The Quasi-Free Electron and Electron Effective Mass, m^*

ECE G201

(Partly adapted from Prof. Hopwood)

Quasi-Free Electron:

This is the **BIG** approximation in looking at electrons in crystals.

- What is a Quasi-Free Electron?
    - Under some conditions (often found in devices) electrons behave like free particles with an effective mass that is different than the mass in vacuum.
    - We want to understand this approximation.
    - We also want to understand when effects beyond this approximation occur in devices.

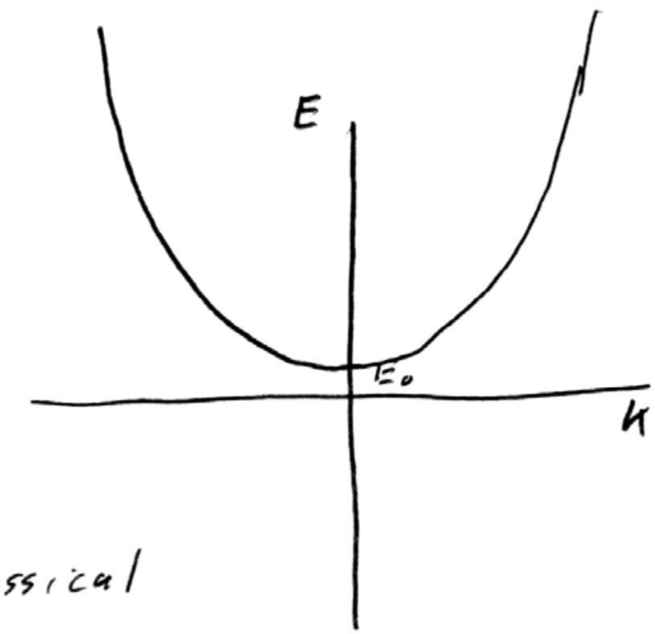
Copy!

Velocity associated with the center of mass of the particle is $V_g = \frac{dx}{dt} = \frac{1}{\hbar}\frac{dE}{dk}$

Schrodinger equation: for free particle $\frac{d^2\Psi(x)}{dx^2} + \frac{2m_0}{\hbar^2}(E-E_0)\Psi(x) = 0$

$$k \equiv \sqrt{\frac{2m_0}{\hbar^2}(E-E_0)}$$

$$E = \frac{k^2\hbar^2}{2m_0} + E_0$$



$$V_g = \frac{1}{\hbar}\frac{dE}{dk} = \frac{\hbar k}{m_0}$$

$p \leftrightarrow \hbar k$

momentum

$p = mV$

$\frac{p}{m} = V$

} classical

Copy!

$p \leftrightarrow \hbar k$

momentum

$$\left.\begin{aligned} p &= mV \\ \frac{p}{m} &= V \end{aligned}\right\} \text{classical}$$

$$\left. E = \frac{p^2}{2m} + E_0 \right\} \text{classical}$$

↑ kinetic ↑ potential

$$\left. E = \frac{\hbar^2 k^2}{2m_0} + E_0 \right\} \text{quantum}$$

$$p = \hbar k$$

$$p = \frac{h}{\lambda}$$

$$\lambda = \frac{h}{p}$$

De Broglie Relationship!

$$E = \frac{\hbar^2 k^2}{2m_0} + E_0$$

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m_0}$$

$$\boxed{m_0 = \hbar^2 \left(\frac{d^2E}{dk^2}\right)^{-1}}$$

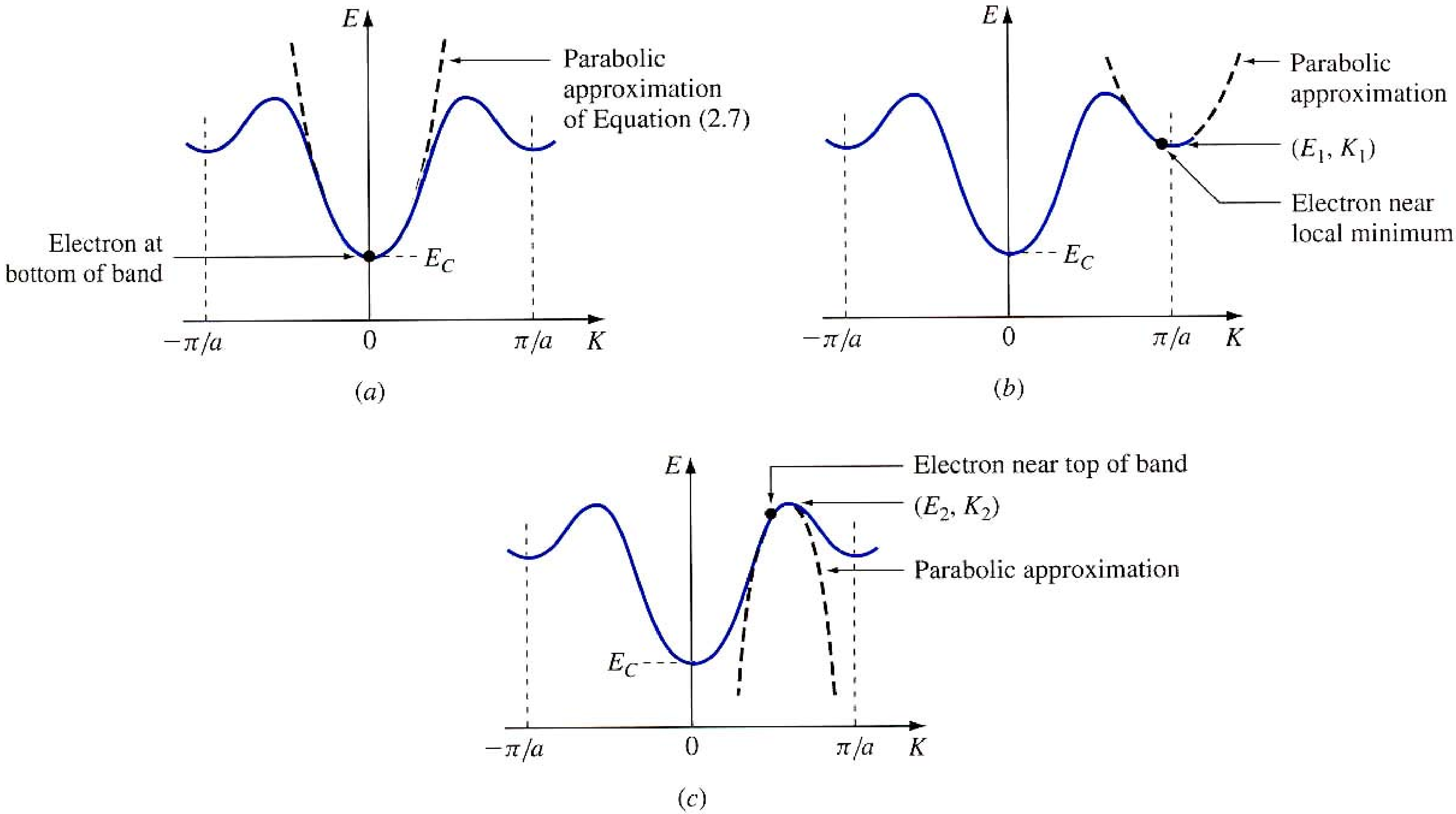


Figure 2.1 The *E*-*K* diagram for (a) an electron at the bottom of the conduction band at $K = 0$, where the velocity and kinetic energy are both zero and thus the total energy is equal to the potential energy; (b) an electron in a local minimum, where it has a different effective mass, and (c) an electron near the top of the band.

Goal: show that an electron behaves like a particle with mass $m^* = \hbar^2(d^2E/dK^2)^{-1}$

- Recall that the electron energy is related to the frequency of the electron wave

  $E = \hbar\omega$

- and the group velocity of the wave is the velocity of the electron

  $v_g = d\omega/dK = 1/\hbar \; dE/dK$ (as in text)

- The *acceleration* of a particle is given by the time-derivative of its velocity:

$$a = dv_g/dt = {}^{d}/_{dt}({}^{d\omega}/_{dK})$$
$$= {}^{d}/_{dK}({}^{d\omega}/_{dK}){}^{dK}/_{dt}$$
$$= (1/\hbar^2)\,{}^{d}/_{dK}({}^{d\hbar\omega}/_{dK})({}^{d\,(\hbar K)}/_{dt})$$
$$= (1/\hbar^2)\,(d^2E/dK^2)({}^{d\,(\hbar K)}/_{dt})$$

This is the term we are looking to show is:

$$(1/\hbar^2)\,(d^2E/dK^2) = 1/m^*$$

What is ${}^{d\,(\hbar K)}/_{dt}$?

If we apply an external force on the electron, for example an electric field ($F_{ext}=q\mathcal{E}$), then we will do work on the electron:

$$dW_e = F_{ext}dx = F_{ext}(v_g dt) \quad \ldots\text{since } v_g = dx/dt$$

$$= F_{ext}({}^{d\omega}/_{dK})dt$$

Doing work on the electron increases its energy

$dW_e = F_{ext}({}^{d\omega}/_{dK})dt = dE$

$= (dE/dK)dK$

$= [d(\hbar\omega)/dK]dK$

$= \hbar\ ({}^{d\omega}/_{dK})dK$

therefore: $F_{ext}dt = \hbar dK$

or $F_{ext} = {}^{d\,(\hbar K)}/_{dt}$

note: since $F=d(mv)/dt$,

$\hbar K$ is called the "crystal momentum"

Finally…

$a = (1/\hbar^2)\,(d^2E/dK^2)(^{d\,(\hbar K)}/_{dt})$

and

$F_{ext} = {}^{d(\hbar K)}/_{dt}$

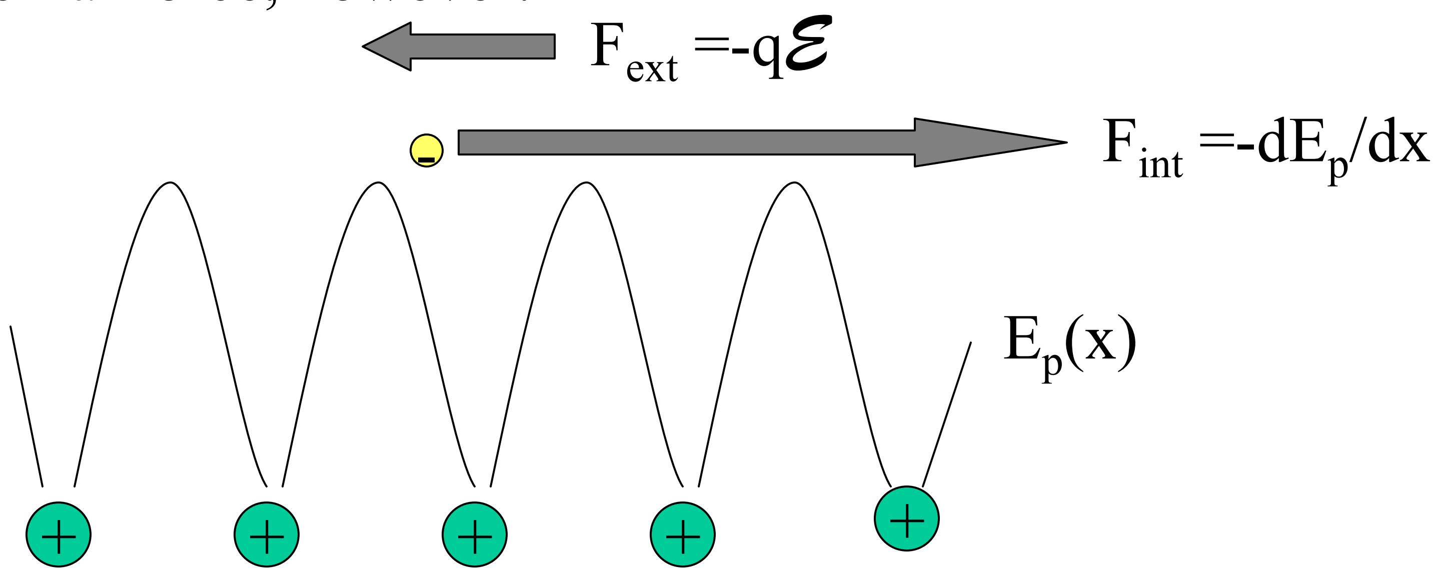
gives us

$a = (1/m^*)F_{ext}$ or $F_{ext} = m^*a$

Where $m^* = [(1/\hbar^2)\,(d^2E/dK^2)]^{-1} = \hbar^2\,(d^2E/dK^2)^{-1}$

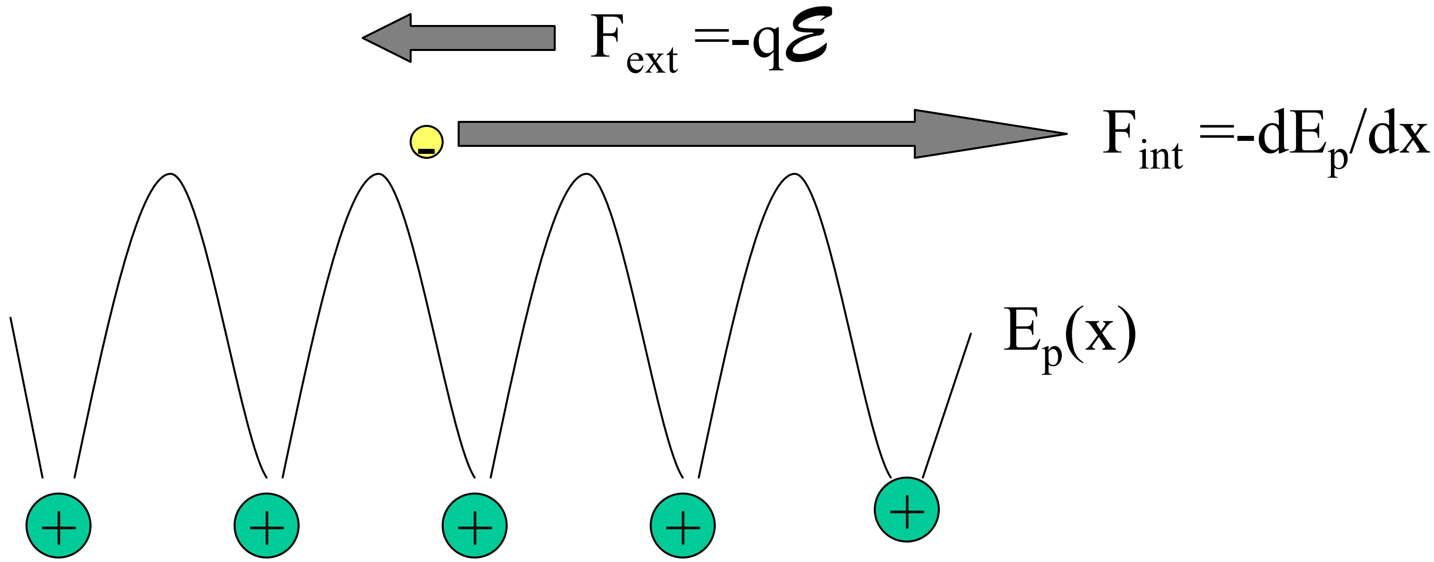
Interpretation

- The electron is subject to internal forces from the lattice (ions and core electrons) AND external forces such as electric fields
- In a crystal lattice, the net force may be opposite the external force, however:



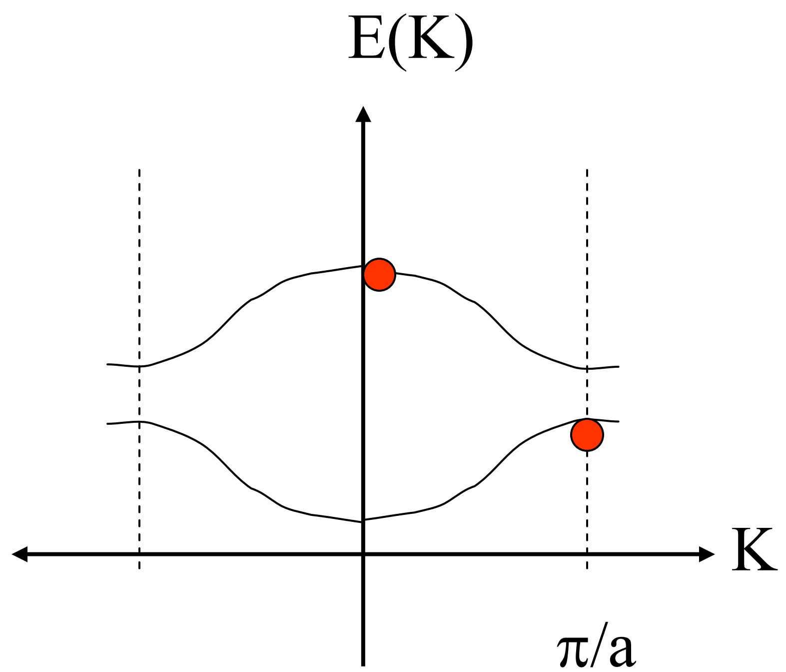
Interpretation

- electron acceleration is not equal to F_{ext}/m_e, but rather…
- $a = (F_{ext} + F_{int})/m_e == F_{ext}/m^*$
- The dispersion relation E(K) compensates for the internal forces due to the crystal and allows us to use *classical* concepts for the electron as long as its mass is taken as m^*



The Hole

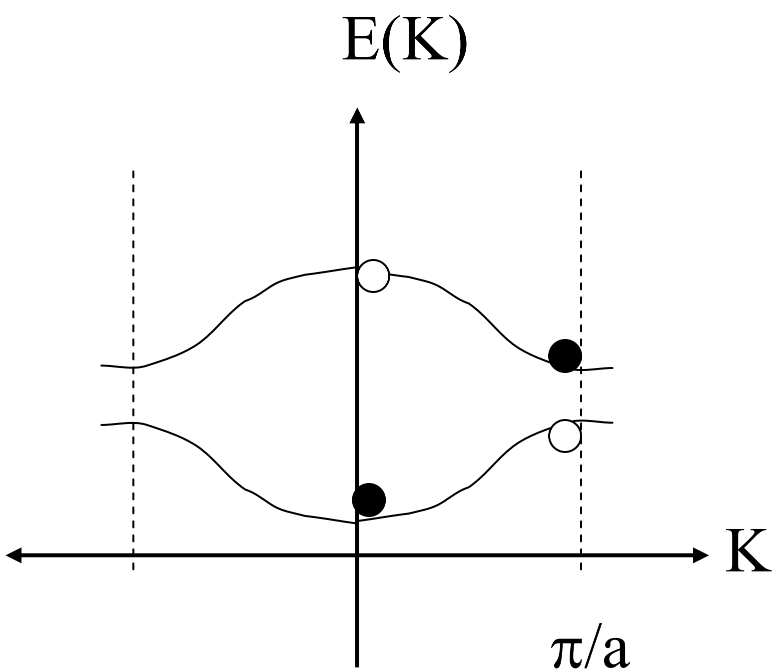
- The hole can be understood as an electron with negative effective mass
- An electron near the top of an energy band will have a negative effective mass
- A negatively charged particle with a negative mass will be <u>accelerated</u> like a positive particle with a positive mass (a hole!)

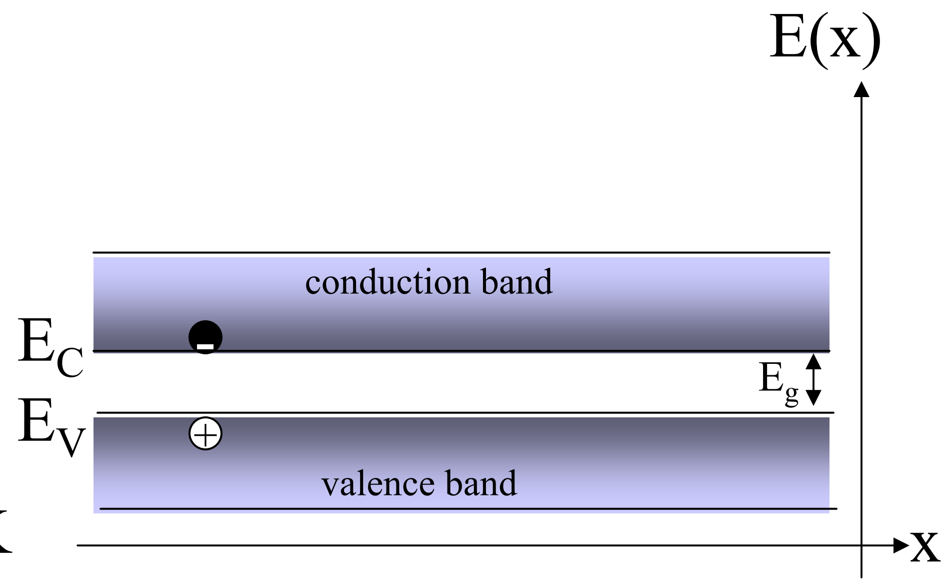


$$F = m^* a = Q\mathcal{E}$$

Without the crystal lattice, the hole cannot exist. It is an artifact of the periodic potential (E_p) created by the crystal.

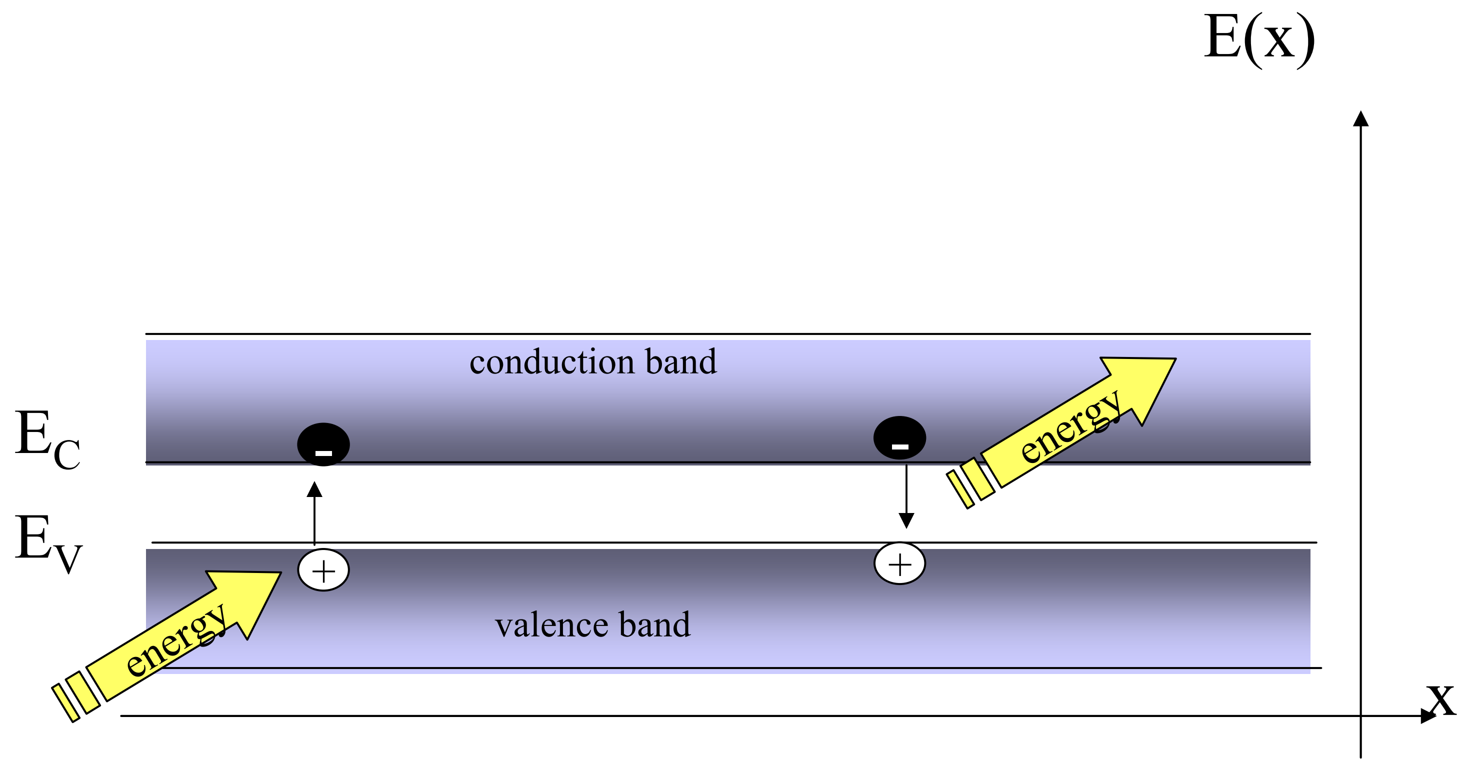
E(K) and E(x)

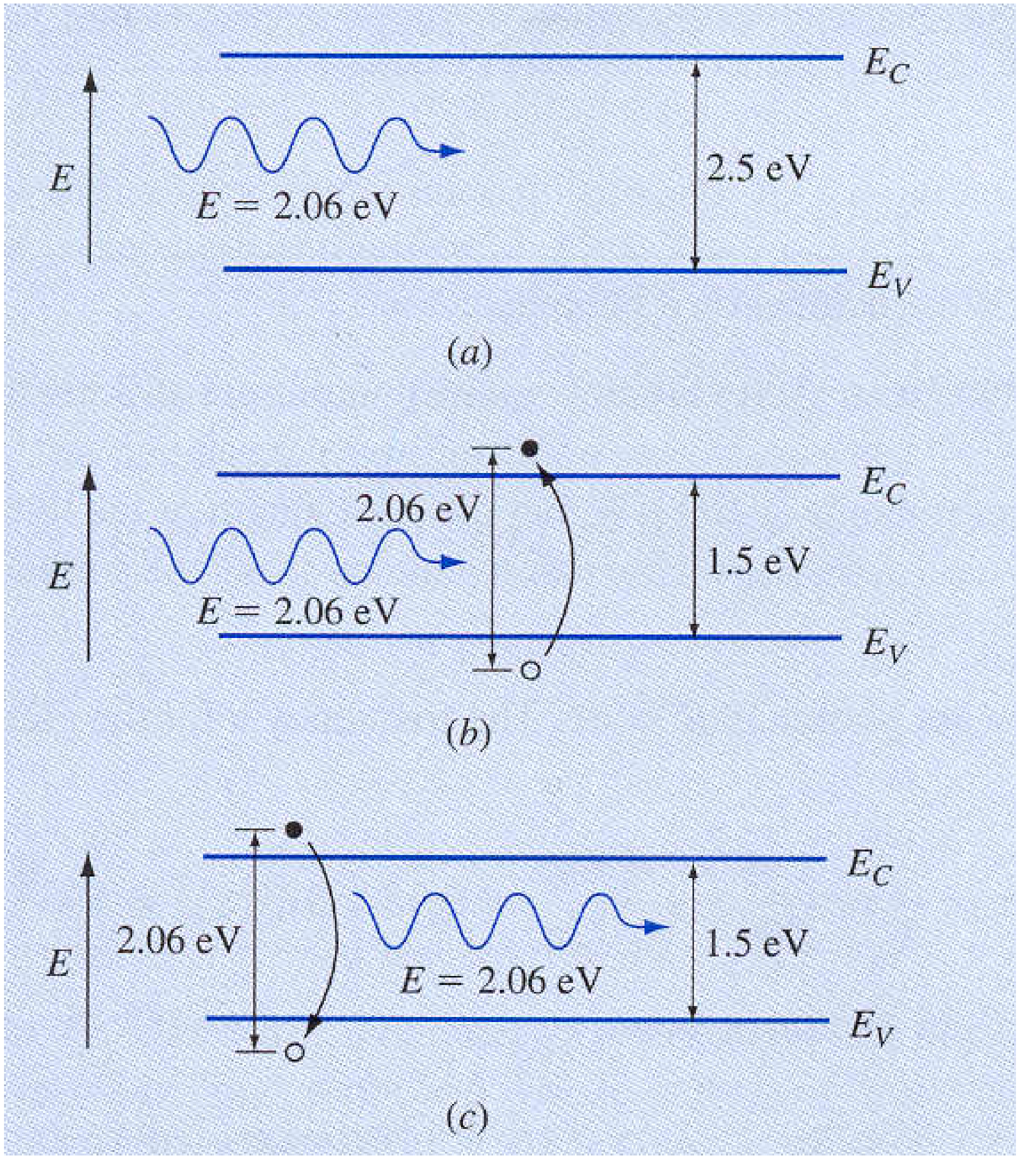




Generation and Recombination

of electron-hole pairs

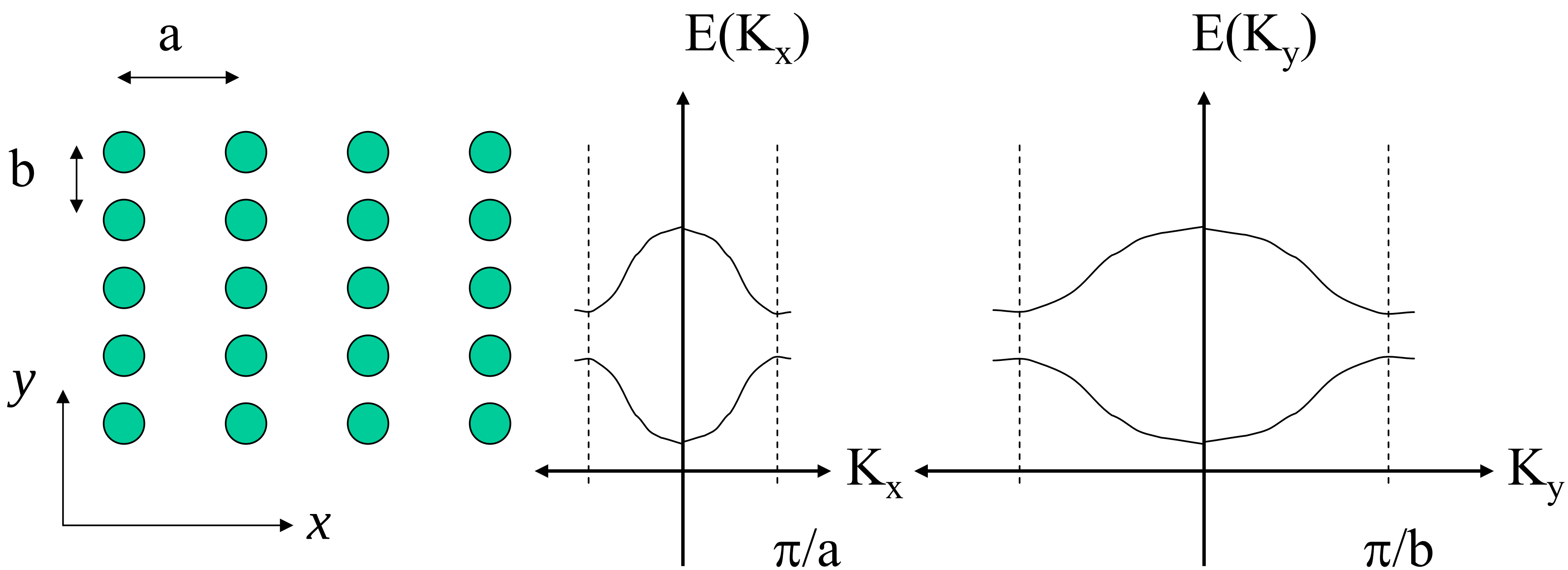




$$E(\text{eV})\lambda(\mu\text{m}) = 1.24 \qquad \text{Golden Rule} \tag{1.74}$$

Non-cubic lattices:

(FCC, BCC, diamond, etc.)



Different lattice spacings lead to different curvatures for E(K) and <u>effective masses</u> that depend on the direction of motion.

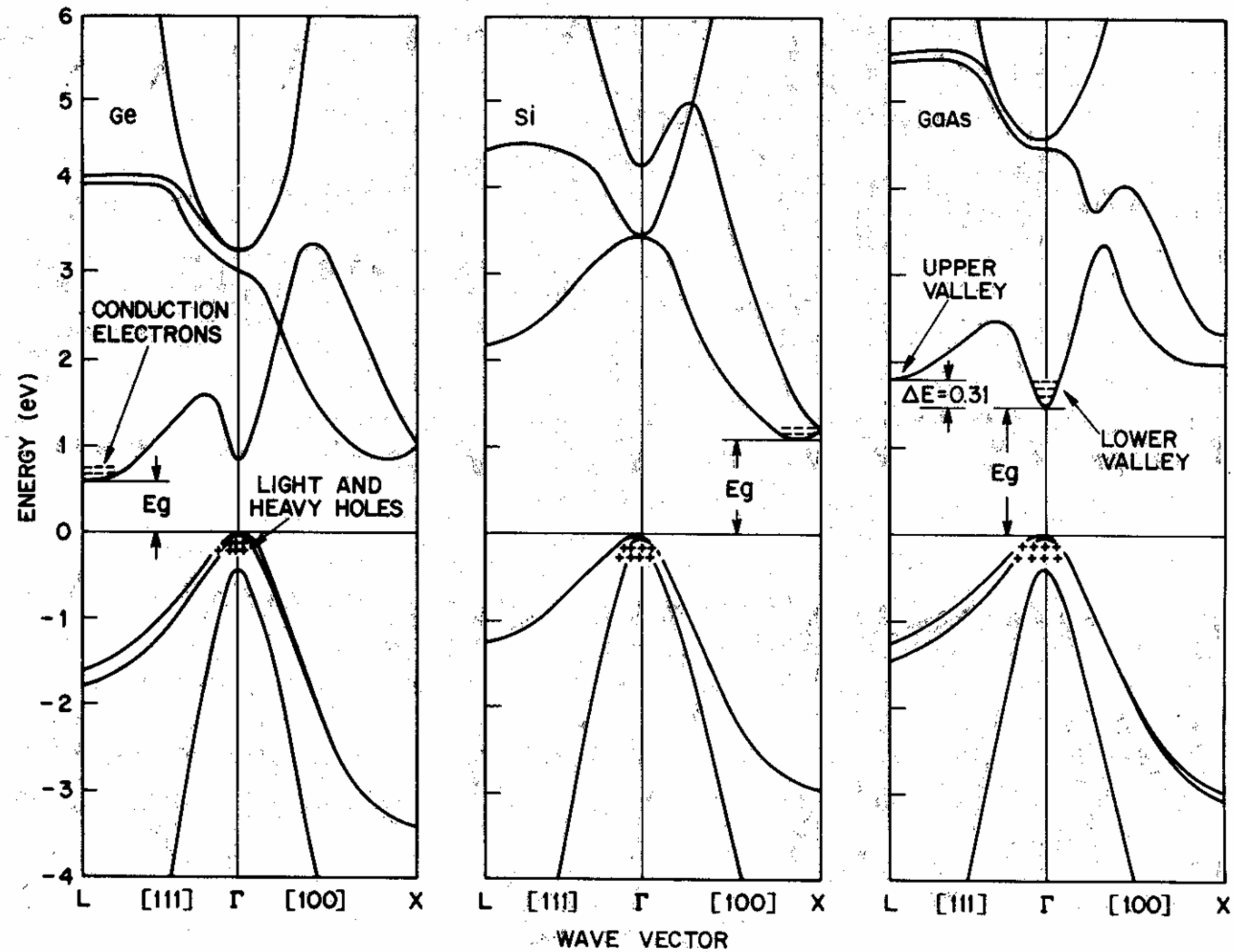
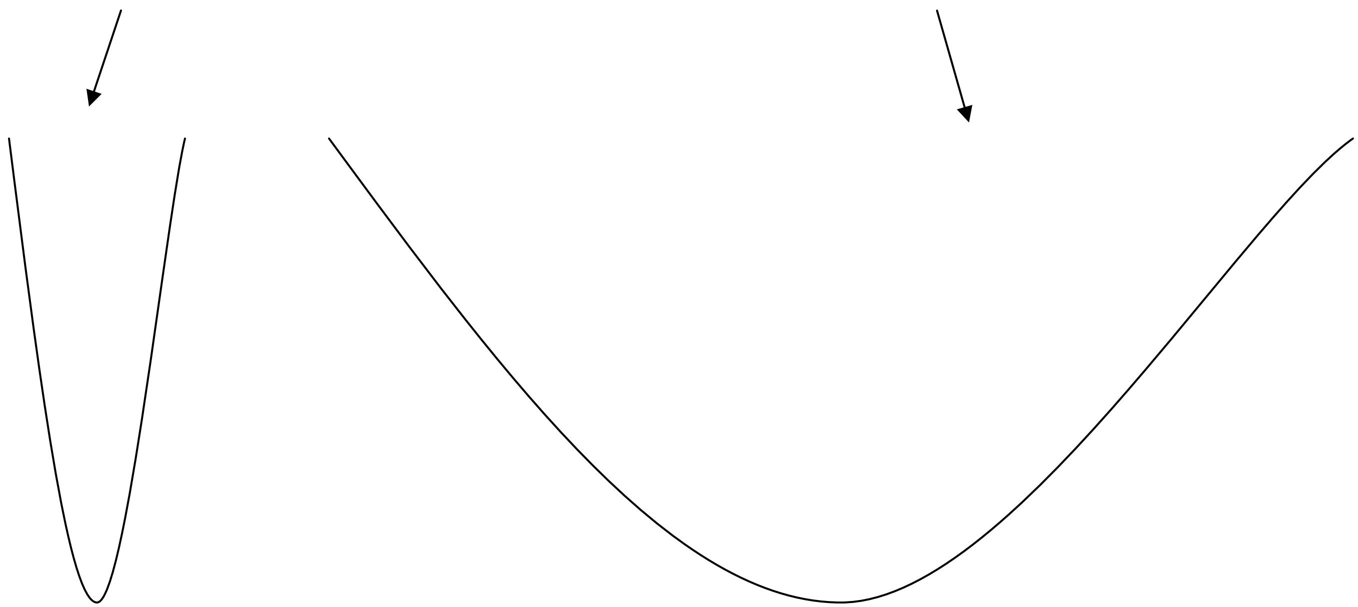


Fig. 5 Energy-band structures of Ge, Si, and GaAs, where E_g is the energy bandgap. Plus (+) signs indicate holes in the valence bands and minus (−) signs indicate electrons in the conduction bands. (After Chelikowsky and Cohen, Ref. 17.)

(from S.M. Sze, 1981)

Memory Aid

"a hairpin is lighter than a frying pan"



light m^*
(larger d^2E/dK^2)

heavy m^*
(smaller d^2E/dK^2)

Notes on E(K)

- The extrema for the conduction and valence bands are at different values of K for silicon and germanium
  - these are called *indirect* bandgap semiconductors
- The conduction band minimum and valence band maximum both occur at K=0 for GaAs
  - this is called a *direct* bandgap semiconductor

Light Emission

- energy (E) and momentum (ħK) must be conserved
- energy is released when a quasi-free electron recombines with a hole in the valence band:

$$\Delta E = E_g$$

  - does this energy produce light (photon) or heat (phonon)?
- indirect bandgap: ΔK is large
  - but for a direct bandgap: $\Delta K=0$
- photons have very low momentum
  - but lattice vibrations (heat, phonons) have large momentum
- Conclusion: recombination (e^-+h^+) creates
  - *light* in direct bandgap materials (GaAs, GaN, etc)
  - *heat* in indirect bandgap materials (Si, Ge)