6.730 Physics for Solid State Applications

Lecture 21:

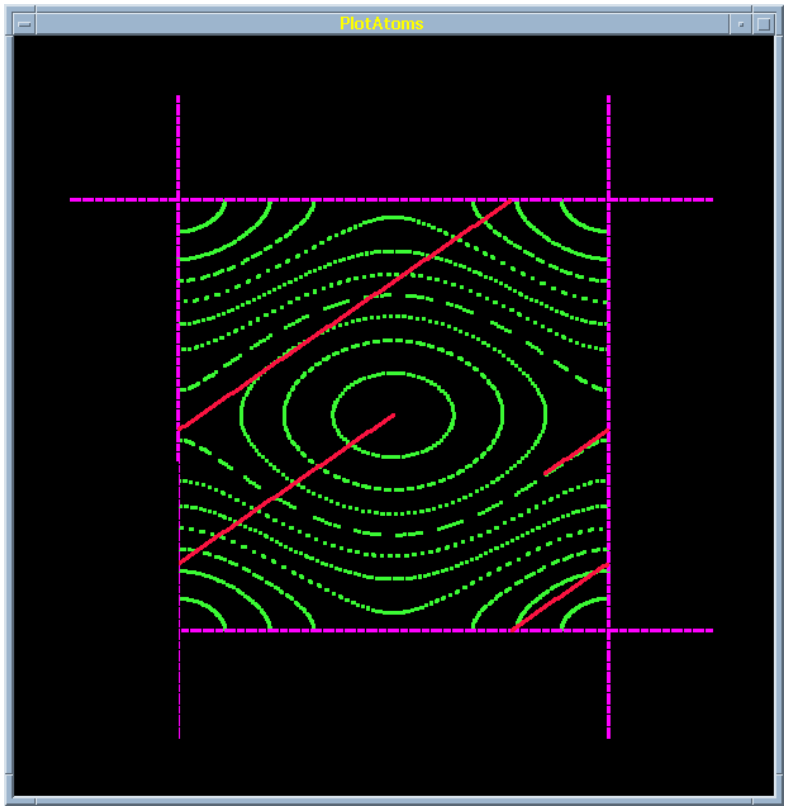
Outline

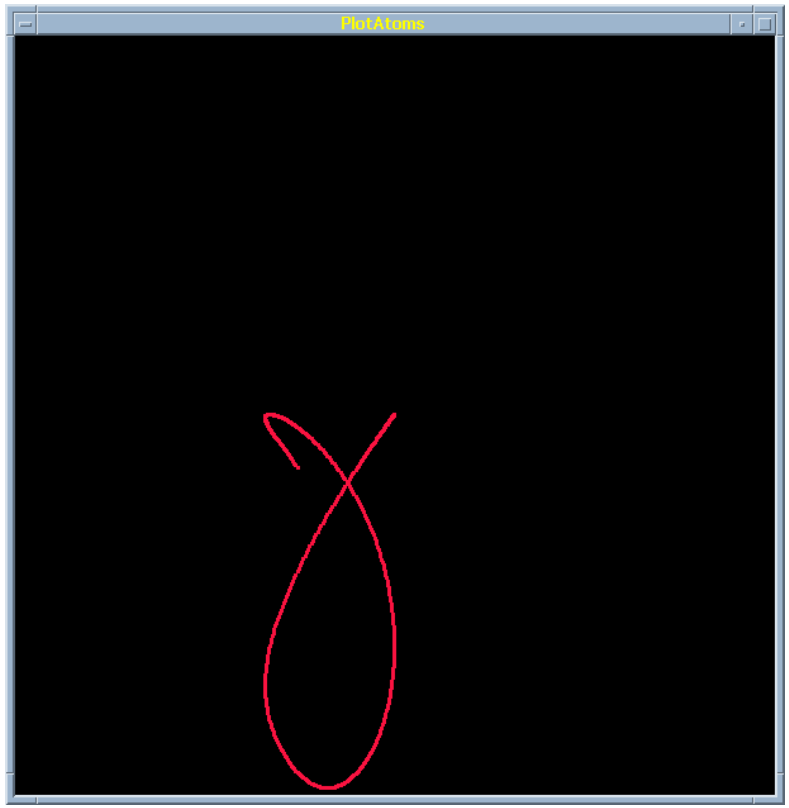
- Dynamical Effective Mass
- Fermi Surfaces
- Electrons and Holes

Semiclassical Equations of Motion

$$< v_n(k) >= \frac{< p >}{m} = \frac{1}{\hbar}\nabla_k E_n(k)$$

$$F_{ext} = \hbar\frac{dk}{dt}$$





http://www.physics.cornell.edu/sss/ziman/ziman.html

Semiclassical Equations of Motion

$$< \mathbf{v_n(k)} >= \frac{< \mathbf{p} >}{\mathbf{m}} = \frac{\mathbf{1}}{\hbar}\nabla_{\mathbf{k}}\mathbf{E_n(k)}$$

$$\mathbf{F_{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}$$

Lets try to put these equations together….

$$a(t) = \frac{dv}{dt} = \frac{1}{\hbar}\frac{\partial}{\partial t}\frac{\partial E_N(k)}{\partial k} = \frac{1}{\hbar}\frac{\partial^2 E_N(k)}{\partial k^2}\frac{dk}{dt}$$

$$= \left[\frac{1}{\hbar^2}\frac{\partial^2 E_N(k)}{\partial k^2}\right] F_{\text{ext}}$$

Looks like Newton's Law if we define the mass as follows…

$$m^*(k) = \hbar^2\left(\frac{\partial^2 E_N(k)}{\partial k^2}\right)^{-1}$$

dynamical effective mass

→ mass changes with k…so it changes with time according to k

Dynamical Effective Mass (3D)

Extension to 3-D requires some care,

F and a don't necessarily point in the same direction

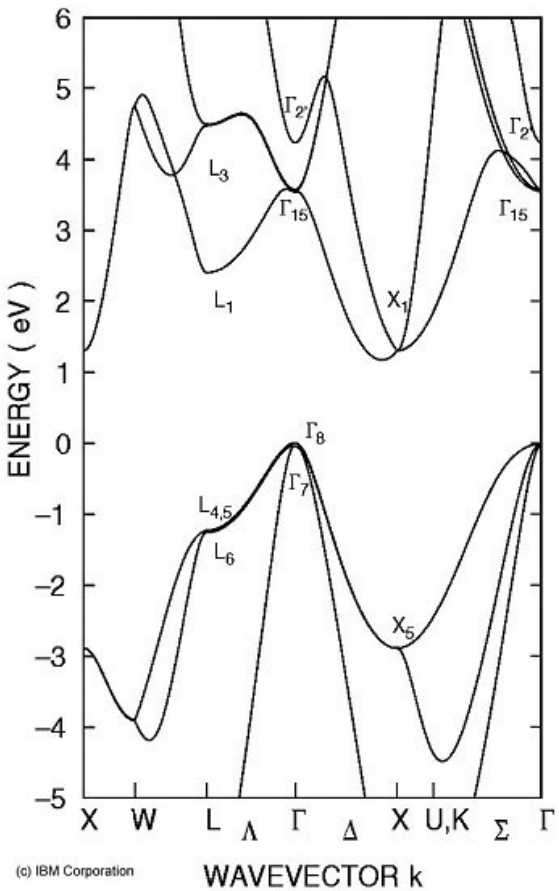
$$\mathbf{a} = \overline{\overline{\mathbf{M}}}^{-1}\mathbf{F}_{\text{ext}} \quad \text{where} \quad \overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2}\frac{\partial^2 E_N}{\partial k_i \partial k_j}$$

$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} \frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\ \frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\ \frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}} \end{pmatrix}\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}$$

Dynamical Effective Mass (3D)
Ellipsoidal Energy Surfaces

Fortunately, energy surfaces can often be approximate as…

$$E_N(k) = E_c + \frac{\hbar^2}{2}\left(\frac{(k_x - k_x^0)^2}{m_t} + \frac{(k_y - k_y^0)^2}{m_t} + \frac{(k_z - k_z^0)^2}{m_l}\right)$$



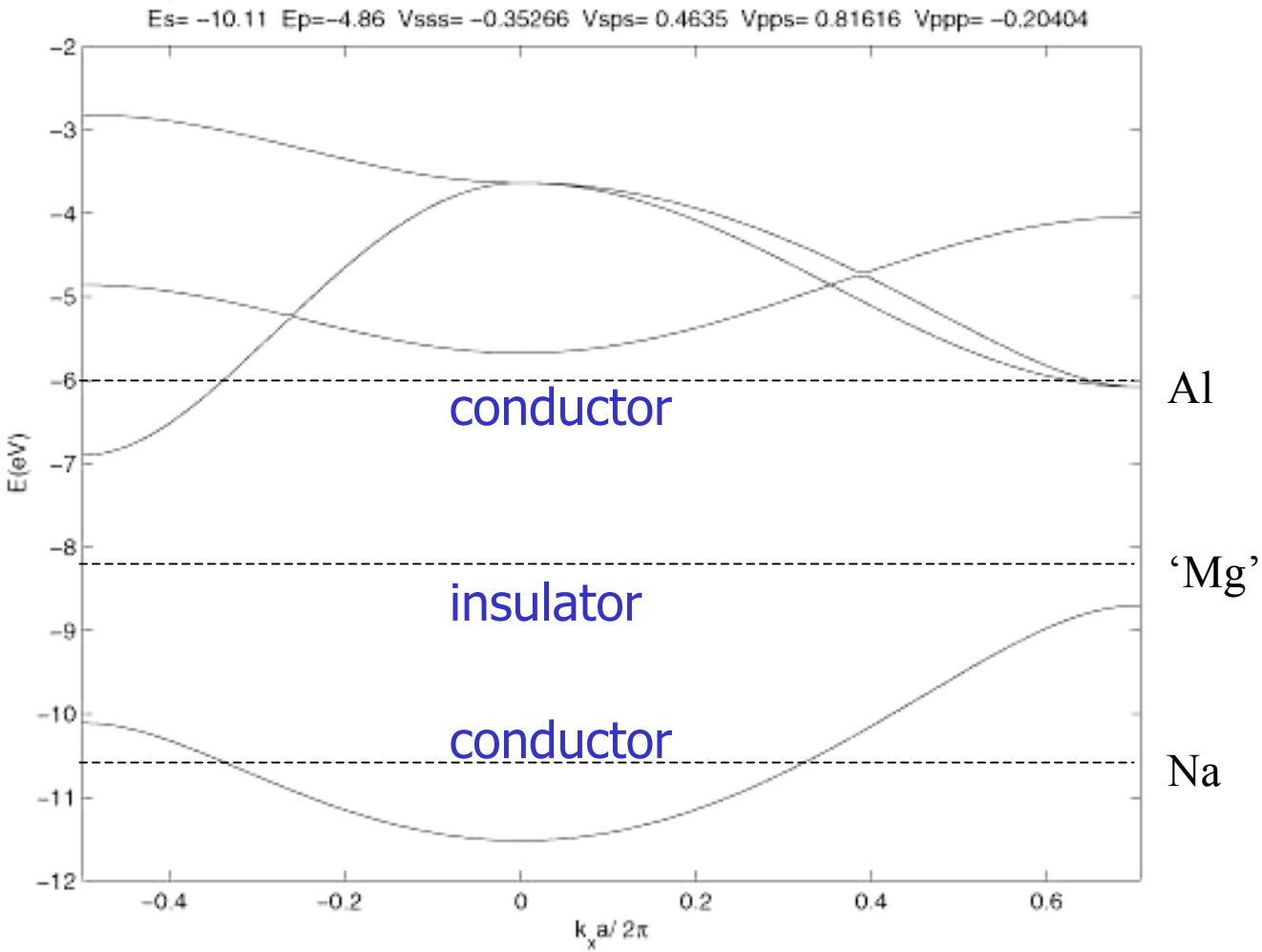
$$\overline{\overline{\mathbf{M}}}^{-1} = \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_l} \end{pmatrix}$$

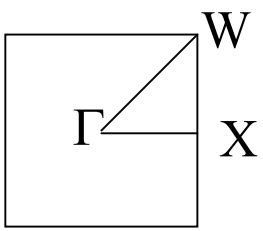
$$\overline{\overline{\mathbf{M}}} = \begin{pmatrix} m_t & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_l \end{pmatrix}$$

2D Monatomic Square Crystals

Dispersion Relations

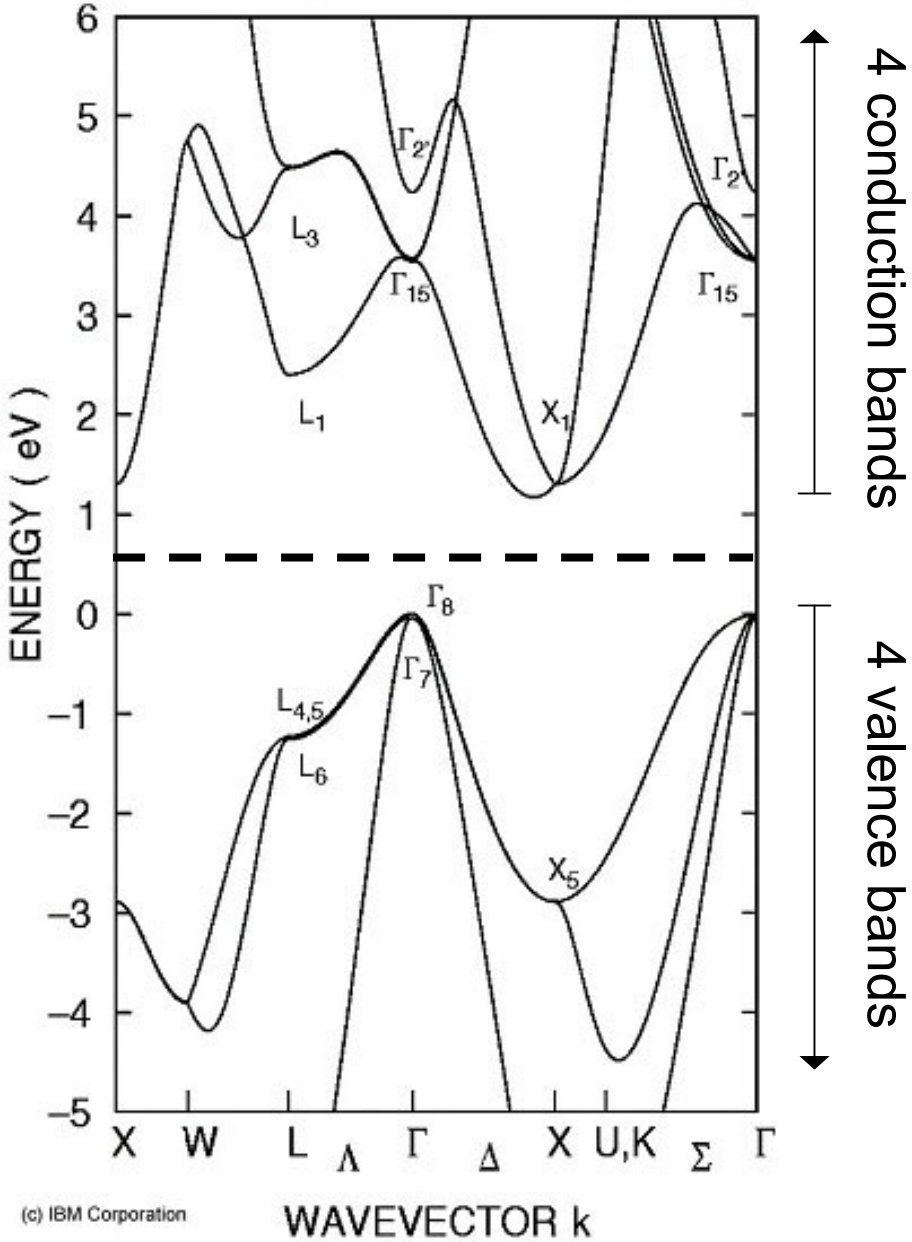
$a = 5.5$ A





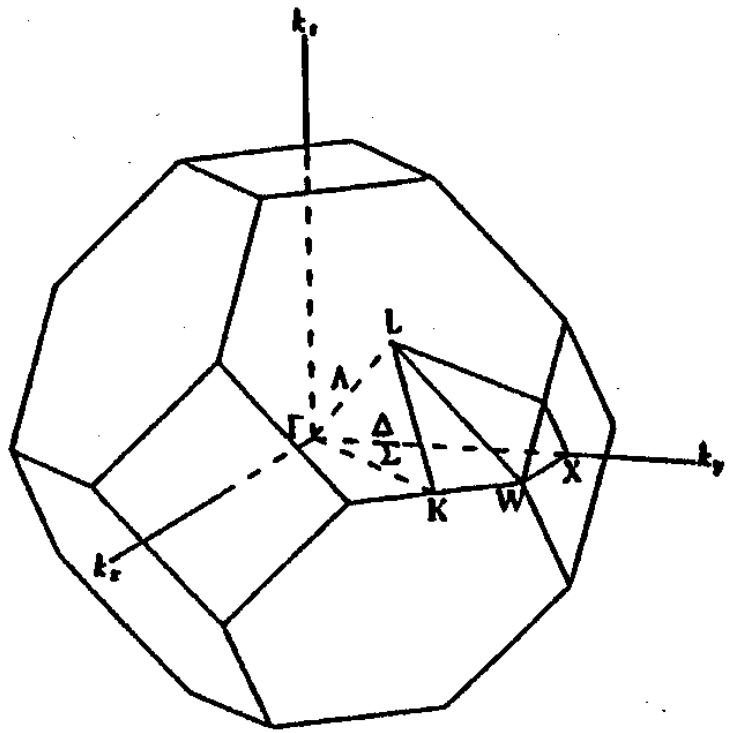
I	II	III	IV	V	VI	VII	VIII
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar

Silicon Bandstructure

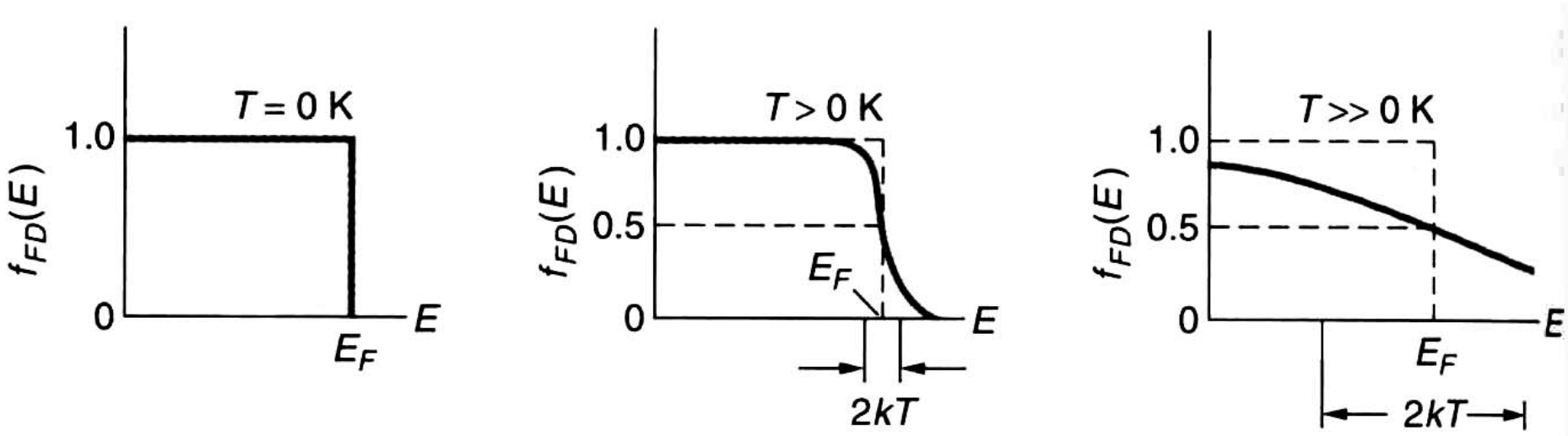


Si: [Ne] $3s^2\ 3p^2$

4 e- per silicon atom
2 silicon atoms per lattice site
total: 8 electrons at each site



Finite Temperatures



$$n = \frac{N}{V} = \int_{-\infty}^{\infty} \frac{1}{1 + e^{(E_{\mathbf{k}} - \mu)/k_B T}} 2 \frac{d^3\mathbf{k}}{(2\pi)^3}$$

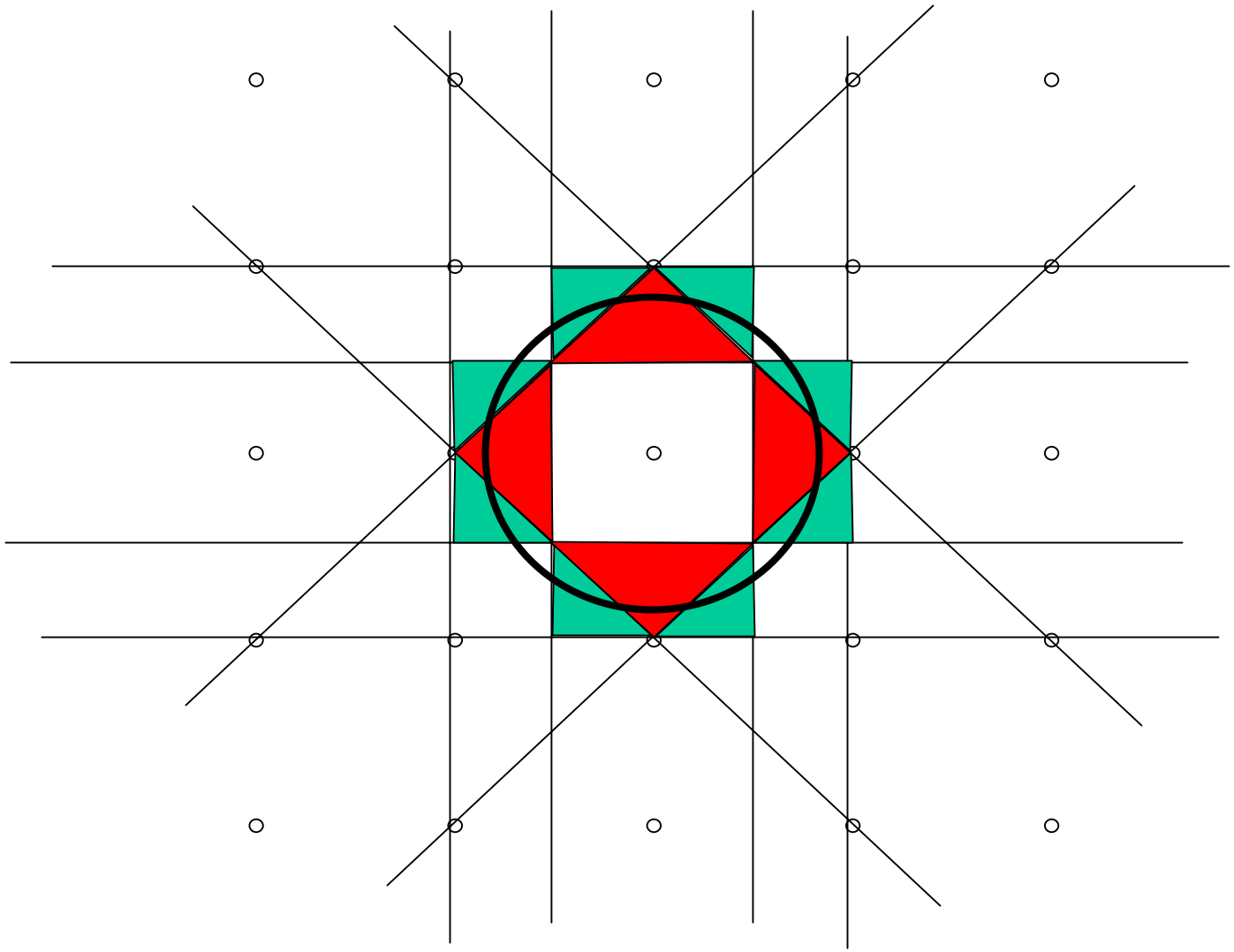
$$\frac{E_{\text{total}}}{V} = \int_{-\infty}^{\infty} E_{\mathbf{k}} \frac{1}{1 + e^{(E_{\mathbf{k}} - \mu)/k_B T}} 2 \frac{d^3\mathbf{k}}{(2\pi)^3}$$

Free Electron Fermi Surfaces (2D)

T=0

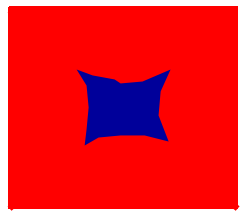
For free electrons energy surfaces are simple spheres (circles)…

Valence (# of electrons) determines radius of energy surface…

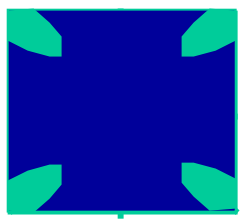


1st zone

2nd zone



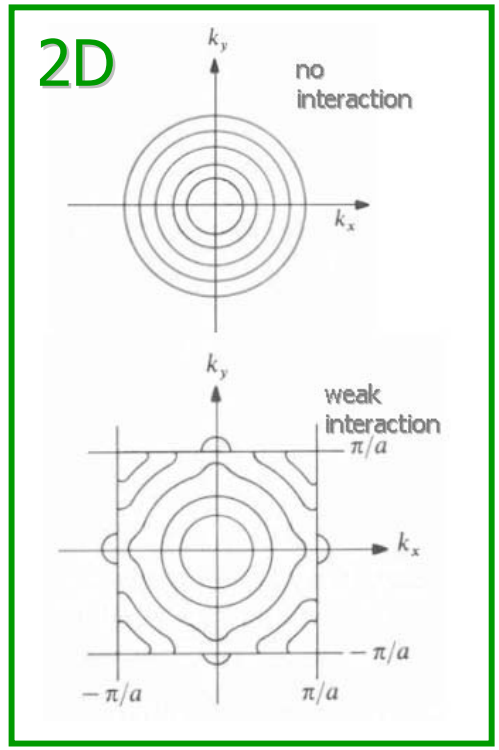
3rd zone



Fermi Surfaces (3D)

When k near to BZ boundary:

⇨ E contours become distorted

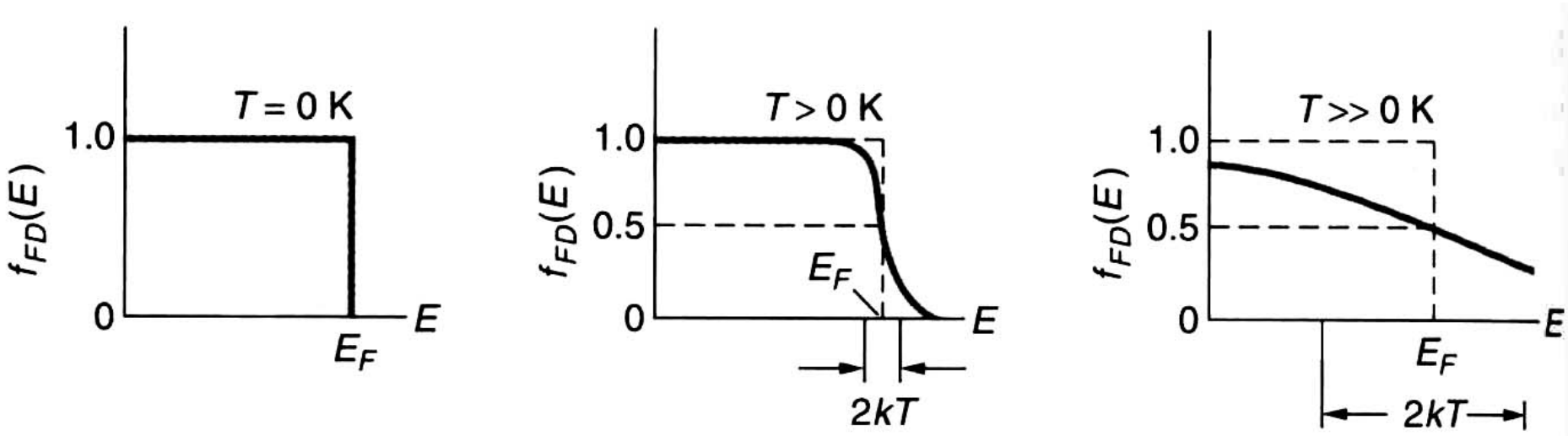


Fermi Surfaces (3D)

N_e = 1 monovalent metals, e.g. Na, Cu, with values ~ f.e. theory

other cases, e.g. Be (N_e=2), Al (N_e=3), there are serious differences

Finite Temperatures



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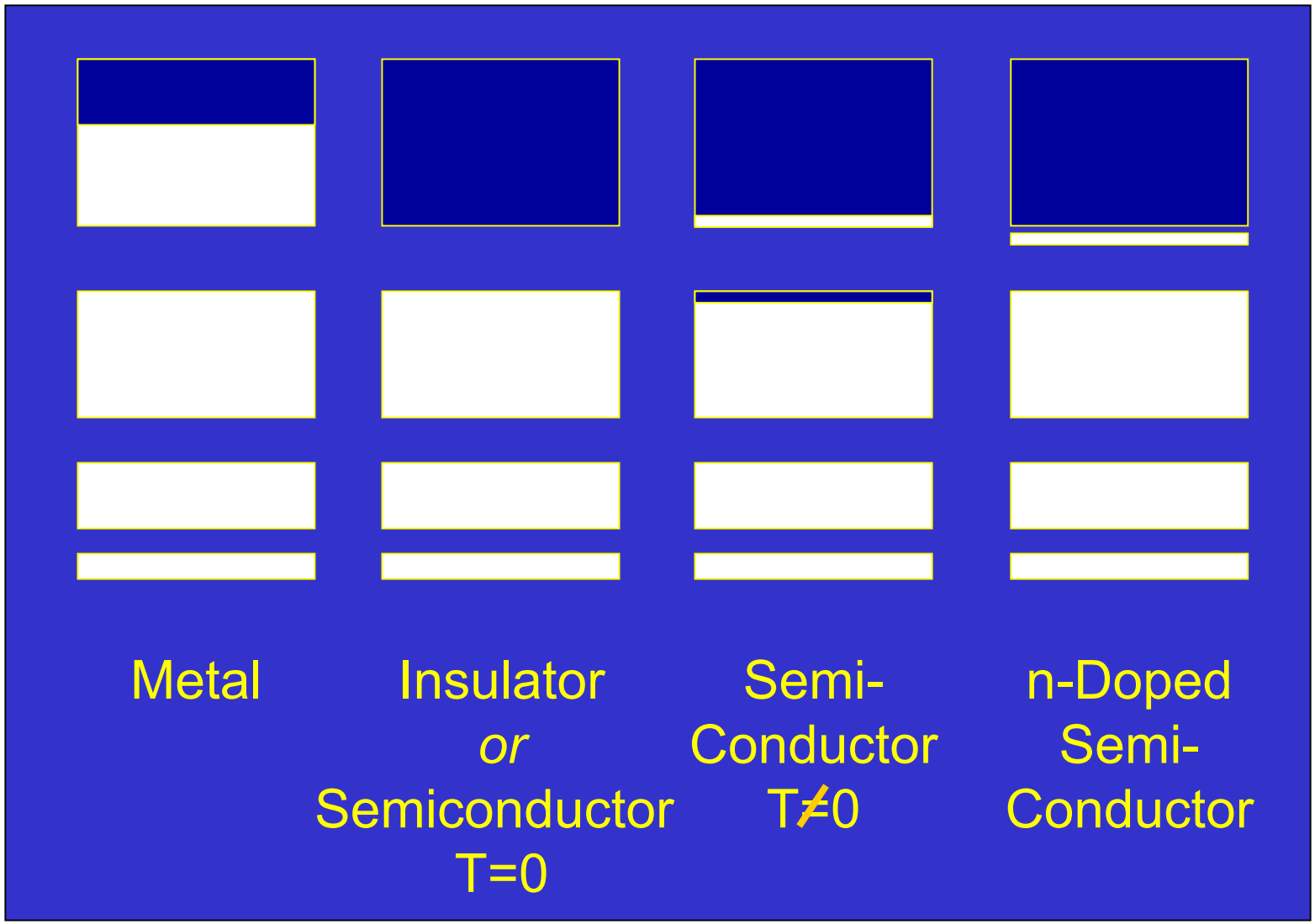
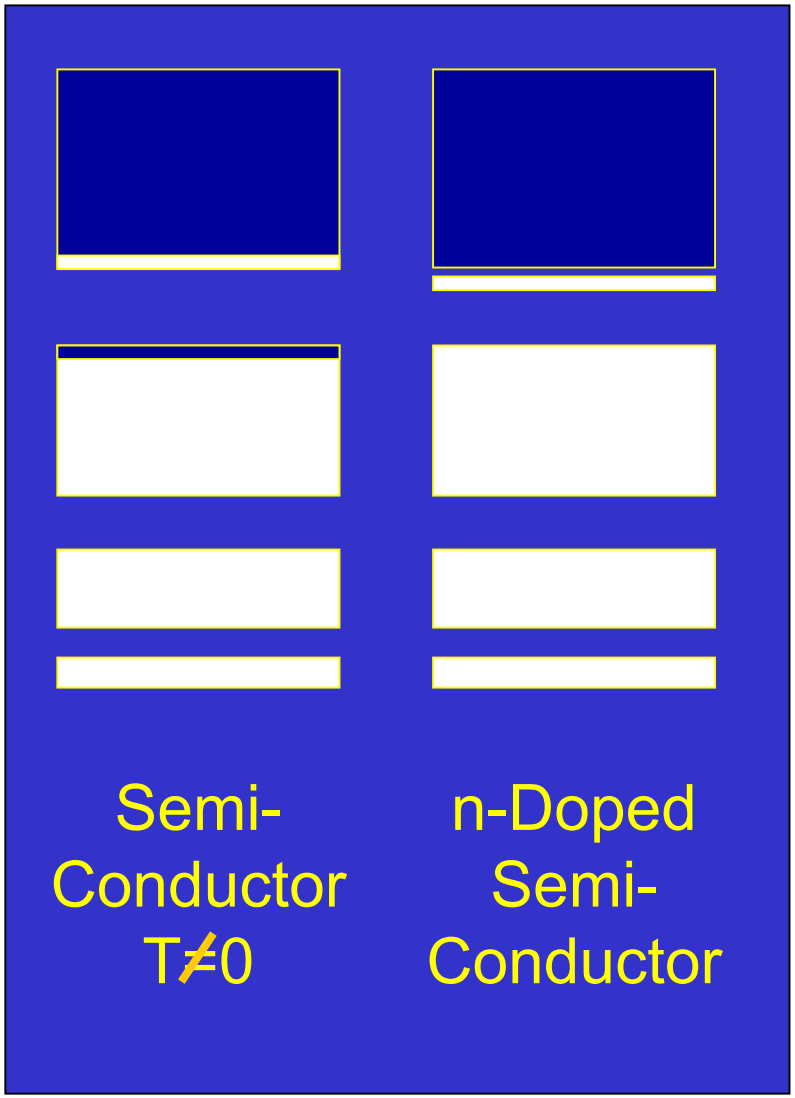
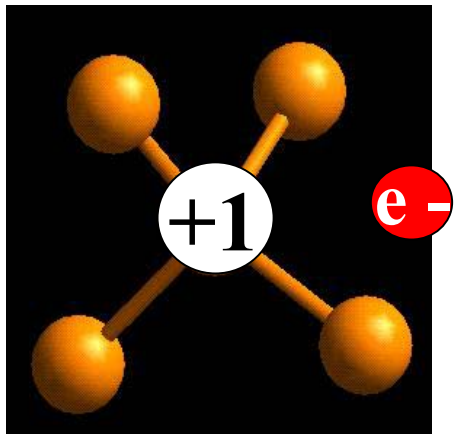
Overview of Electron Distributions

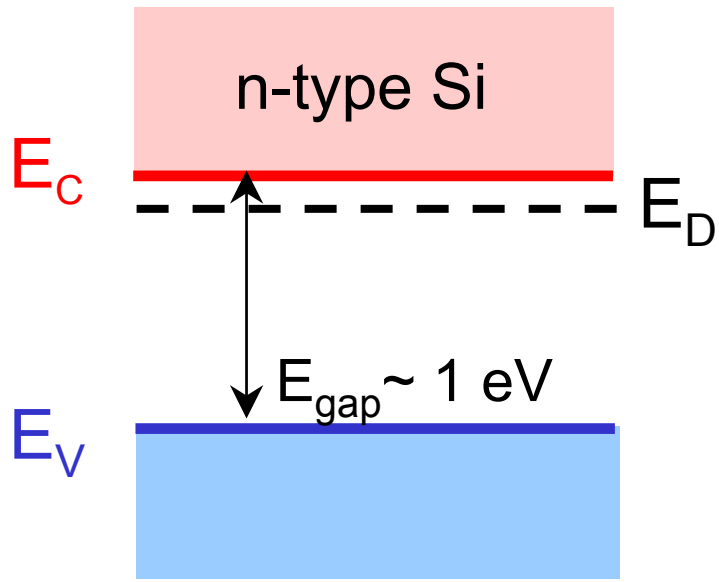


Electron Distributions in Doped Semiconductors

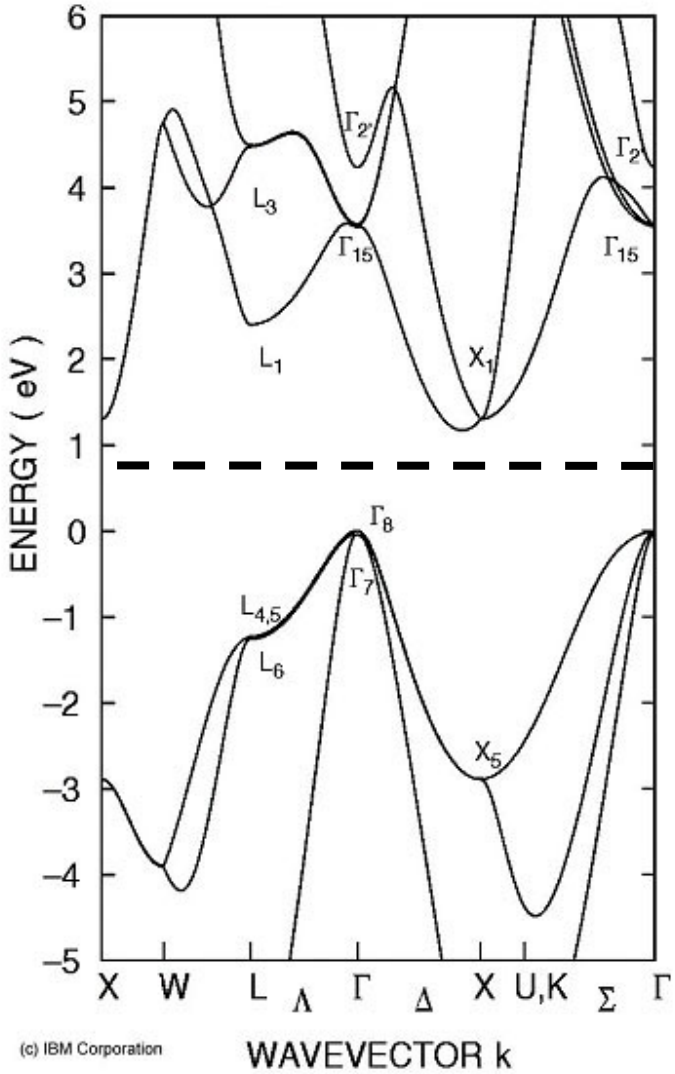


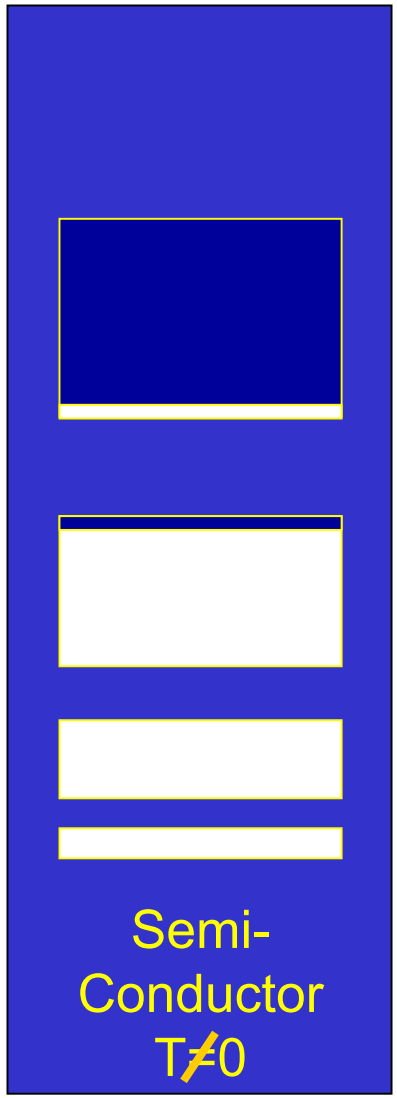


$$E_d = E_c - \frac{13.56\, m^*}{l^2 \epsilon^2 \, m} \text{ eV}$$



Electron and Holes

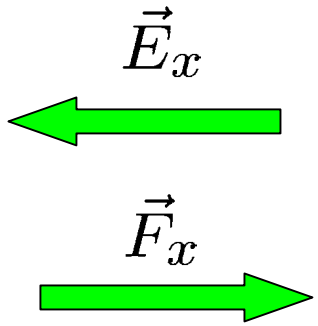




Electrons in conduction band

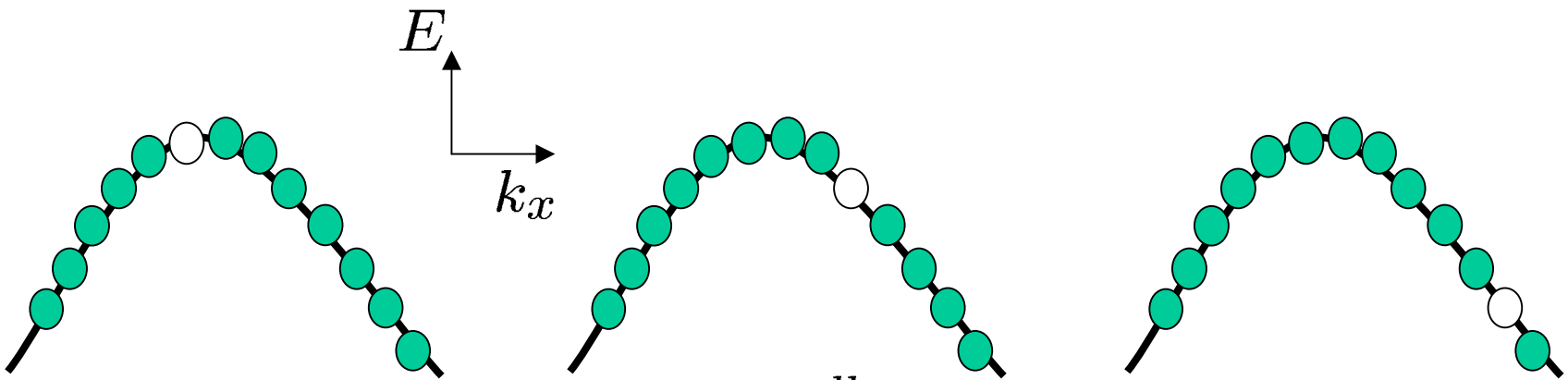
Holes in valence band

Motion of Valence Electrons



electrons have negative charge

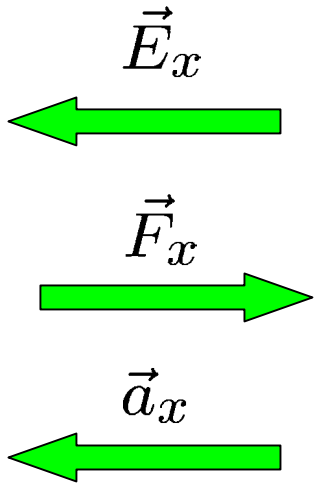
k-space



$$F_x = \hbar \frac{dk_x}{dt}$$

Valence electrons (and vacancy) all move in the positive k_x direction…

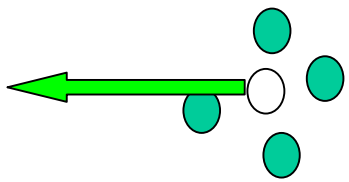
Motion of Valence Electrons



electrons have negative charge

valence electrons have negative mass !

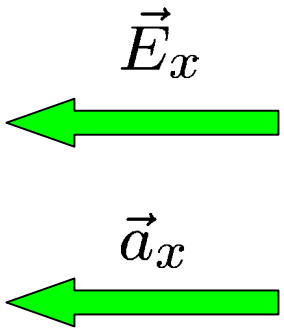
Real space



Vacancy ends up moving in the direction of the electric field as if it had a positive charge

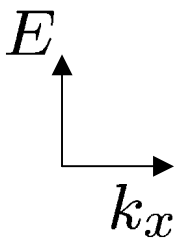
Hole is a quasi-particle with positive charge and positive mass…

Motion of Valence Electrons



Hole is a quasi-particle with positive charge and positive mass…

k-space



hole dispersion