“Complementi di Fisica” Lecture 18

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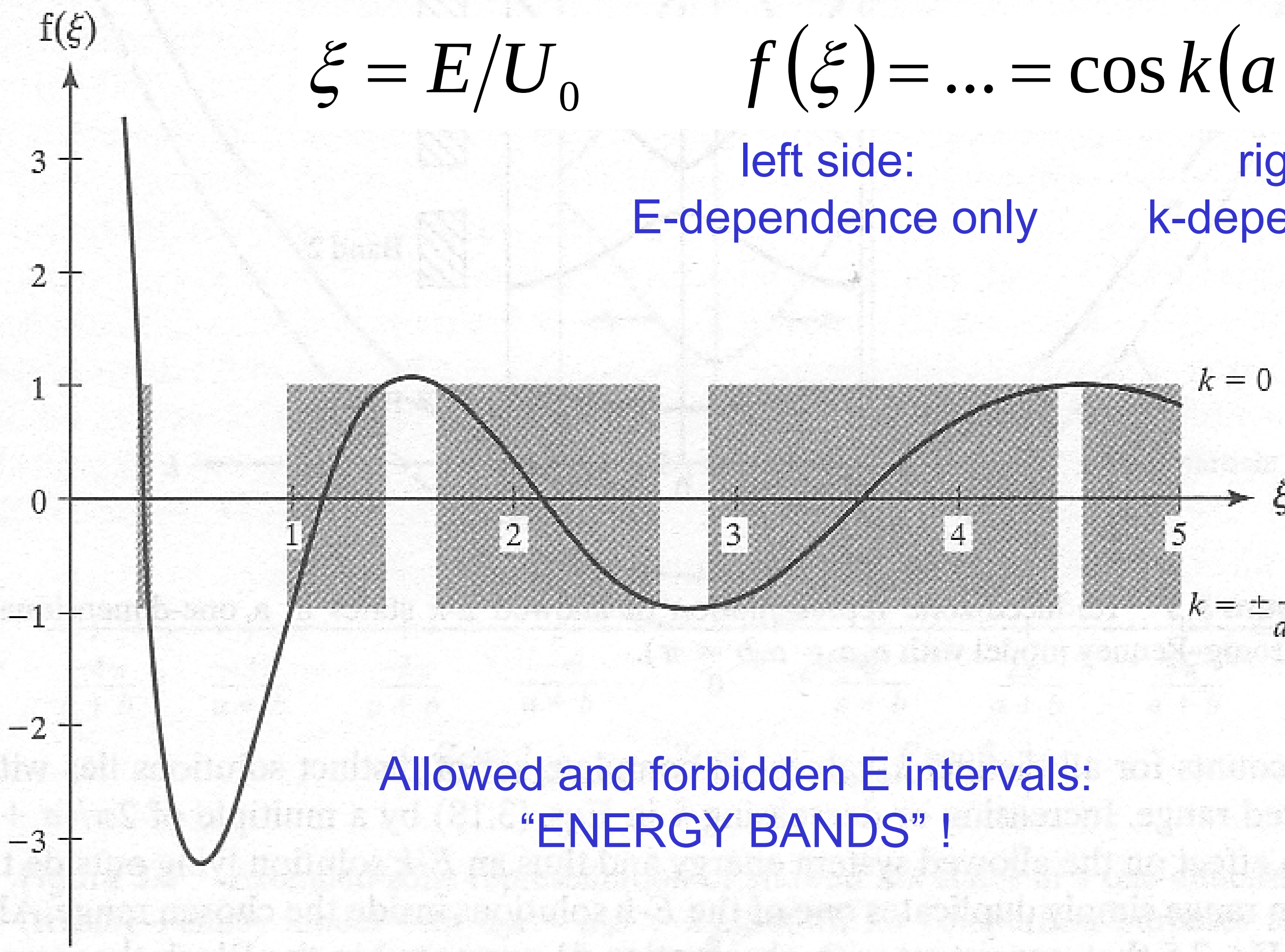
Course Outline - Reminder

- The physics of semiconductor devices: an introduction
- Quantum Mechanics: an introduction
  - Reminder on waves
  - Waves as particles and particles as waves (the crisis of classical physics); atoms and the Bohr model
  - The Schrȍdinger equation and its interpretation
  - (1-d) free and confined (infinite well) electron; wave packets, uncertainty relations; barriers and wells; periodic potential
  - (3-d) Hydrogen atom, angular momentum, spin
  - Systems with many particles
- Advanced semiconductor fundamentals (bands, etc…)
  - Energy bands, effective mass, …
  - …

Lecture 18 - outline

- Reminder: the E-k relation in the Kronig-Penney model, Brillouin zones etc.
- Particle motion and effective mass
  - Wave packets in crystals
  - Group velocity variations due to external forces: “effective mass”
  - E-k relations close to band edges;
    - positive and negative effective mass;
    - nearly constant effective mass;
  - Carriers and electrical current; electrons and holes
- Extrapolation to 3-d
  - Brillouin zones; E-k diagrams; constant energy surfaces
  - Effective mass tensor;
  - effective mass measurements

Kronig-Penney: allowed E values



$$\xi = E/U_0 \qquad f(\xi) = \ldots = \cos k(a+b)$$

left side: E-dependence only

right side: k-dependence only

$\cos k(a+b) = +1$
$k(a+b) = 0$

$\cos k(a+b) = -1$
$k(a+b) = \pm\pi$

Allowed and forbidden E intervals: “ENERGY BANDS” !

Figure 3.3 Graphical determination of allowed electron energies. The left-hand side of the Eqs. (3.18) Kronig–Penney model solution is plotted as a function of $\xi = E/U_0$. The shaded regions where $-1 \leq f(\xi) \leq 1$ identify the allowed energy states $(\alpha_0 a = \alpha_0 b = \pi)$. Specific example

Unreduced Bloch E-k diagram

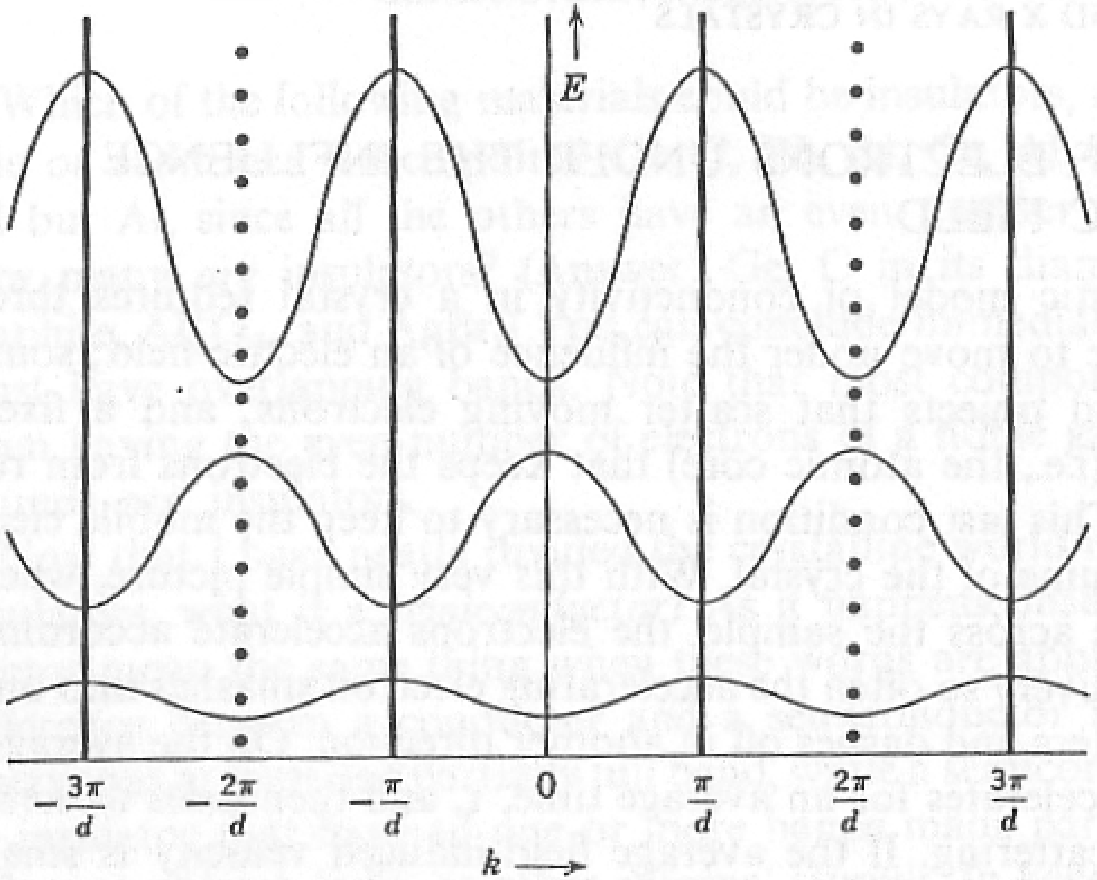


Figure 2.18 Complete unreduced Bloch diagram. Any interval of $2\pi/d$ along the k axis (a *zone*) contains a complete set of solutions. The usual set of zones is indicated by the bold vertical lines.

Brillouin zones (1-d)

- Some properties of the E-k relation from the Kronig-Penney model, that can be generalized to more realistic potentials:
  - Allowed energy intervals or "bands" from: $-1 \leq \cos k(a+b) \leq +1$

$$\xi = E/U_0 \qquad f(\xi) = \ldots = \cos k(a+b)$$

  - The smallest absolute values for k corresponding to E values in each "band" are:

$$\cos k(a+b) = +1 \qquad \cos k(a+b) = -1$$
$$k(a+b) = 0 \qquad k(a+b) = \pm\pi$$

  - The k-interval from $-\pi/(a+b)$ to $+\pi/(a+b)$ is called "first Brillouin zone"
  - The E-k relation is periodic in k, with period = $2\pi/(a+b)$, since k is the argument of the funcion cos k(a+b)
  - Adjacent k intervals are called "2nd, 3rd, … Brillouin zone" (see fig.)
  - dE/dk = 0 at zone boundaries (k=0, $\pm\pi/(a+b)$, …)

Kronig-Penney: E-k relation

"extended zone representation" of allowed E-k states, compared with "free particle"

"reduced zone representation" of allowed E-k states

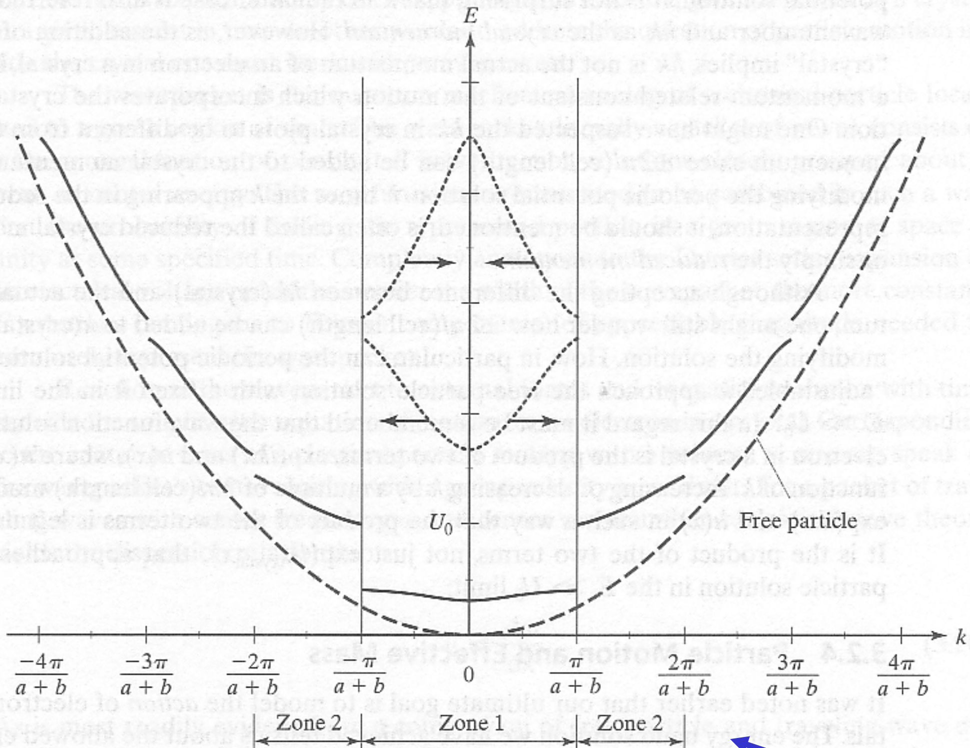


Figure 3.6 Extended-zone representation of allowed E-k states in a one-dimensional crystal (Kronig–Penney model with $\alpha_0 a = \alpha_0 b = \pi$). Shown for comparison purposes are the free-particle E-k solution (dashed line) and selected bands from the reduced-zone representation (dotted lines). Arrows on the reduced-zone band segments indicate the directions in which these band segments are to be translated to achieve coincidence with the extended-zone representation. Brillouin zones 1 and 2 are also labeled on the diagram.

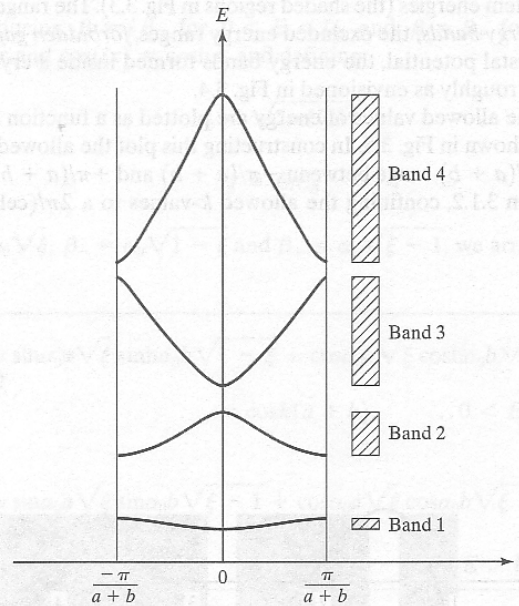


Figure 3.5 Reduced-zone representation of allowed E-k states in a one-dimensional crystal (Kronig–Penney model with $\alpha_0 a = \alpha_0 b = \pi$).

"Brillouin zones"

Particle motion and effective mass

Wave packets

Group velocity variations

Band edges

Carriers and electrical current

Wave packets in crystals

- The Bloch "plane wave" solutions, with eigenvalue E and two possible values of k in the first Brillouin zone, correspond to electrons that have well defined energy but are completely delocalized in space (equal probability to be anywhere in the crystal)

- Partial localization can be achieved, like for free particles, by wave packets = superposition of Bloch "plane waves"

- Wave-packets (or their centers) move with velocity that can be identified with the "group velocity"

$$v_g = \frac{d\omega}{dk} \quad \Rightarrow \quad v_g = \frac{1}{\hbar}\frac{dE}{dk}$$

Group velocity variations: effective mass

- What happens if an “external” force is applied, for instance an external electric field (the lattice forces are already included in the Bloch wave functions!) ?
  - “force” $\Rightarrow$ “change in particle energy” or absorbed power $\Rightarrow$ “changes in group velocity” $\Rightarrow$ “acceleration” $\Rightarrow$ “effective mass”:

$$dE = F dx = F v_g dt, \quad v_g = \frac{1}{\hbar}\frac{dE}{dk} \quad \Rightarrow$$

$$\Rightarrow F = \frac{1}{v_g}\frac{dE}{dt} = \frac{1}{v_g}\frac{dE}{dk}\frac{dk}{dt} = \hbar\frac{dk}{dt} = \frac{d(\hbar k)}{dt}$$

$$\Rightarrow \frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d}{dk}\left(\frac{dE}{dk}\right)\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}\frac{d(\hbar k)}{dt}$$

Formally similar to Newton’s law, if…

$$a_g = \frac{dv_g}{dt} = \frac{F}{m^*}$$

… if this coefficient Is interpreted as an “effective mass”

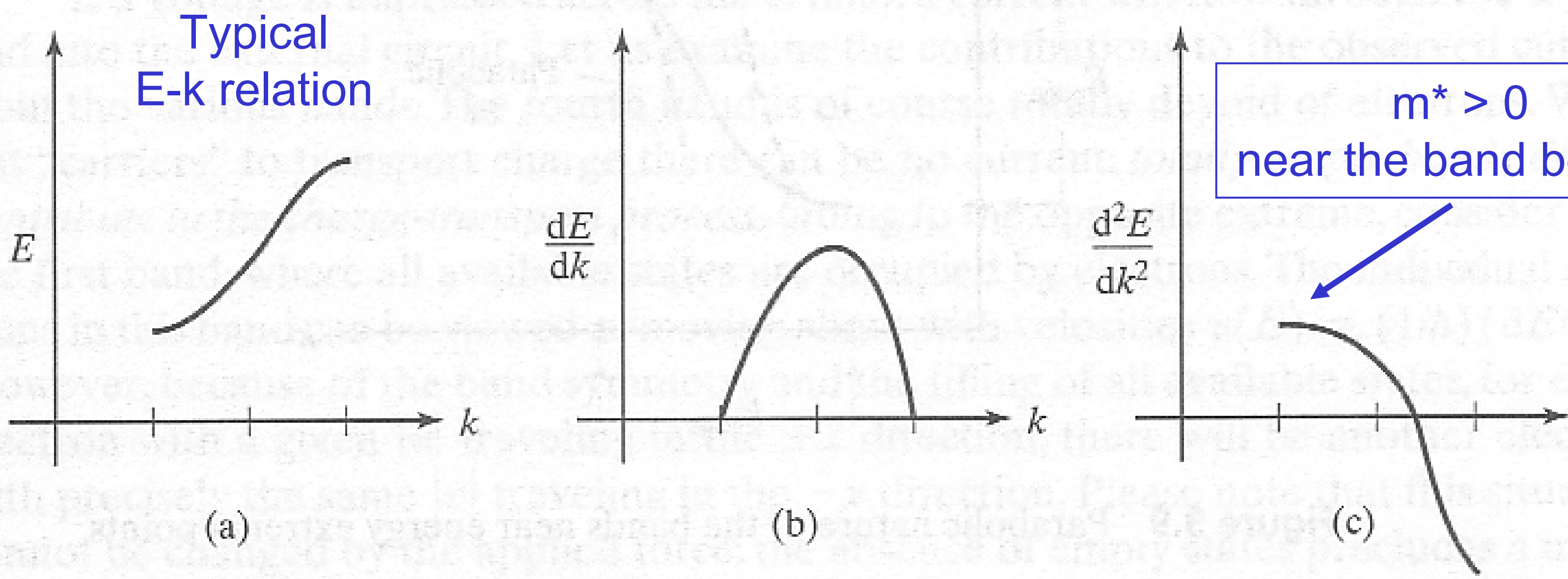
$$m^* = \frac{1}{\frac{1}{\hbar^2}\frac{d^2E}{dk^2}}$$

Effective mass

$$F = m^* \frac{dv_g}{dt} \qquad m^* = \frac{1}{\frac{1}{\hbar^2}\frac{d^2E}{dk^2}}$$

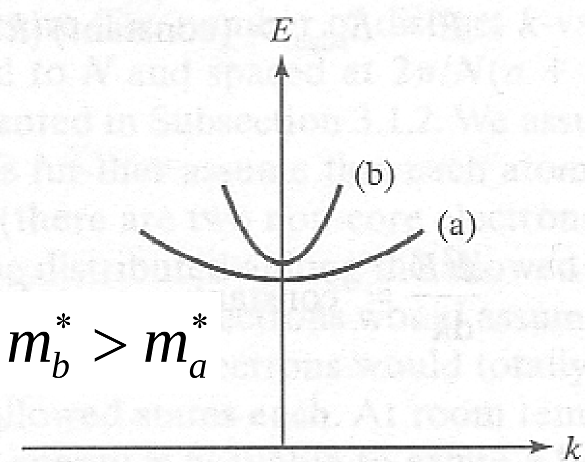
- m* is really a coefficient describing crystal-wave interaction, not the well known classical inertial mass;
- however it would be quite useful to treat the Bloch wave packet as a particle following the familiar Newtonian mechanics
- This is possible only if m* is nearly constant
  - This happens close to band edges!
- However, keep in mind the following peculiarities:
  - negative effective masses !?
  - non-constant effective masses !?
  - “tensor” instead of “scalar” masses (see later, 3-d) !?

Effective mass and E-k near band edges



m* > 0
near the band bottom

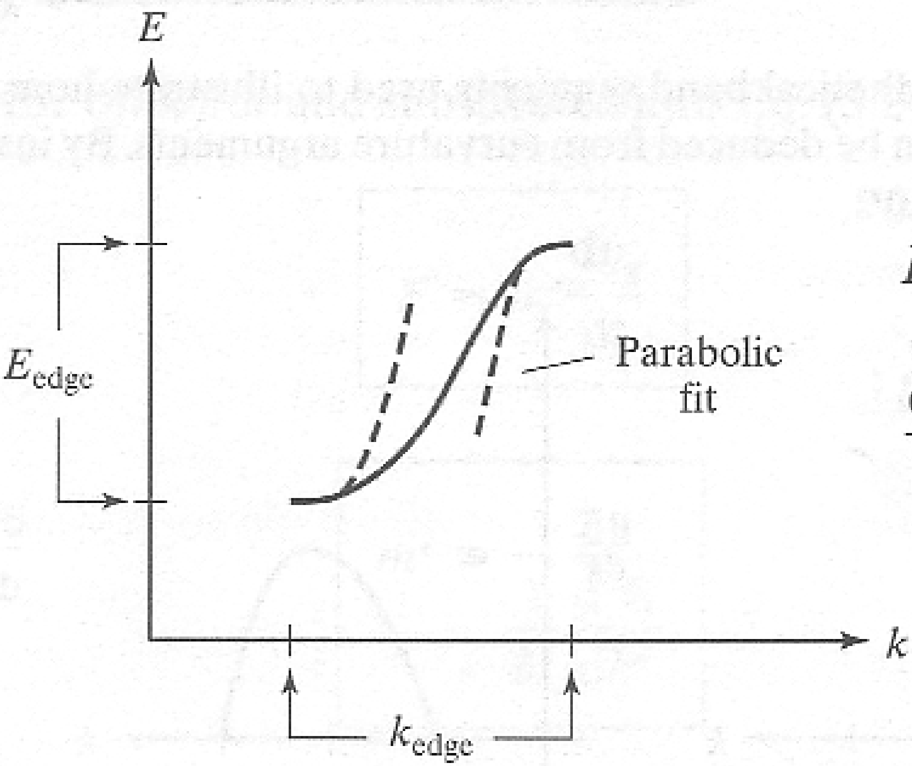
m* < 0
near the band top



$$m_b^* > m_a^*$$

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

Effective mass and E-k near band edges



near the band edges:

$$E - E_{edge} \simeq (\text{constant})(k - k_{edge})^2$$

$$\frac{d^2E}{dk^2} \simeq \text{constant} \qquad \ldots E \text{ near } E_{edge}$$

… the effective mass is approximately constant (energy-independent)!

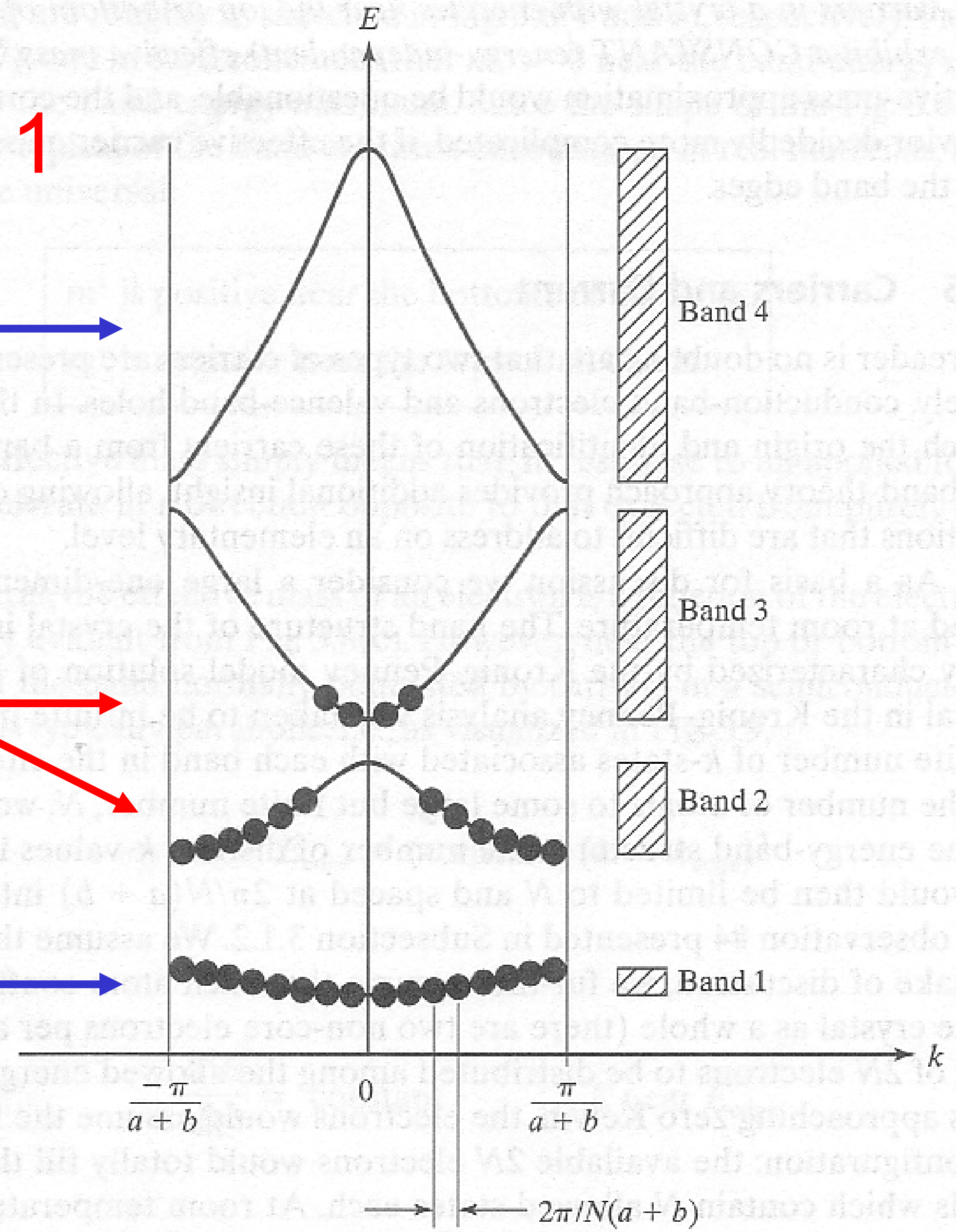
$$m^* = \frac{1}{\dfrac{1}{\hbar^2}\dfrac{d^2E}{dk^2}}$$

Carriers and electrical current - 1

Empty band: no current

Partially filled bands contribute to current

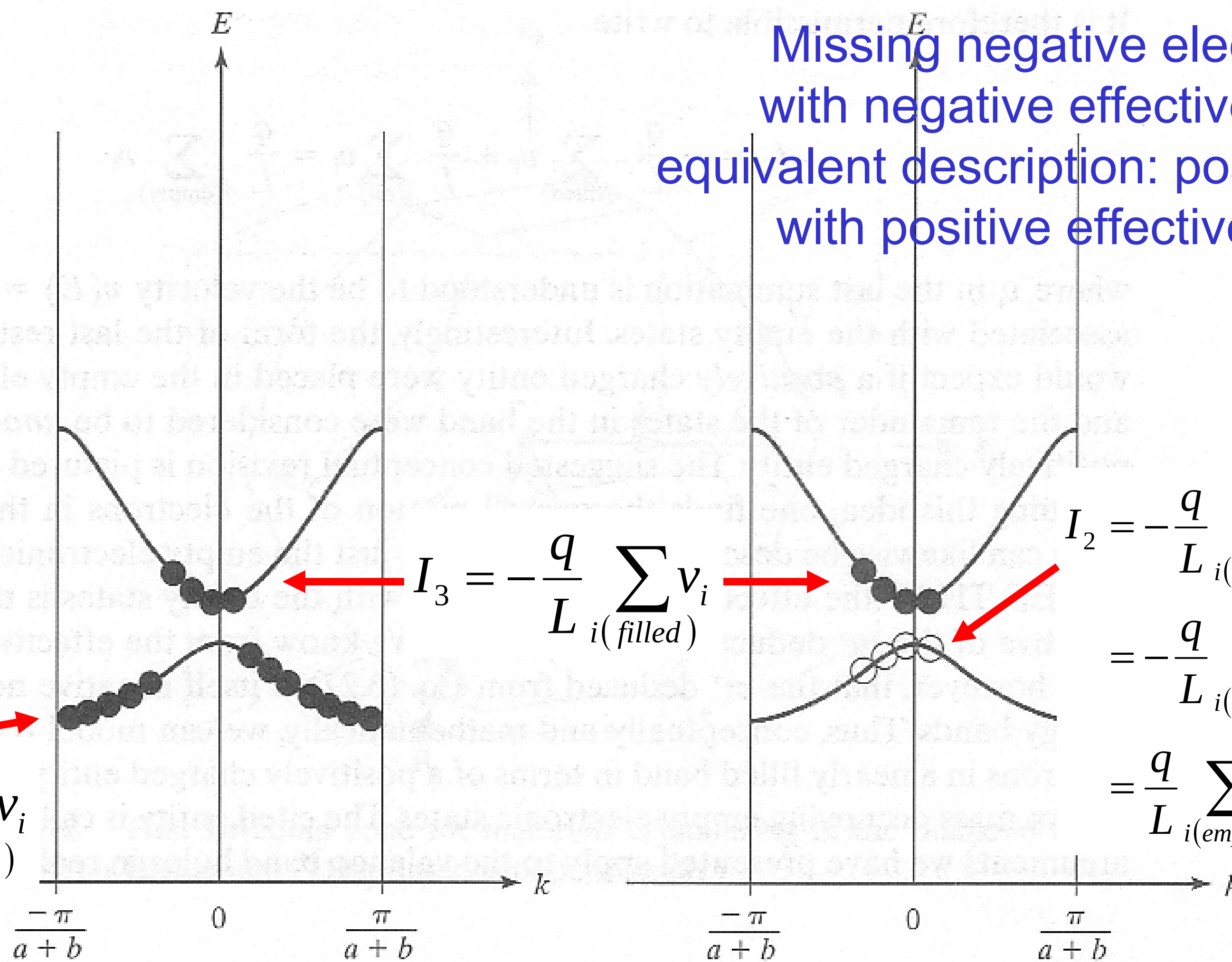
Full band: no current



Carriers and electrical current - 2

Two equivalent descriptions: holes!

Missing negative electrons,
with negative effective mass:
equivalent description: positive holes,
with positive effective mass



$$I_2 = -\frac{q}{L}\sum_{i(filled)} v_i$$

$$I_3 = -\frac{q}{L}\sum_{i(filled)} v_i$$

$$I_2 = -\frac{q}{L}\sum_{i(filled)} v_i = -\frac{q}{L}\sum_{i(filled)} v_i + \frac{q}{L}\sum_{i(all)} v_i = \frac{q}{L}\sum_{i(empty)} v_i$$

Extrapolation to 3-d

Brillouin zones

E-k diagrams

Constant-energy surfaces

Tensor effective mass

Brillouin zones in 2-d and 3-d

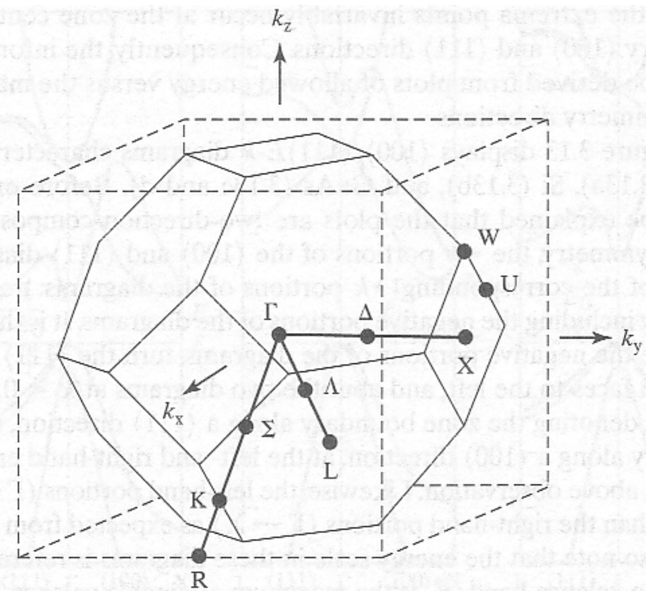


Figure 3.12 First Brillouin zone for materials crystallizing in the diamond and zincblende lattices. (After Blakemore.[1] Reprinted with permission.)

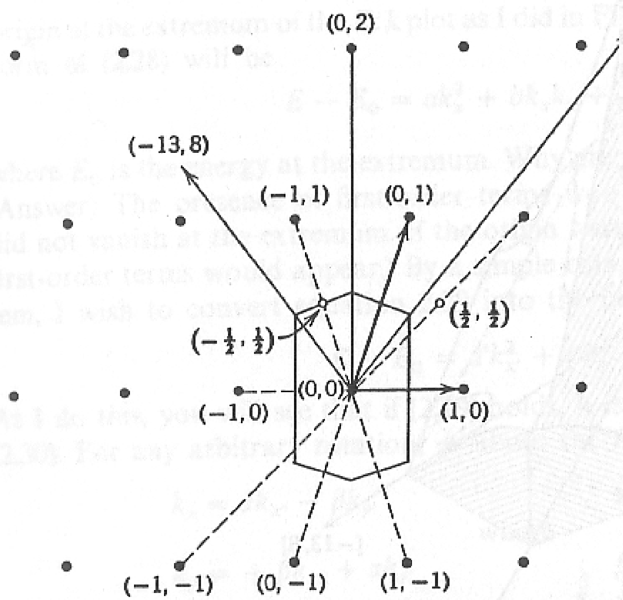
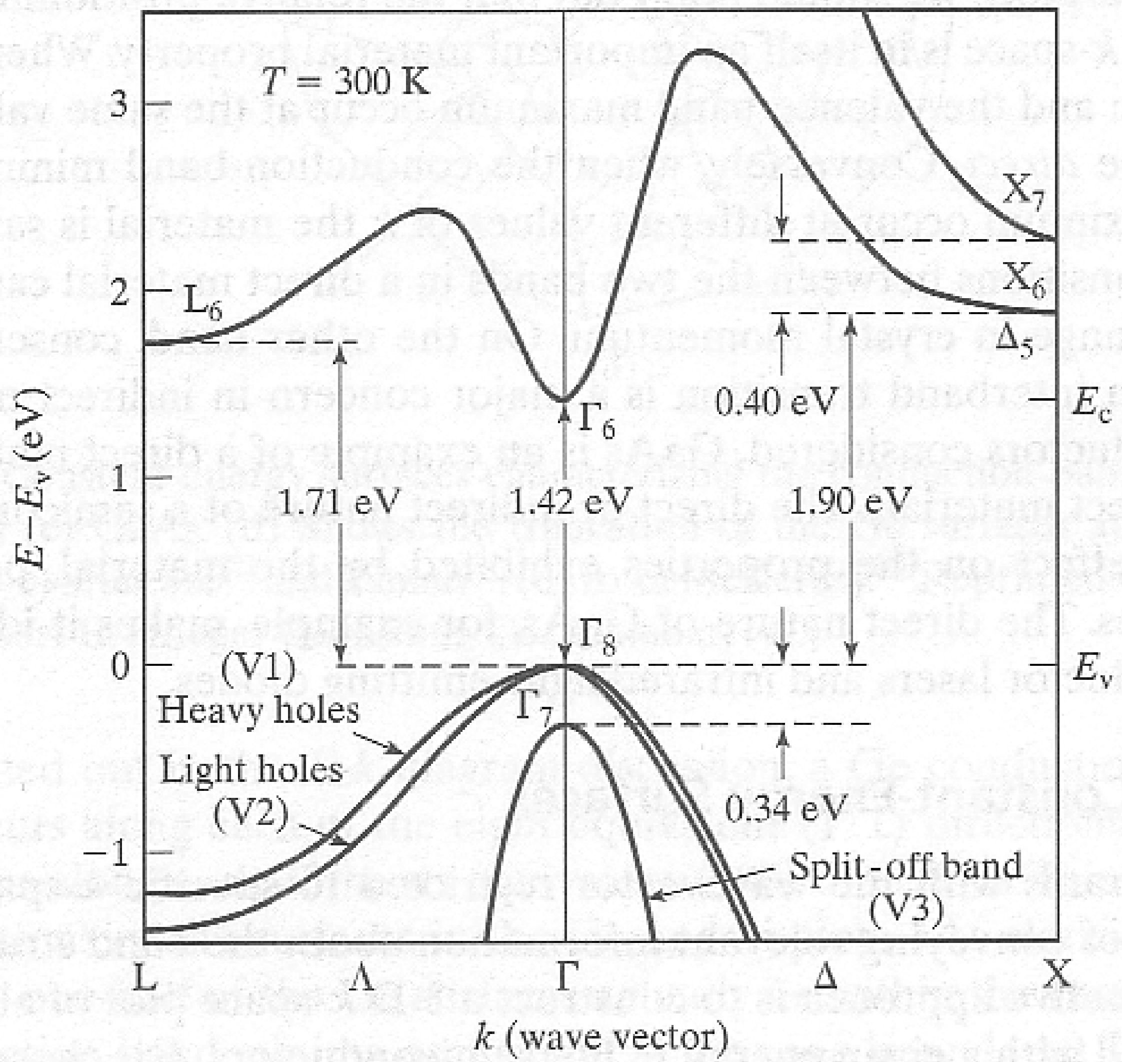
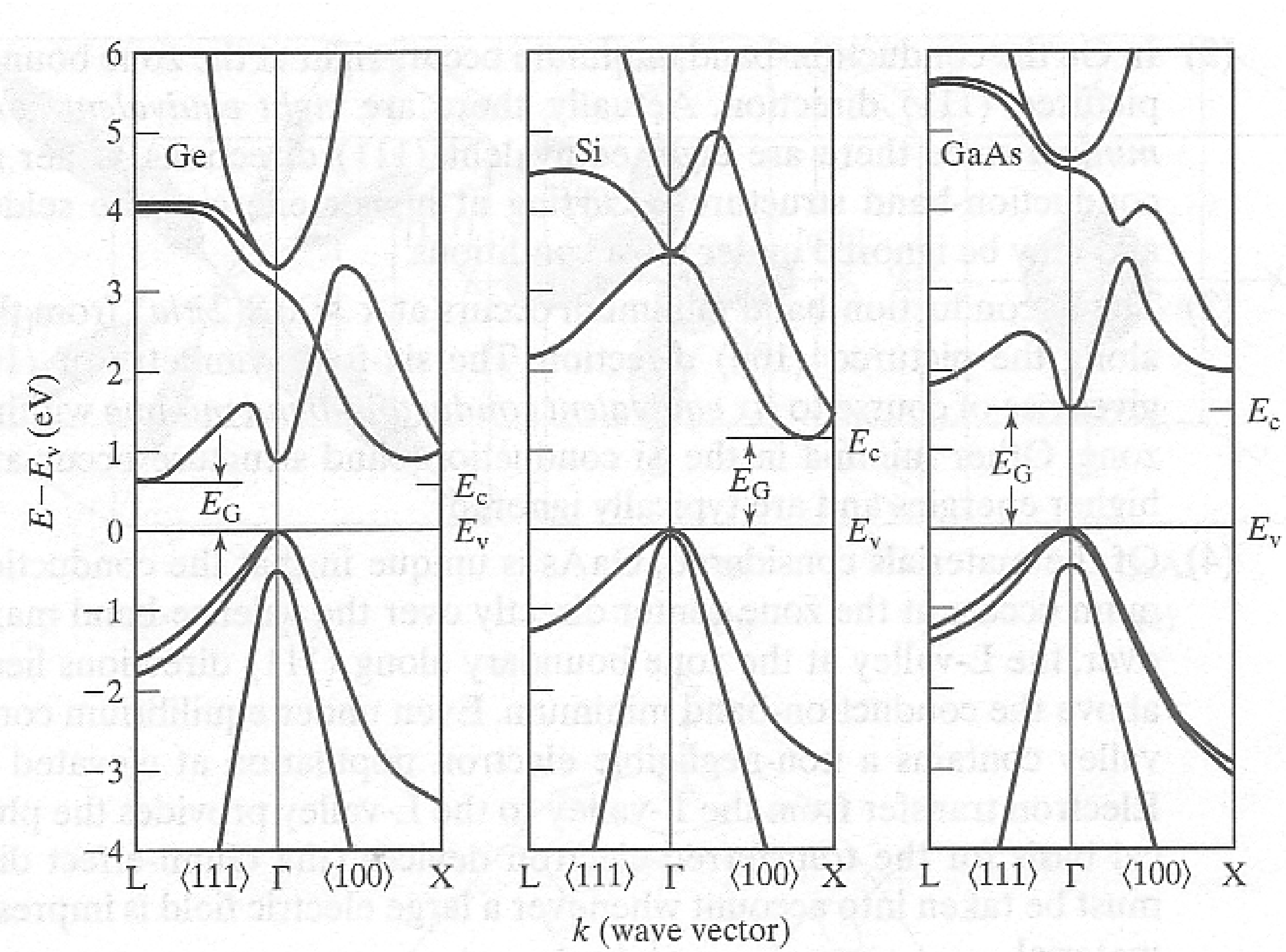


Figure 2.20 Construction of the first Brillouin zone for a general two-dimensional reciprocal lattice.

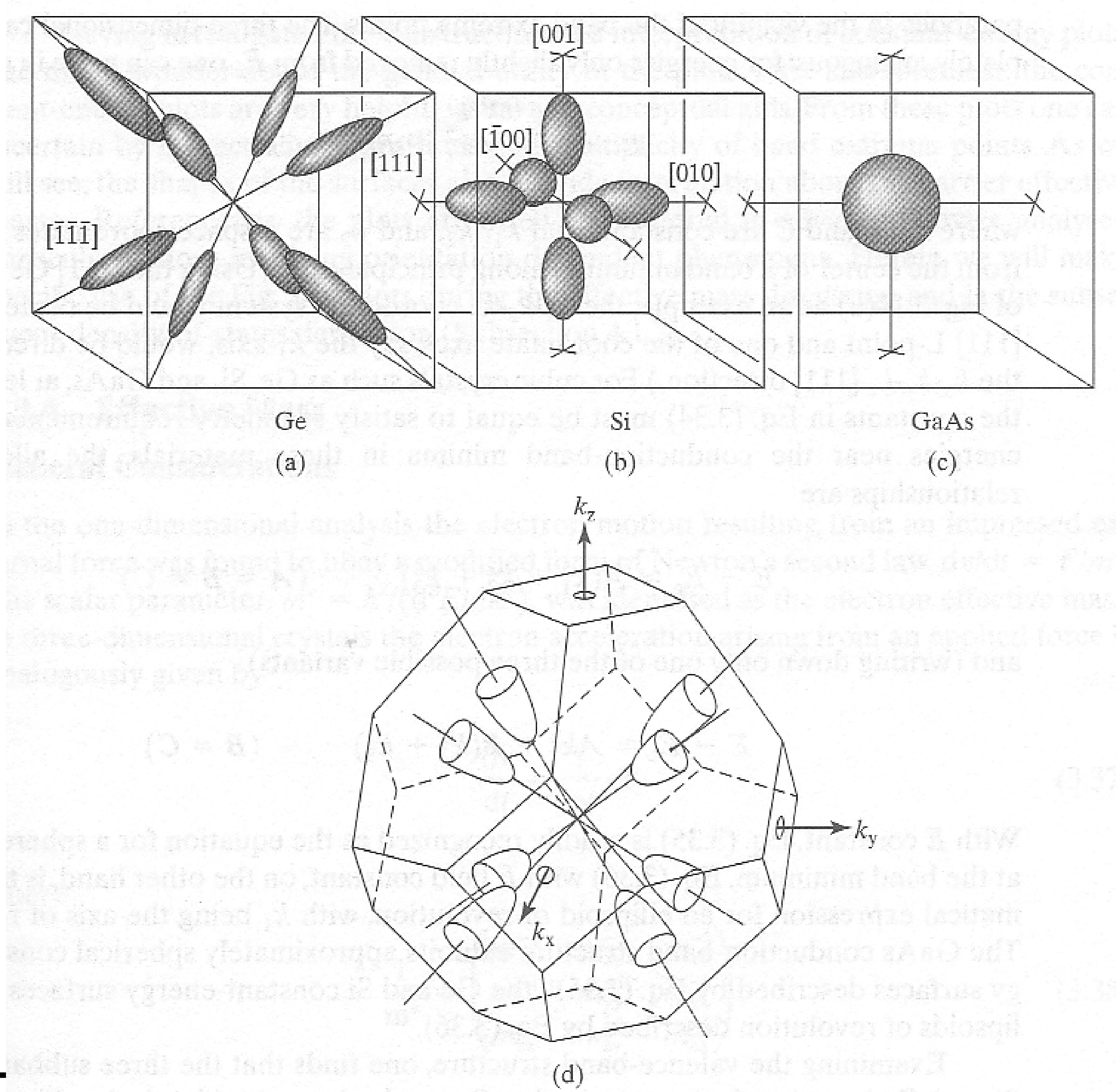
E-k diagrams - 1



E-k diagrams - 2



“Constant energy” surfaces



Tensor Effective Mass

In the one-dimensional analysis the electron motion resulting from an impressed external force was found to obey a modified form of Newton's second law, $dv/dt = F/m^*$. The scalar parameter, $m^* = \hbar^2/(d^2E/dk^2)$, was identified as the electron effective mass. In three-dimensional crystals the electron acceleration arising from an applied force is analogously given by

$$\frac{d\mathbf{v}}{dt} = \frac{1}{\mathbf{m}^*} \cdot \mathbf{F} \tag{3.37}$$

where

$$\frac{1}{\mathbf{m}^*} = \begin{pmatrix} m_{xx}^{-1} & m_{xy}^{-1} & m_{xz}^{-1} \\ m_{yx}^{-1} & m_{yy}^{-1} & m_{yz}^{-1} \\ m_{zx}^{-1} & m_{zy}^{-1} & m_{zz}^{-1} \end{pmatrix} \tag{3.38}$$

is the inverse effective mass tensor with components

$$\boxed{\frac{1}{m_{ij}} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} \qquad \ldots i,\ j = x,\ y,\ z} \tag{3.39}$$

An interesting consequence of the 3-D equation of motion is that the acceleration of a given electron and the applied force will not be colinear in direction as a general rule. For example, given a force pointing in the $+x$ direction, one obtains

$$\frac{d\mathbf{v}}{dt} = m_{xx}^{-1} F_x \mathbf{a}_x + m_{yx}^{-1} F_x \mathbf{a}_y + m_{zx}^{-1} F_x \mathbf{a}_z \tag{3.40}$$

with $\mathbf{a}_x$, $\mathbf{a}_y$, and $\mathbf{a}_z$ being unit vectors directed along the x, y, and z axes, respectively.

Some effective masses

Table 3.1 Electron and Hole Effective Masses in Ge,[6] Si,[7] and GaAs[1] at 4 K. (All values referenced to the free electron rest mass m_0.)

Effective Mass	Ge	Si	GaAs
m_ℓ^*/m_0	1.588	0.9163	—
m_t^*/m_0	0.08152	0.1905	—
m_e^*/m_0	—	—	0.067†
m_{hh}^*/m_0	0.347	0.537	0.51
$m_{\ell h}^*/m_0$	0.0429	0.153	0.082
m_{so}^*/m_0	0.077	0.234	0.154

† Band edge effective mass. The E-k relationship about the GaAs conduction-band minimum becomes non-parabolic and m_e^* increases at energies only slightly removed from E_c.

Energy gap values

Material	E_G (300 K)	E_G (0)	α	β
Ge	0.663	0.7437	4.774×10^{-4}	235
Si	1.125	1.170	4.730×10^{-4}	636
GaAs	1.422	1.519	5.405×10^{-4}	204

$$E_G(T) = E_G(0) - \frac{\alpha T^2}{(T+\beta)}$$

How do we know m*, E-k, E_G ?

- Accurate measurements of:
  - Cyclotron resonances $\Rightarrow$ effective mass
  - Photon absorption $\Rightarrow$ band gap
  - …
- Good theoretical computations
  - More complicated than the simple 1-d Kronig-Penney model
  - They must take into account the peculiarities of the atomic structure of different elements…
  - They match the data!
- A detailed discussion is beyond the scope of this course
  - Some references will be given for those who are interested to learn more on this.

Lecture 18 - summary

- The solutions of the Schrodinger equation for the simple Kronig-Penney model of a single electron moving in a periodic potential are characterized by the E-k relations, that have a reduced representation in the "1st Brillouin zone".
- The acceleration of a Bloch wave packet due to an external electric field is equivalento to that of a classical particle with an "effective mass" different from the free electron mass.
- The effective mass can be positive, negative; in general, it is a tensor quantity. It is useful in practice because it is approximately constant close to band edges, allowing a simplified semi-classical description of electron motion.
- A complete 3-d description requires a generalization of Brillouin zones, effective mass etc

Lecture 18 - exercises

- Exercise 18.1: Define in words what is meant by a “Brillouin zone”.
- Exercise 18.2: Briefly explain why the current associated with the motion of electrons in a totally filled energy band (a band in which all allowed states are occupied) is identically zero.
- Exercise 18.3: Compare the values of effective masses for electrons in Si that you found on textbooks or in the literature. Are they all equal? By how much do they differ? What may be the origin of the differences?
- Exercise 18.4: What is the value of the band gap E_G that you expect for si at T=500K ? (At 300K it is E_G = 1.125 eV). What may be the origin of the change with temperature?