FYS3410 - Vår 2016 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/v16/index.html

Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17, 18, 20)

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2016 FYS3410 Lectures (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17,18,20)

Module I – Periodic Structures and Defects (Chapters 1-3, 20)

M18/1: 9-12 am	**Introduction. Crystal bonding. Periodicity and lattices, Brag diffraction and Laue condition, reciprocal space**	**3h**
W20/1 cancelled		
M25/1: 9-12 am	**Ewald construction, interpretation of a diffraction experiment , Brag planes, and Brillouin zones**	**3h**
W27/1 cancelled		
M01/2: 10-12 am	**Elastic strain and structural defects in crystals**	**2h**
W03/2: 9-10 am	**Atomic diffusion in solids**	**1h**
M08/2: 10-12 am	**Summary of Module I**	**2h**

Module II – Phonons (Chapters 4 and 5)

W10/2: 9-10 am	**Vibrations in monoatomic and diatomic chains of atoms**	**1h**
M15/2: 10-12am	**Periodic boundary conditions, phonons and density of states (DOS)**	**2h**
W17/2: 9-10 am	**Planck distribution**	**1h**
M22/2 : 10-12am	**Lattice heat capacity: Dulong-Petit, Einstein, and Debye models**	**2h**
W24/2 cancelled		
M29/2: 9-12am	**Comparison of different models for lattice heat capacity, thermal conductivity with phonons**	**3h**
W02/3: 9-10 am	**Thermal expansion**	**1h**
M07/3: 10-12am	**Summary of Module II.**	**2h**

Module III – Electrons (Chapters 6, 7, 18 - pp.528-530, and Appendix D)

W09/3: 9-10 am	**Free electron gas (FEG) versus free electron Fermi gas (FEFG)**	**1h**
M14/3: 10-12am	**DOS of FEFG in 3D. Effect of temperature – Fermi-Dirac distribution**	**2h**
W16/3: 9-10 am	**Heat capacity of FEFG in 3D**	**1h**
W30/3: 9-10 am	**DOS in 2D - quantum wells**	**1h**
M04/4: 10-12am	**DOS in 1D and 0D, i.e. quantum wires and quantum dots; transport properties of electrons**	**2h**
W06/4: 9-10 am	**Origin of the energy band gap**	
M11/4: 10-12am	**Nearly free electron model. Kronig-Penney model. Empty lattice approximation.**	**2h**
W13/4: 9-10 am	**Number of orbitals in a band**	**1h**
M18/4: 10-12am	**Summary of Module III.**	**2h**

Module IV – Semiconductors and interfaces (Chapters 8, 9-pp 223-231, 17)

W20/4: 9-10 am	**Metals versus semiconductors. Surfaces and interfaces.**	**1h**
M25/4: 9-12 am	**Effective mass method.**	**3h**
W27/4: 9-10 am	**Intrinsic carrier generation – elctrons and holes.**	**1h**
M02/5: 9-12 am	**Localized levels for hydrogen-like impurities – donors and acceptors. Doping.**	**3h**
W04/5: 9-10 am	**Carrier statistics in semiconductors**	**1h**
M09/5: 9-12 am	**p-n junctions**	**3h**
W11/5: 9-10 am	**Optoelectronic semiconductor properties and devices**	**1h**
M18/5: 9-12 am	**Device demonstrations. Summary of Module IV**	**3h**

Repetition

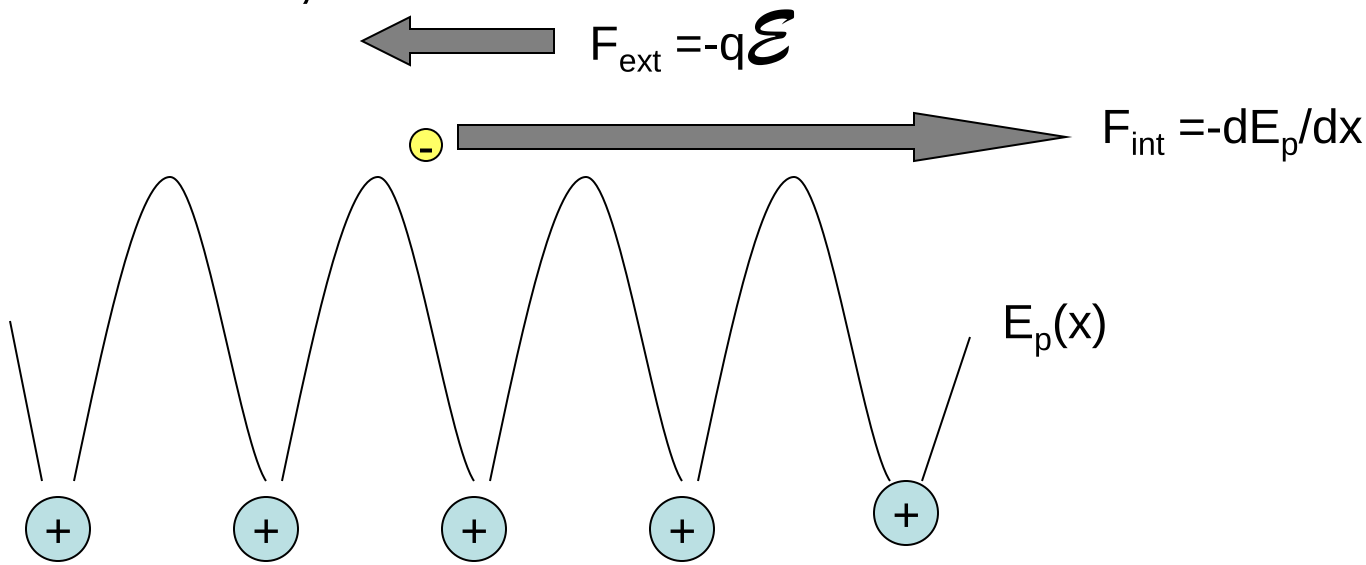
M23/5 9-12 am	**The course in a nutshell**	**2h**
W25/5, M30/5 and W1/6 cancelled		

Exam during week 22 (tentatively 30-31/5)

Lecture 18: Effective mass

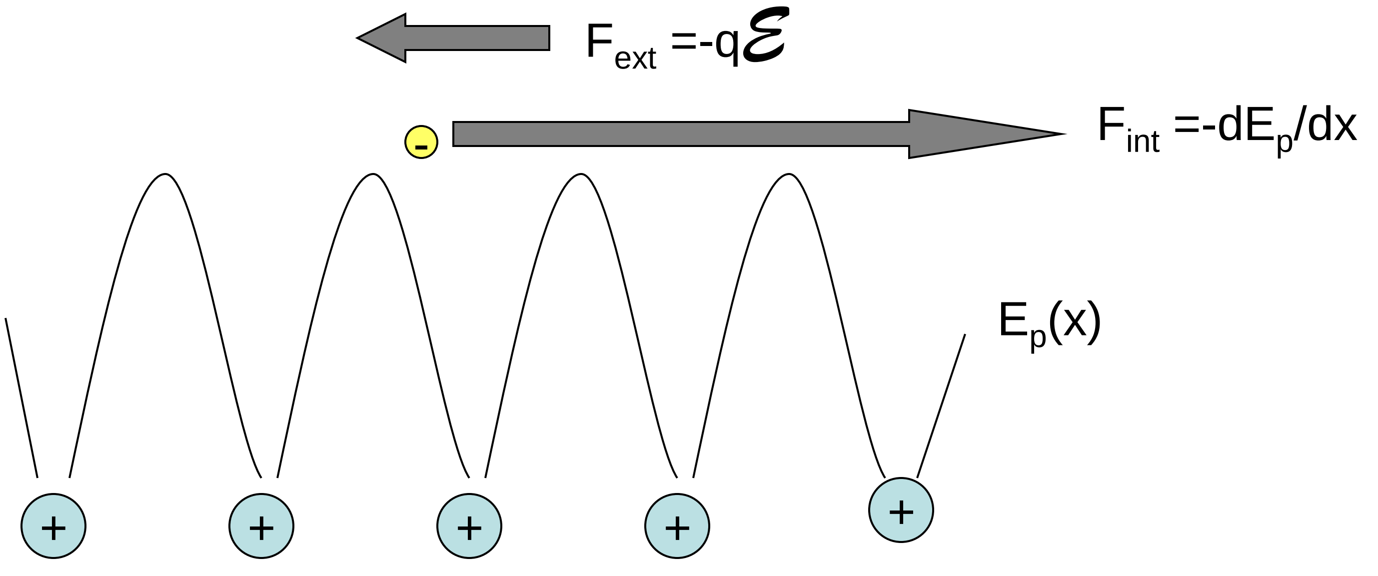
Internal and external forces affecting an electron in crystal

- 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:



Internal and external forces affecting an electron in crystal

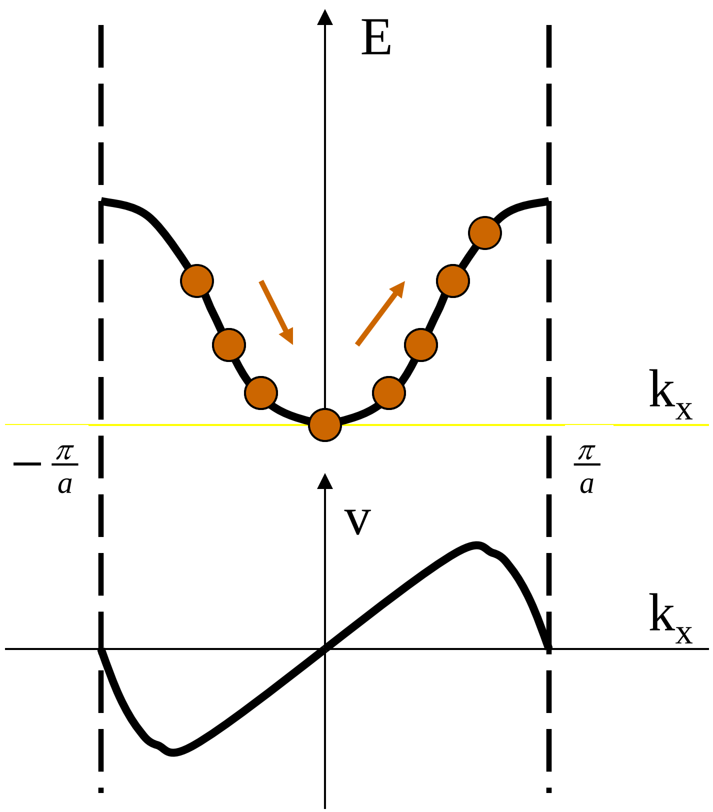
- electron acceleration is not equal to F_{ext}/m_e, but rather…
- $a = (F_{ext} + F_{int})/m_e == F_{ext}/m^*$
- The dispersion relation E(K) compensates for the internal forces due to the crystal and allows us to use *classical* concepts for the electron as long as its mass is taken as m^*



Dynamics of electrons in a band

The external electric field causes a change in the k vectors of all electrons:

$$\vec{F} = \hbar \frac{d\vec{k}}{dt} = -e\vec{E} \longrightarrow \frac{d\vec{k}}{dt} = \frac{-e\vec{E}}{\hbar}$$

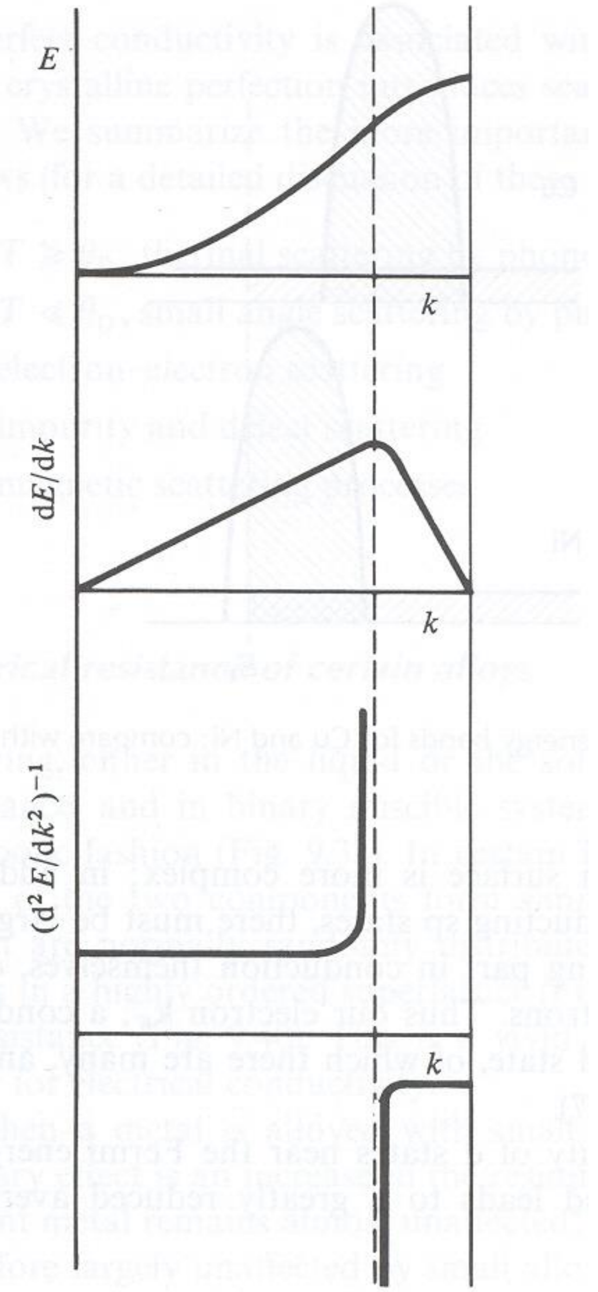


If the electrons are in a partially filled band, this will break the symmetry of electron states in the 1st BZ and produce a net current. But if they are in a filled band, even though all electrons change k vectors, the symmetry remains, so J = 0.

When an electron reaches the 1st BZ edge (at k = π/a) it immediately reappears at the opposite edge (k = -π/a) and continues to increase its k value.

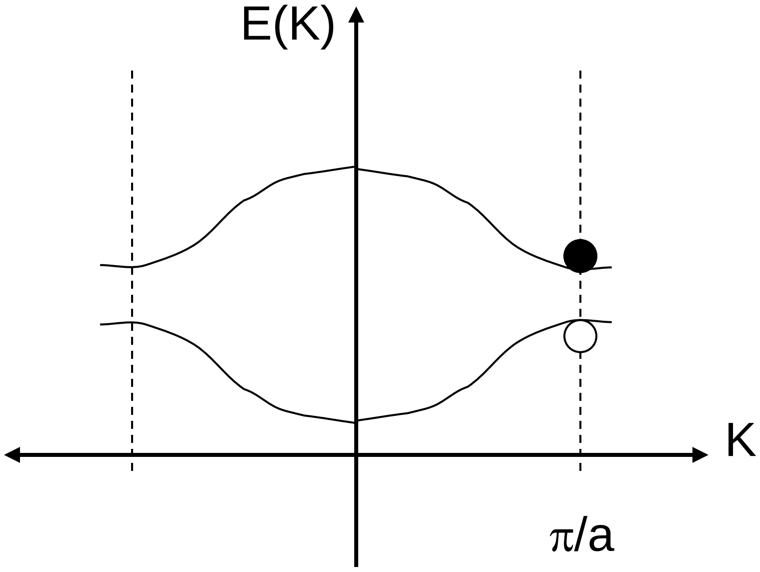
As an electron's k value increases, its velocity increases, then decreases to zero and then becomes negative when it re-emerges at k = -π/a!!

Dynamics of electrons in a band



Hole - an electron near the top of an energy band

- 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!)

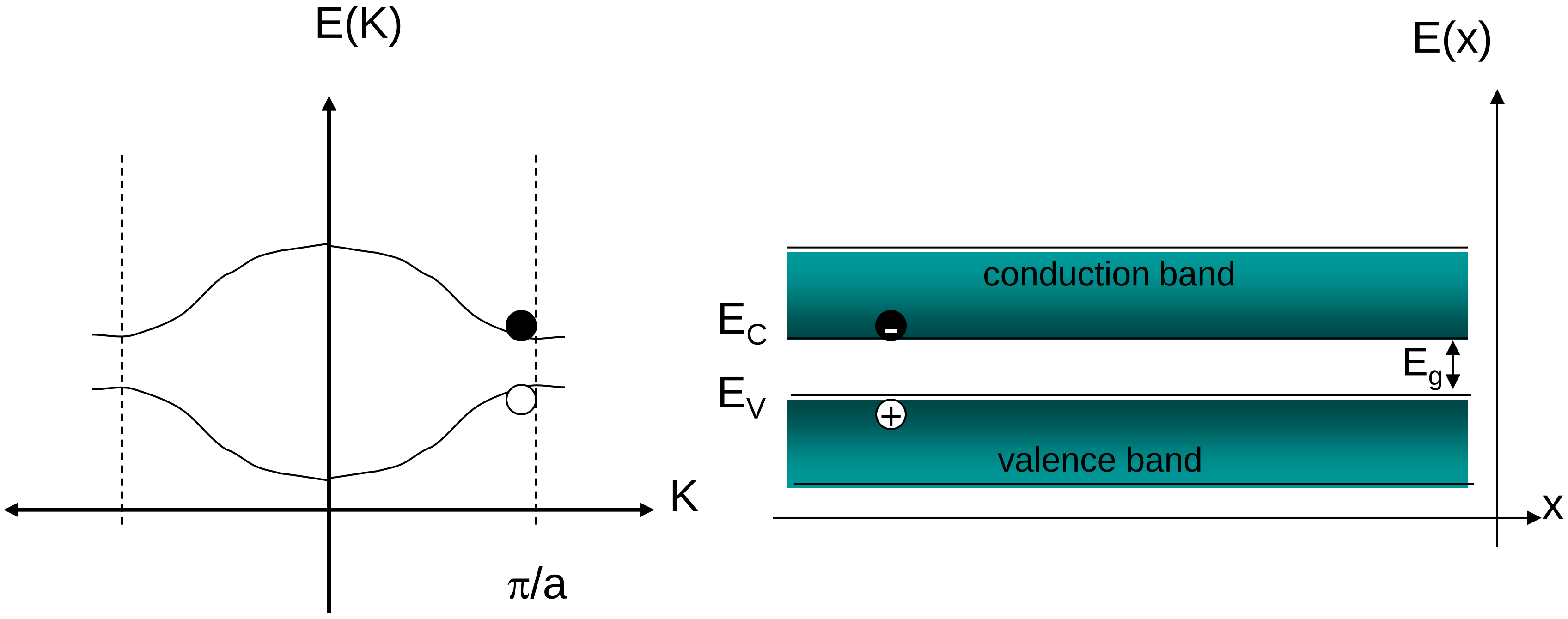


$F = m^{*}a = Q\mathcal{E}$

Without the crystal lattice, the hole would not exist!

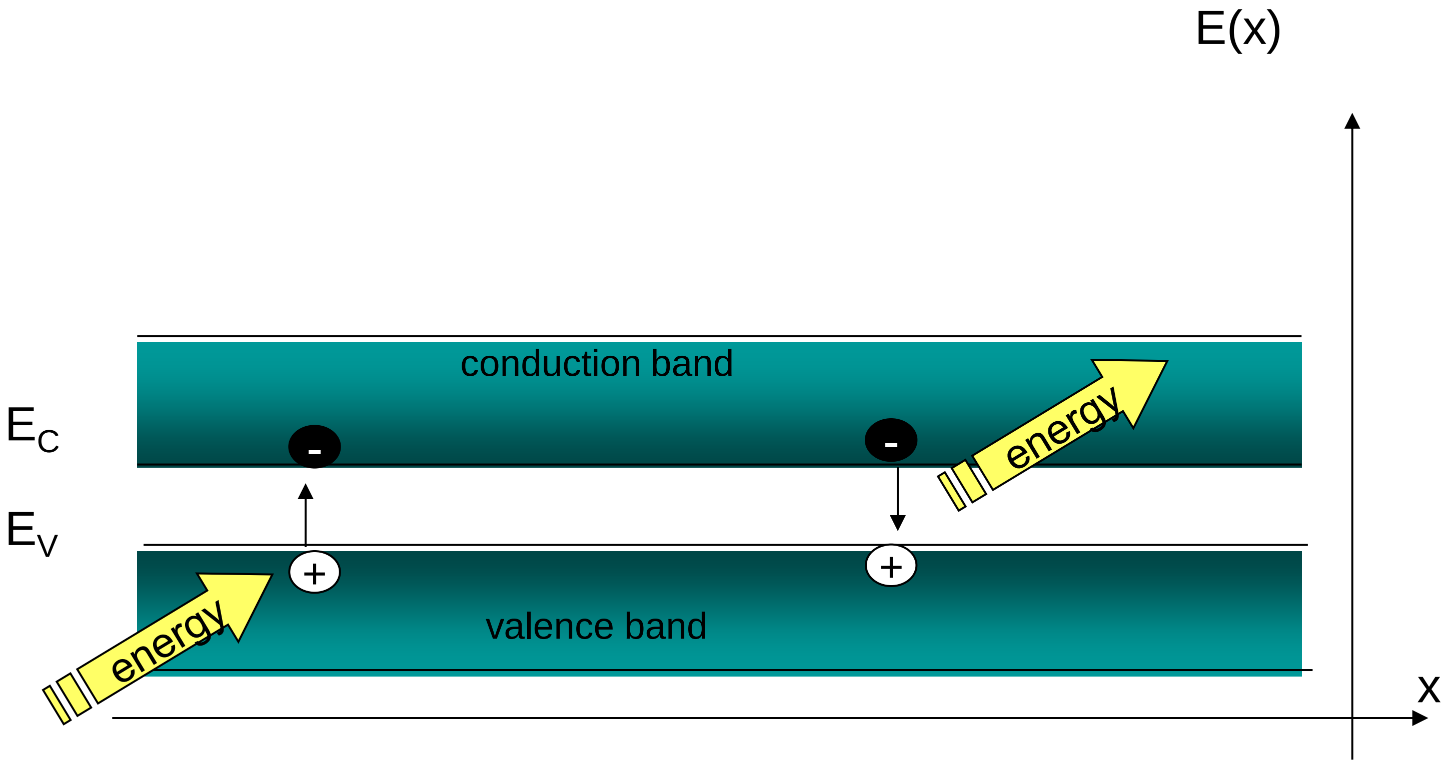
The hole is a pure consequence of the periodic potential operating in the crystal!!!

E(K) and E(x)

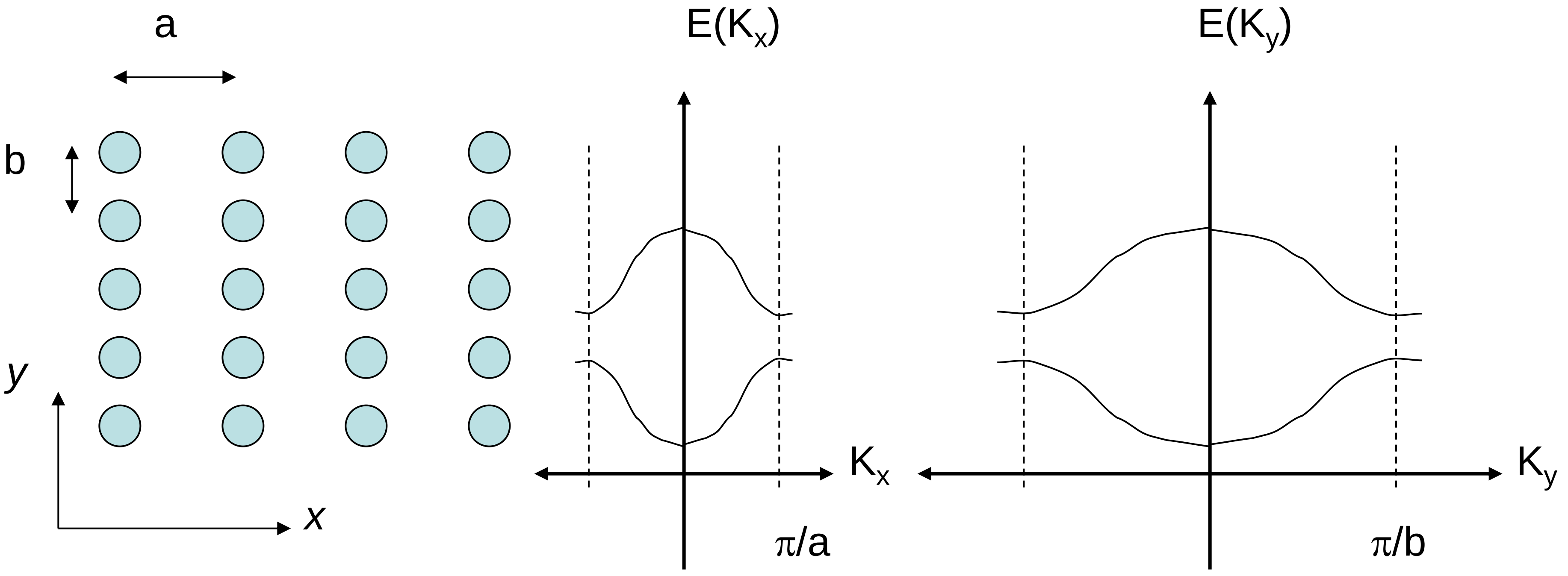


Generation and Recombination

of electron-hole pairs



Real 3D lattices, e.g. FCC, BCC, diamond, etc.



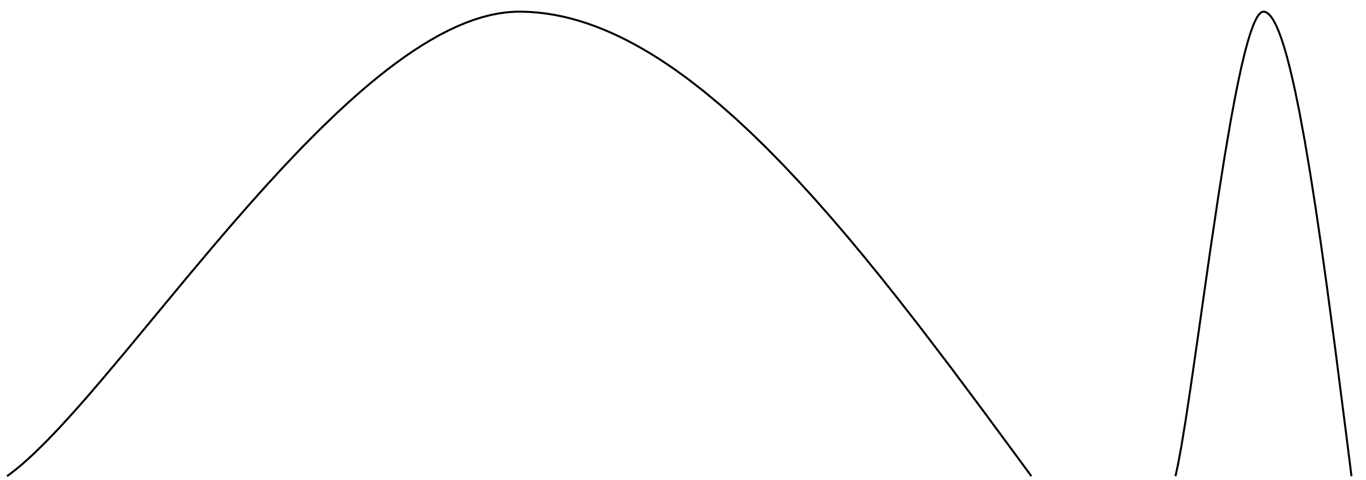
Different lattice spacings lead to different curvatures for E(K) and effective masses that depend on the direction of motion.

Real 3D lattices, e.g. FCC, BCC, diamond, etc.

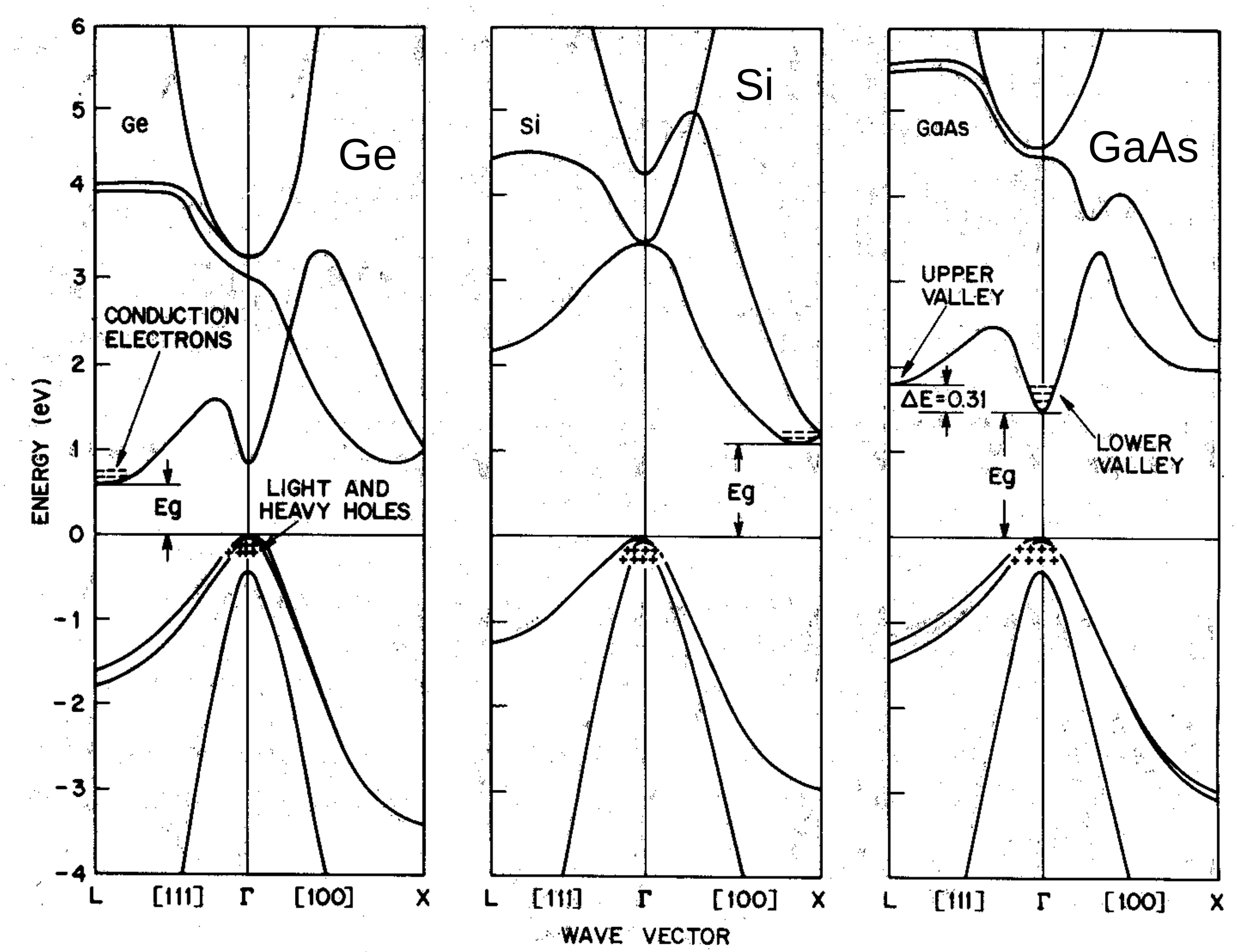
$$m_{c,ij}^{-1} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

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

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



Real 3D lattices, e.g. FCC, BCC, diamond, etc.



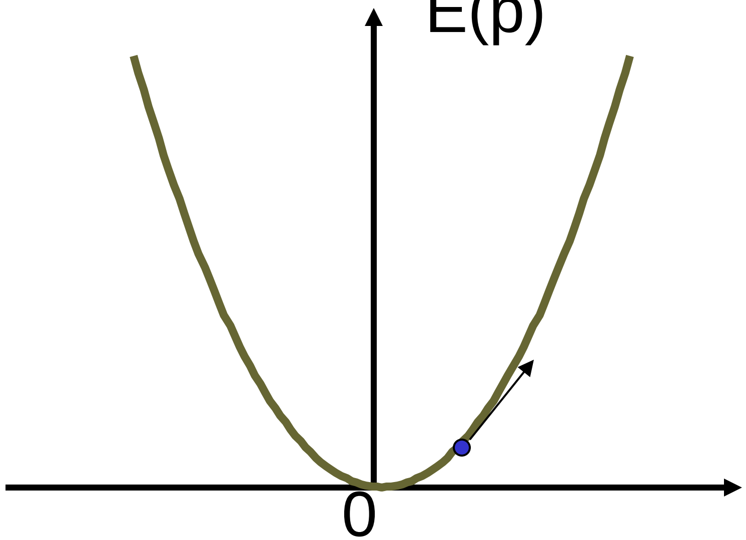
Direct and inderect band gap in semiconductors

- energy (E) and momentum ($\hbar K$) 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)

Motion of free electrons



Consider free electron

Dispersion relation

$$\mathrm{E} = p^2/2m_0 = (p_x^2 + p_y^2 + p_z^2)/2m_0 \quad \boldsymbol{p} = m_0\boldsymbol{v}$$

Newton's law of motion

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{F} \quad m_0\frac{d\boldsymbol{r}}{dt} = \boldsymbol{p}$$

Velocity

$$v_x = \frac{p_x}{m_0} = \frac{\partial \mathrm{E}}{\partial p_x} \quad \boldsymbol{v} = v_x\hat{x} + v_y\hat{y} + v_z\hat{z} = \frac{\partial \mathrm{E}}{\partial p_x}\hat{x} + \frac{\partial \mathrm{E}}{\partial p_y}\hat{y} + \frac{\partial \mathrm{E}}{\partial p_z}\hat{z} = \frac{\partial \mathrm{E}}{\partial \boldsymbol{p}}$$

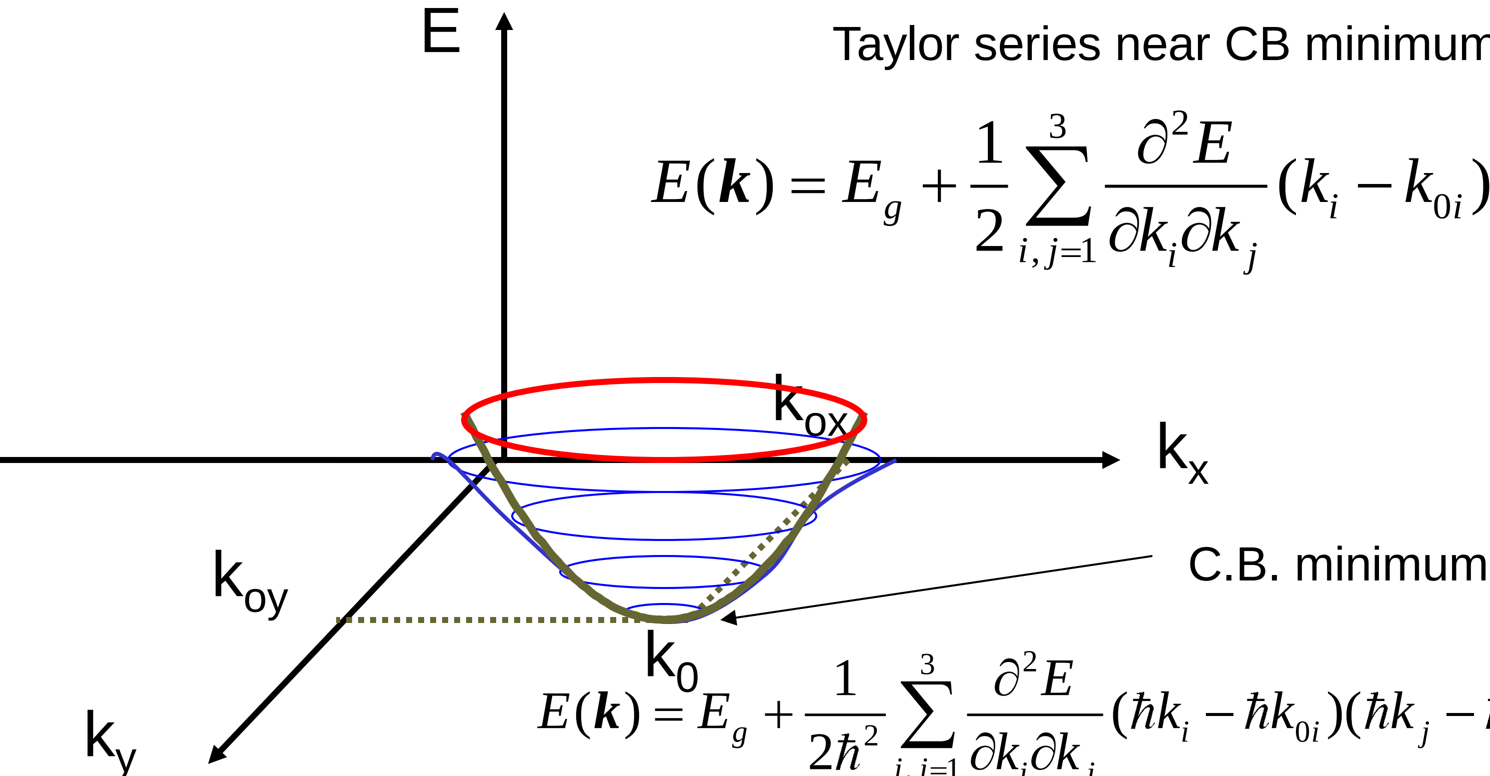
Mass

$$m_0^{-1} = \frac{\partial^2 \mathrm{E}}{\partial p_x^2} = \frac{\partial^2 \mathrm{E}}{\partial p_y^2} = \frac{\partial^2 \mathrm{E}}{\partial p_z^2}$$

Effective mass

Taylor series near CB minimum

$$E(\boldsymbol{k}) = E_g + \frac{1}{2}\sum_{i,j=1}^{3}\frac{\partial^2 E}{\partial k_i \partial k_j}(k_i - k_{0i})(k_j - k_{0j}) + \ldots =$$



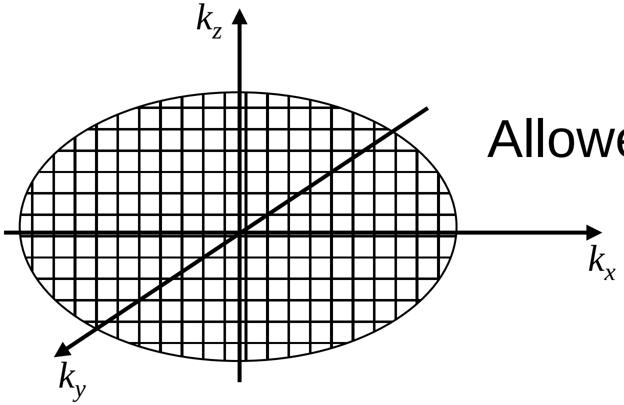
$$E(\boldsymbol{k}) = E_g + \frac{1}{2\hbar^2}\sum_{i,j=1}^{3}\frac{\partial^2 E}{\partial k_i \partial k_j}(\hbar k_i - \hbar k_{0i})(\hbar k_j - \hbar k_{0j}) + \ldots =$$

$$E_g + \frac{1}{2}\sum_{i,j=1}^{3} m_{c,ij}^{-1} p_i p_j + \ldots \quad p_i = \hbar(k_i - k_{0i})$$

Effective mass tensor

$$m_{c,ij}^{-1} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$$

Density of states



Parallelepiped of Volume $V = L_x L_y L_z$

Allowed states satisfy boundary conditions: $k_i L_i = 2\pi n_i$

Each state occupies volume in k space

$$\delta V_k = 8\pi^3 / (L_x L_y L_z) = 8\pi^3 V^{-1}$$

Consider a conduction valley along x or [100] direction

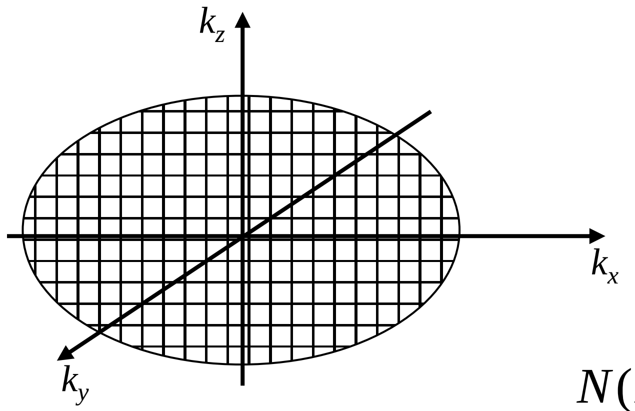
$$E(k) = E_g + \frac{\hbar^2 k_x^2}{2m_L} + \frac{\hbar^2 k_y^2}{2m_T} + \frac{\hbar^2 k_z^2}{2m_T} \qquad \frac{\hbar^2 k_x^2}{2m_L(E-E_g)} + \frac{\hbar^2 k_y^2}{2m_T(E-E_g)} + \frac{\hbar^2 k_z^2}{2m_T(E-E_g)} = 1$$

Half axes $a_x = \sqrt{\frac{2m_L(E-E_g)}{\hbar^2}},\ a_y = \sqrt{\frac{2m_T(E-E_g)}{\hbar^2}},\ a_z = \sqrt{\frac{2m_T(E-E_g)}{\hbar^2}};$

The volume in k-space containing energies less than E

$$V_k(E) = \frac{4}{3}\pi a_x a_y a_z = \frac{4}{3}\pi \left(\frac{2}{\hbar^2}\right)^{3/2} m_L^{1/2} m_T (E-E_g)^{3/2}$$

Density of states



$$V_k(E) = \frac{4}{3}\pi\left(\frac{2}{\hbar^2}\right)^{3/2} m_L^{1/2} m_T (E - E_g)^{3/2}$$

Number of states with energies less than E

$$N(E) = 2 \times V_k(E) / \delta V_k = \frac{V}{3\pi^2}\left(\frac{2}{\hbar^2}\right)^{3/2} m_L^{1/2} m_T (E - E_c)^{3/2}$$

Multiply by number of valleys -G , divide by volume take derivative

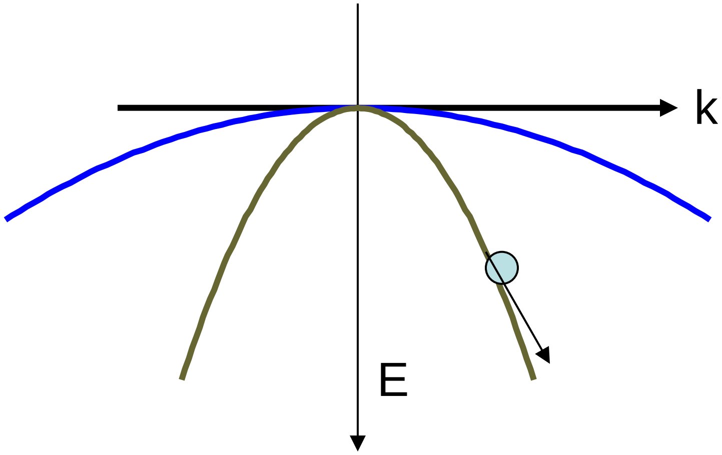
$$g_c(E) = G\frac{\partial N(E)}{\partial E}V^{-1} = \frac{G}{2\pi^2}\left(\frac{2}{\hbar^2}\right)^{3/2} m_L^{1/2} m_T (E - E_g)^{1/2} = \frac{1}{2\pi^2}\left(\frac{2m_n^*}{\hbar^2}\right)^{3/2}(E - E_g)^{1/2}$$

Number of states per unit volume per unit energy –density of states

Effective D.O.S. mass $\quad m_n^* = G^{2/3}\left(m_L m_T^2\right)^{1/3}$

In GaAs $\quad m_n^* = m_c$

Density of states in the valence band



Count energy down

$$g_v(E) = g_{lh}(E) + g_{hh}(E) = \frac{1}{2\pi^2}\left(\frac{2m_{lh}}{\hbar^2}\right)^{3/2} E^{1/2} + \frac{1}{2\pi^2}\left(\frac{2m_{hh}^*}{\hbar^2}\right)^{3/2} E^{1/2} = \frac{1}{2\pi^2}\left(\frac{2m_p^*}{\hbar^2}\right)^{3/2} E^{1/2}$$

Effective D.O.S. mass is $m_p^* = \left(m_{hh}^{3/2} + m_{lh}^{3/2}\right)^{2/3} \sim m_{hh}$