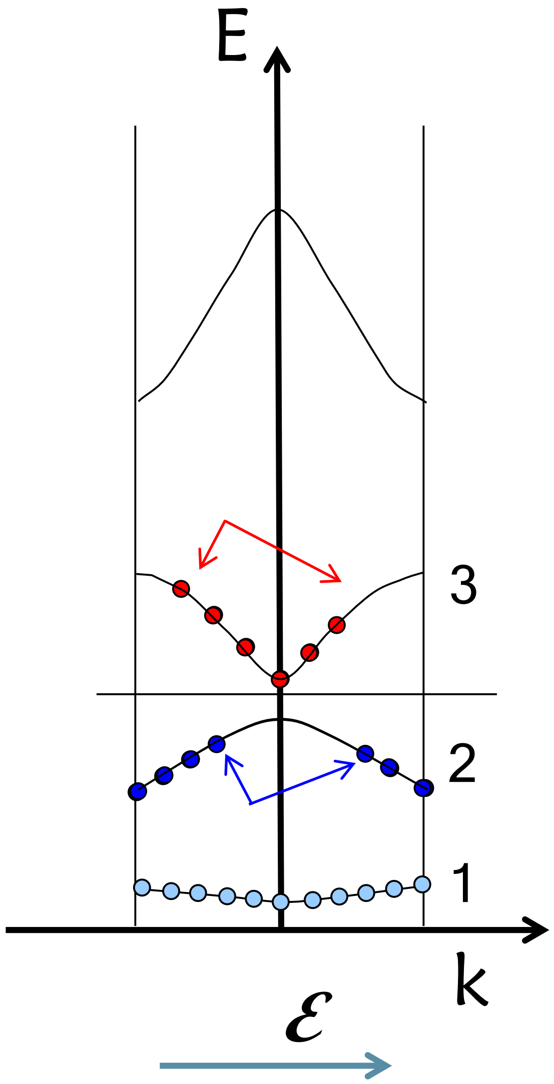
Partial filling can be achieved by:
- Optical excitation
- Thermal excitation
- Doping + a little thermal excitation

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



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

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

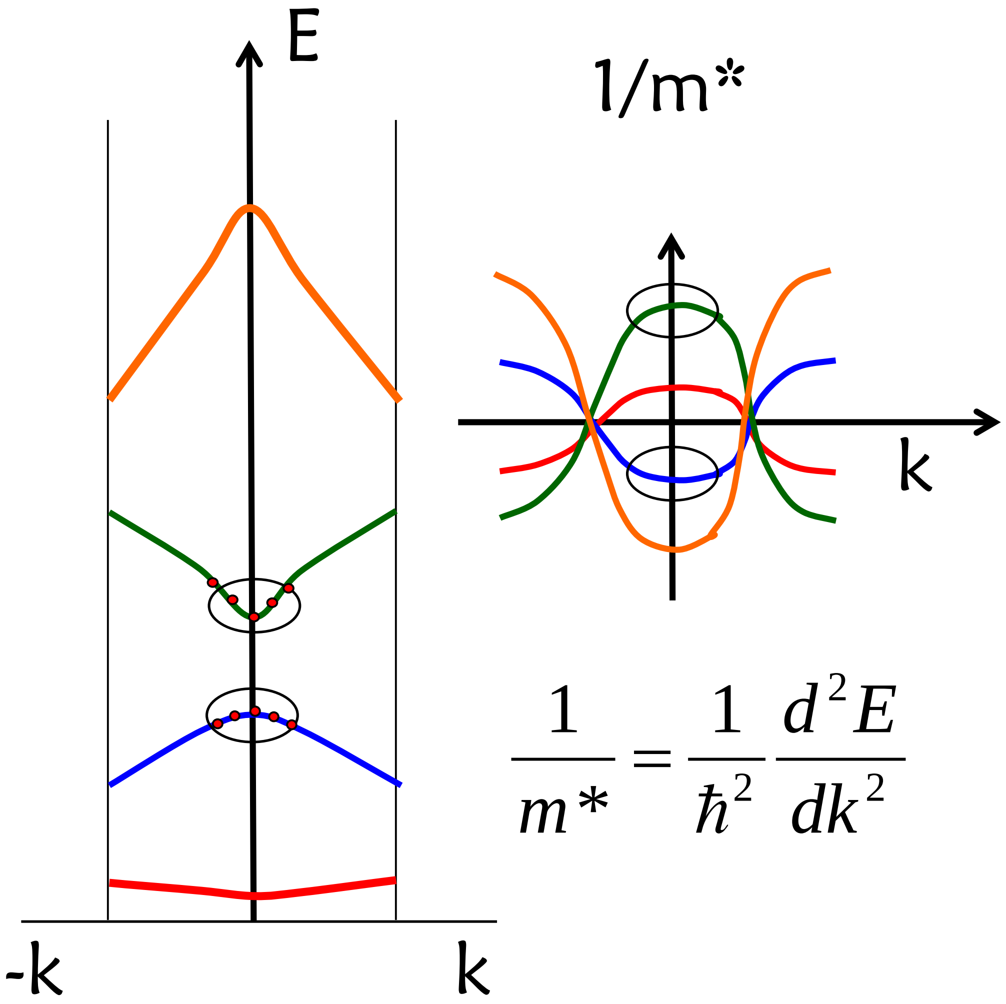
$$= \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

$-v_e$ charge moving with $-v_e$ mass

$+v_e$ charge moving with $+v_e$ 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

Conclusions

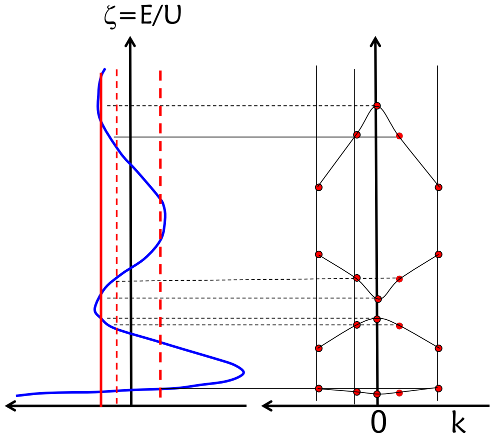
- Solution of Schrodinger equation is relatively easy for systems with well-defined periodicity.
- Kronig-Penney model is analytically solvable. Real band-structures are solved numerically. Such solutions are relatively easy – we will do HW problems on nanohub.org on this topic.

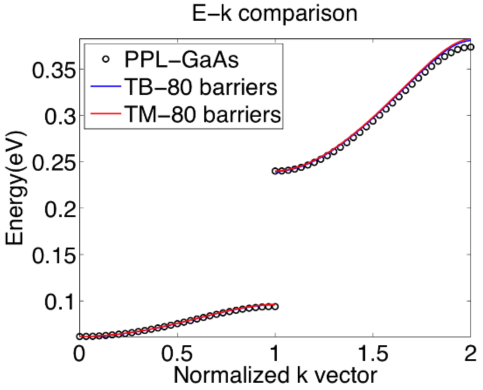
- Electrons can only sit in-specific energy bands.
- Effective masses and band gaps summarize information about possible electronic states.
- Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.

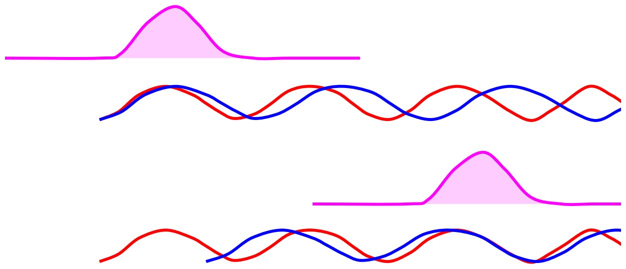
- Of all the possible bands, only a few contribute to conduction. These are often called conduction and valence bands.

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

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







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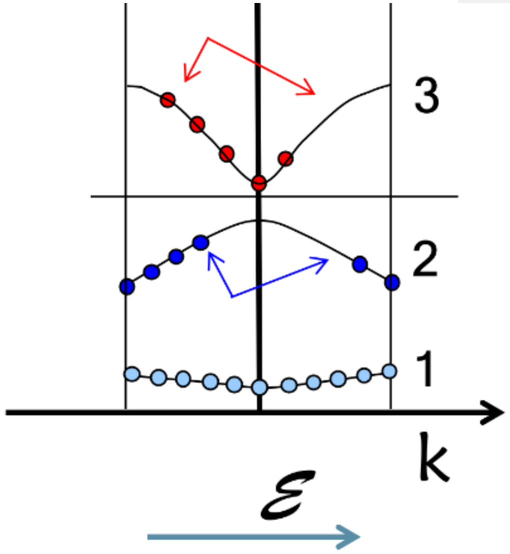

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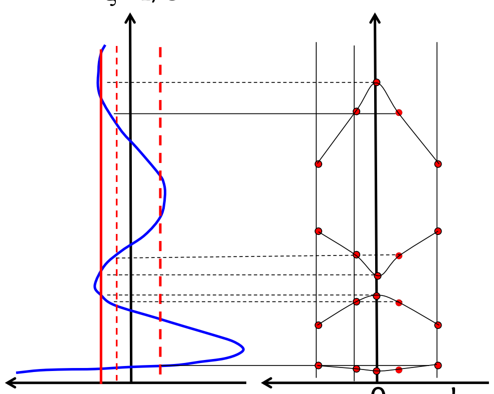

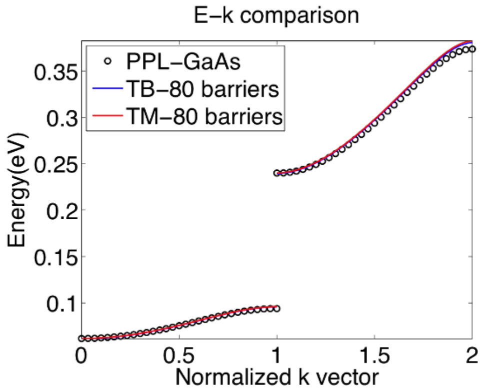

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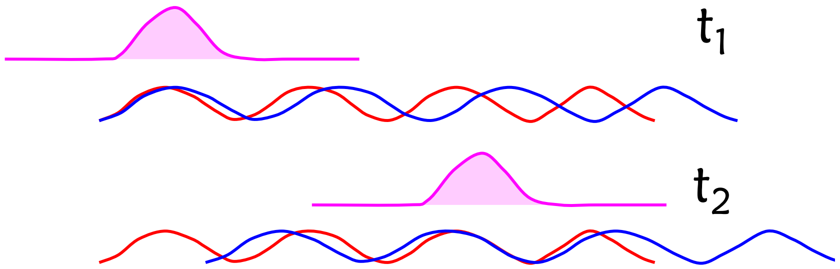

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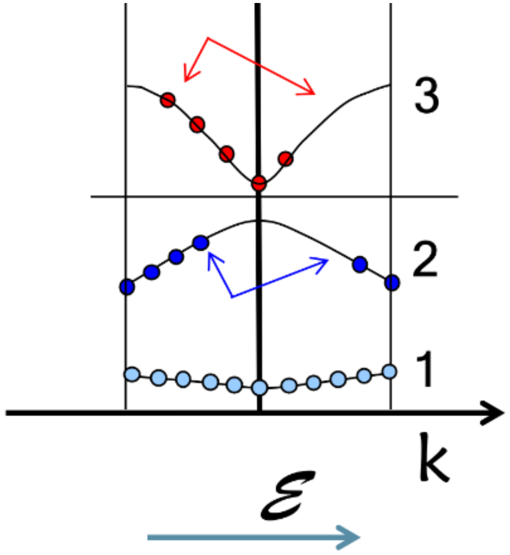

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