PURDUE UNIVERSITY

NCN

www.nanohub.org

EE-606: Solid State Devices
Lecture 6: Energy Bands (continued)

Muhammad Ashraful Alam
alam@purdue.edu

Outline

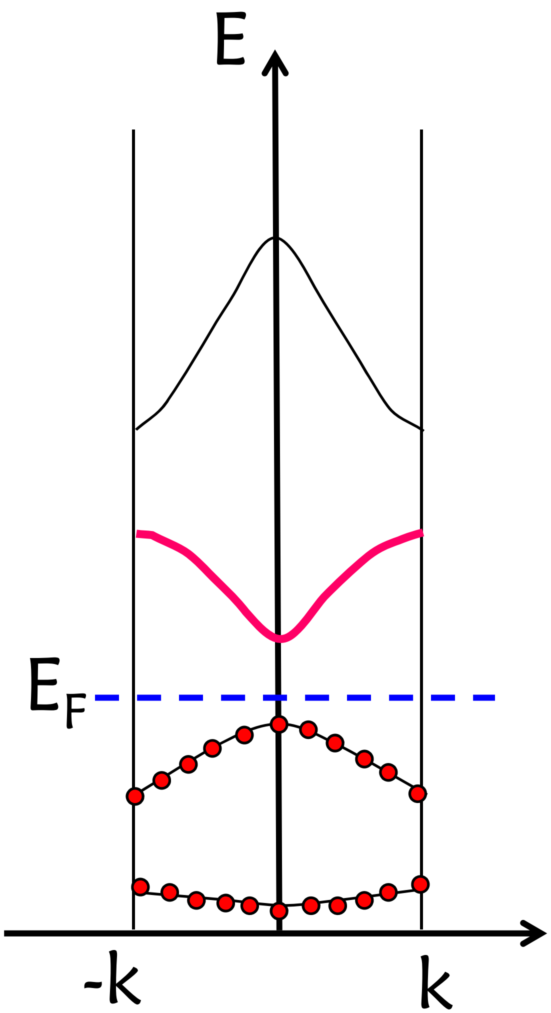
1) **Properties of electronic bands**

2) E-k diagram and constant energy surfaces

3) Conclusions

Reference: Vol. 6, Ch. 3 (pages 63-70)

Electron and Hole fluxes: Filled/Empty Bands

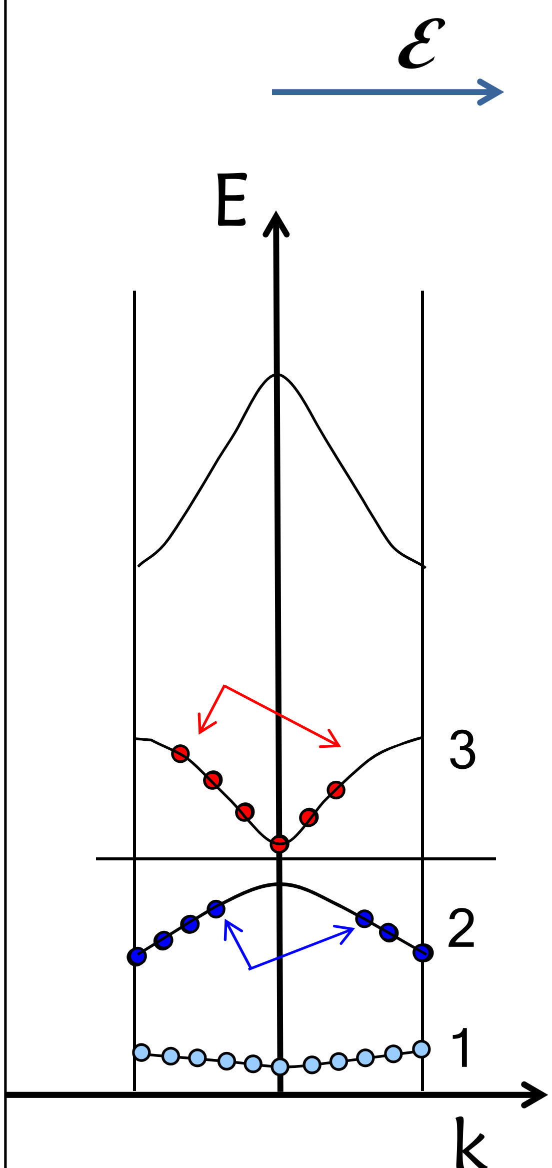


$$J_3 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i = 0$$

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

Filled and empty bands carry no current !

Electron and Hole Fluxes: Partially Filled Bands



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

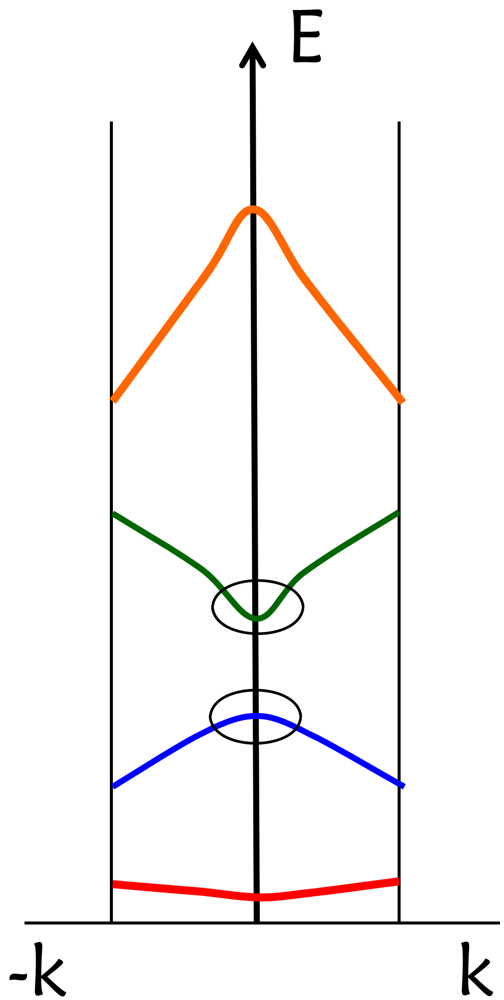
$$J_2 = -\frac{q}{L}\sum_{i(filled)} \upsilon_i = -\frac{q}{L}\sum_{all} \upsilon_i + \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

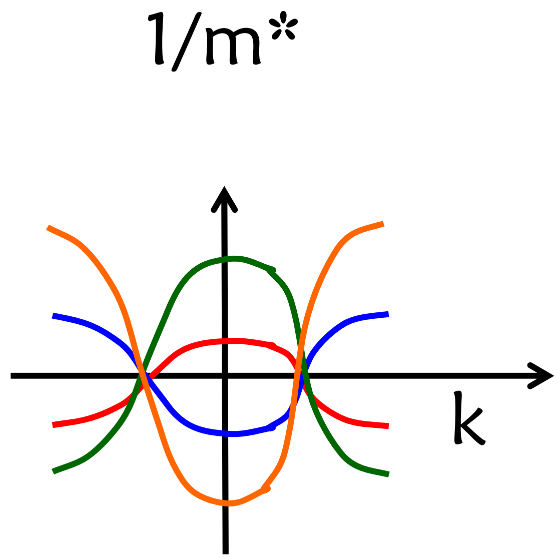
$$= \frac{q}{L}\sum_{i(empty)} |\upsilon_i|$$

-ve charge moving with –ve mass

+ve charge moving with +ve mass

what good is effective mass ?





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

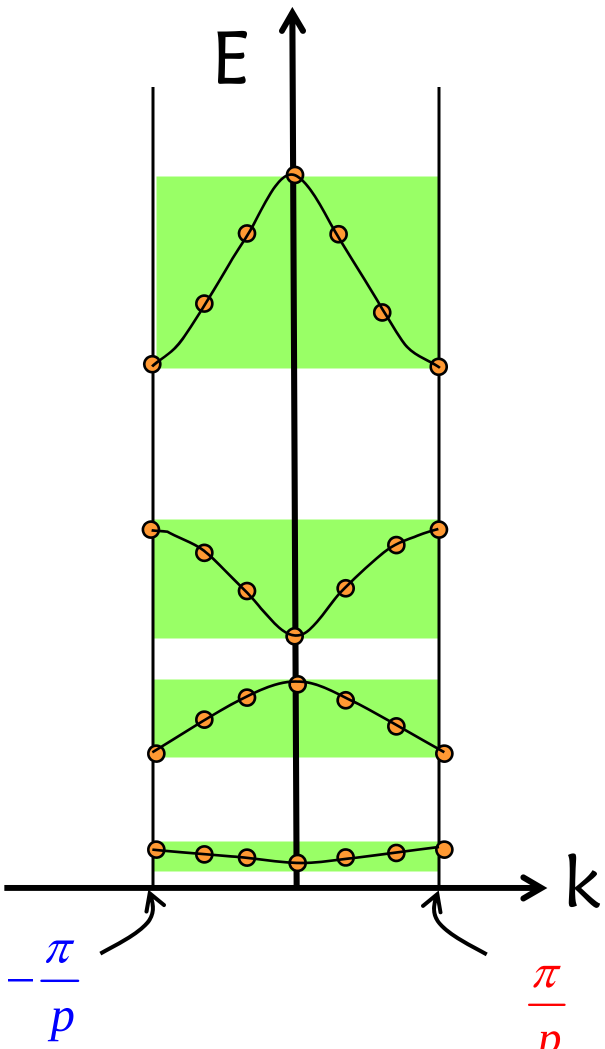
Outline

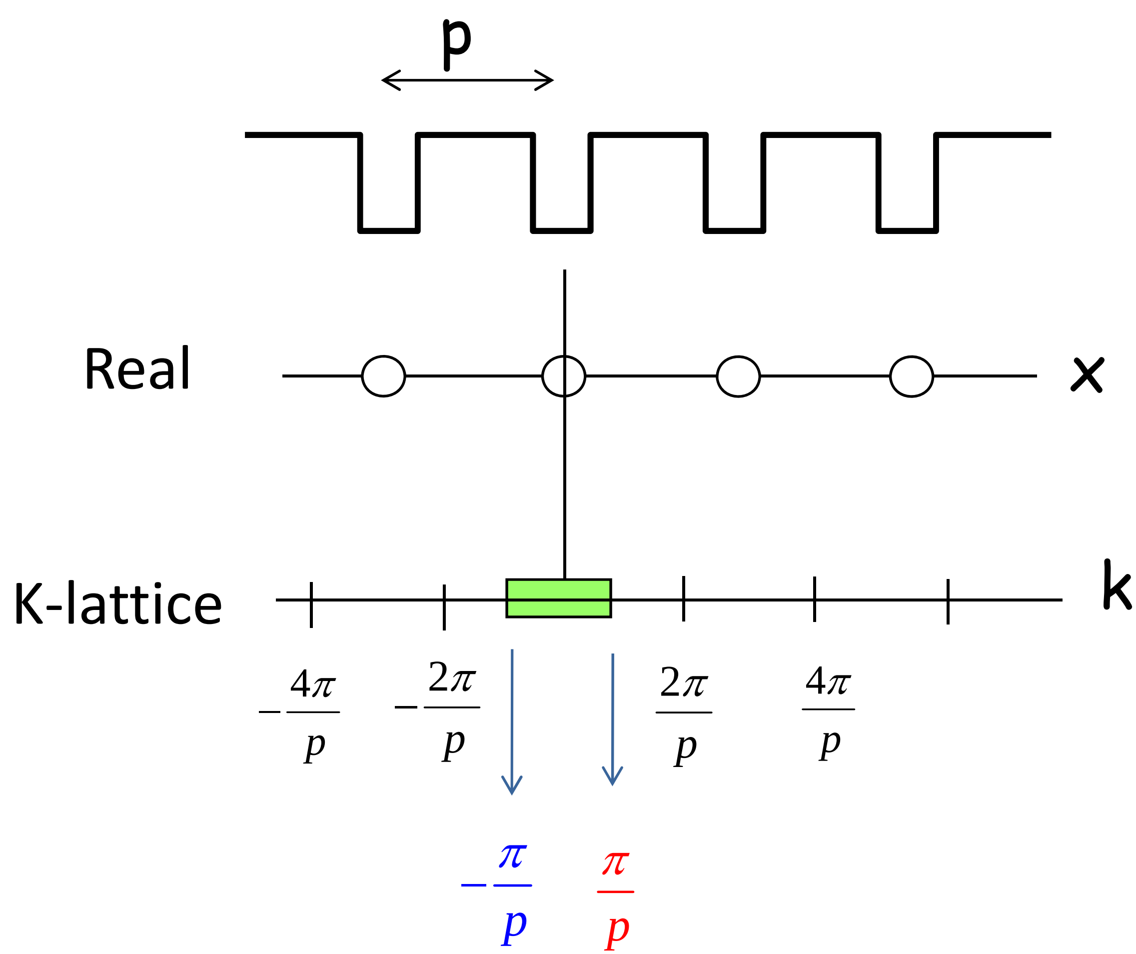
1) Properties of electronic bands

2) **E-k diagram and constant energy surfaces**

3) Conclusions

Solution Space: Brillouin Zone





General rules for Brillouin Zone

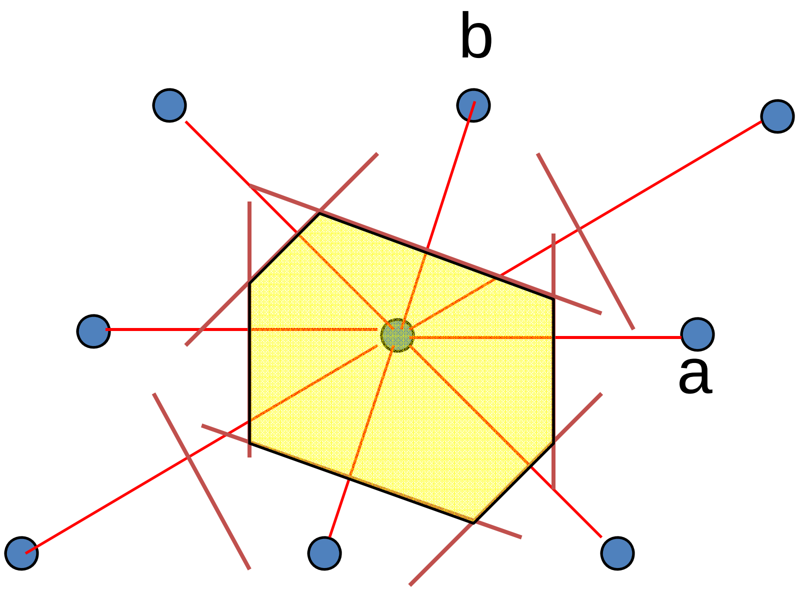
1) Define reciprocal lattice with the following vectors ....

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

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

Wigner-Seitz Method for Reciprocal Space

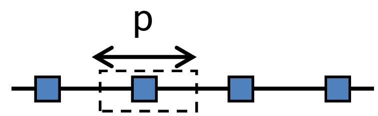
Primitive cell in real space



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

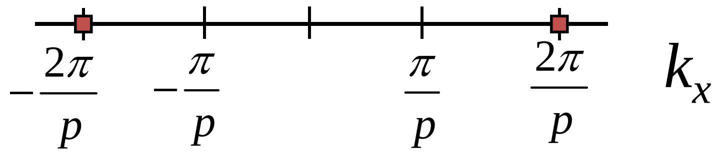
Brillouin Zone for One-dimensional Solids

Real-space

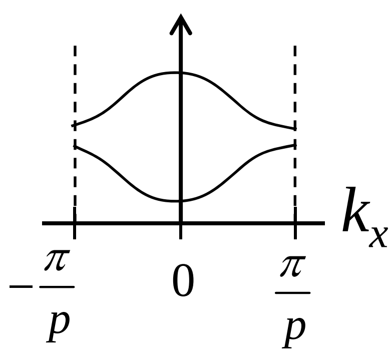


Replacing (a+b) by p …

1st B-Z

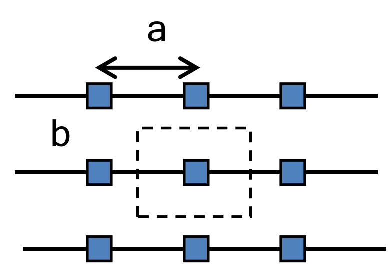


E-k diagram

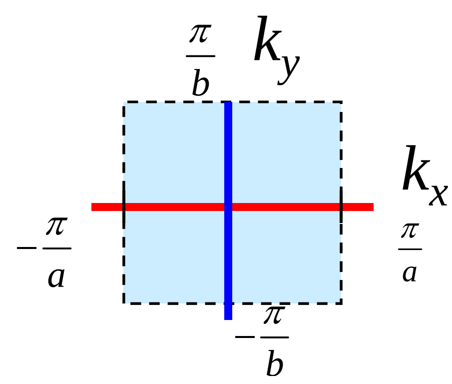


E-k diagram in 2D solids

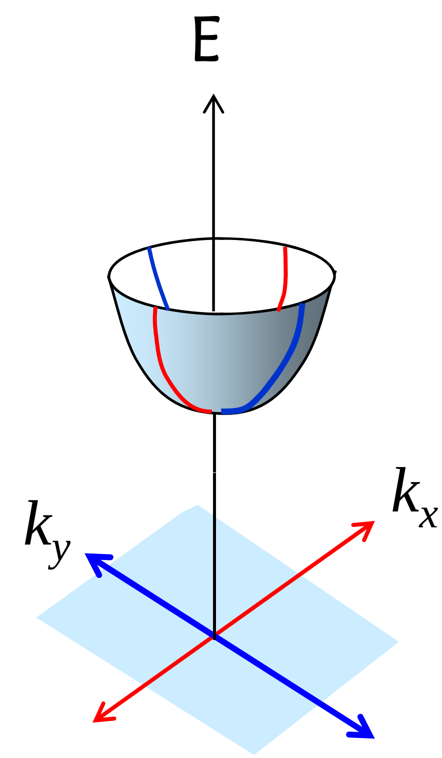
Real-space



1st B-Z

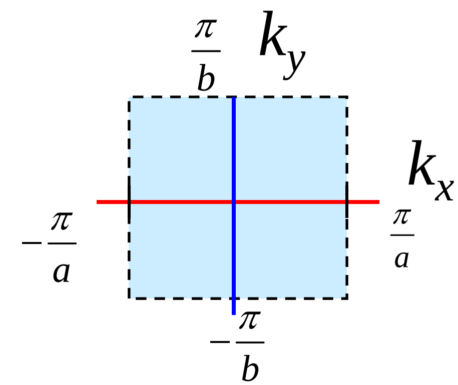


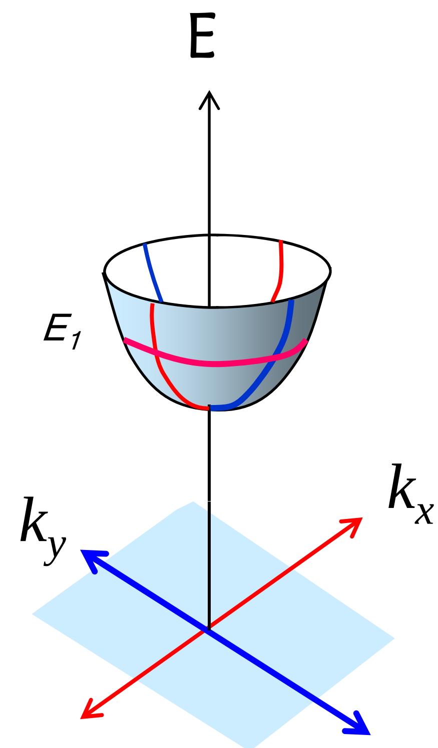
E-k diagram



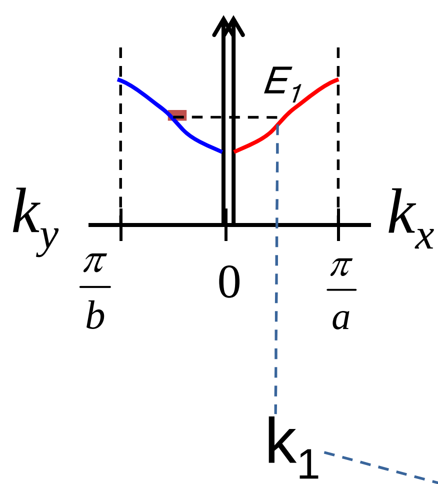
Constant Energy-surface in 2D

1st B-Z

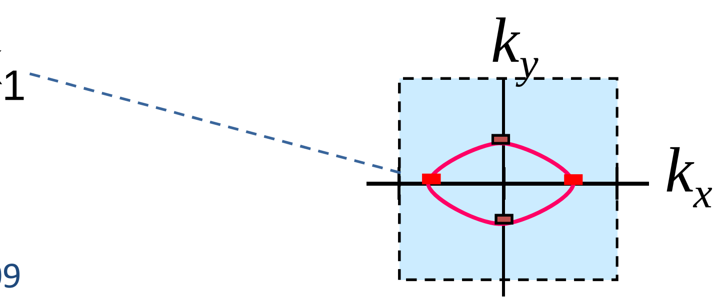




E-k diagram



Const. Energy
Surface



Conclusion

1) Electrons can only sit in-specific energy bands. Effective masses and band gaps summarize information about possible electronic states.

2) Effective mass is not a fundamental concept. There are systems for which effective mass can not be defined.

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

4) 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.

5) Most of the practical problems can only be analyzed by numerical solution.