Class 02
Semiconductor Band Theory

18.02.2025

- ❑ Theoretical background
  - Bloch theorem
  - FE model
- ❑ Kronig-Penney model
  - Strength of the barrier
- ❑ Effective mass and concept of holes

Bloch theorem

$$U(\mathbf{r}) = U(\mathbf{r} + \mathbf{R})$$

Periodic potential

$$H\,\Psi(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r})$$

Schroedinger equation for an electron in a periodic potential

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = A\,\exp(\mathrm{i}\,\mathbf{k}\,\mathbf{r})\,u_{n\mathbf{k}}(\mathbf{r})\,.$$

Wavefunction of the electron in a periodic potential

$$u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R})$$

Bloch function (periodic in space)

$$E_n(\mathbf{k}) = E_n(\mathbf{k} + \mathbf{G})\,.$$

Eigenvalue of the electron (periodic in the reciprocal space)

The eigenvalue is a function of the wavector (reciprocal space)

Each state is defined by a wavevector k

Free electron model

$$U(\mathbf{r}) = U(\mathbf{r} + \mathbf{R})$$

Periodic potential

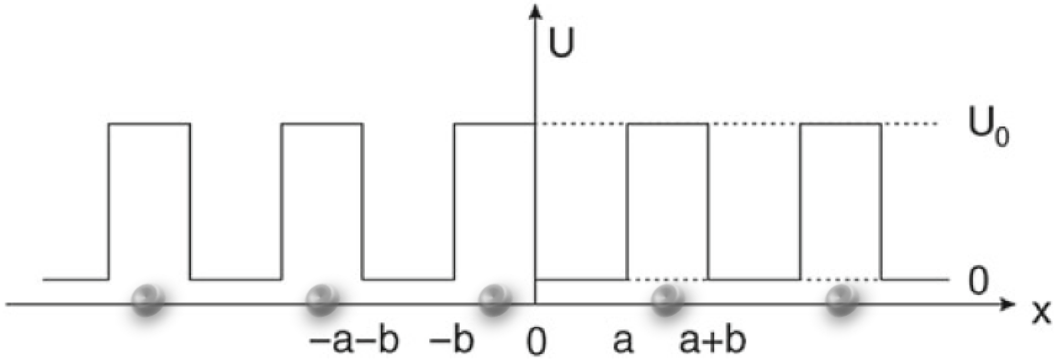
$$H\,\Psi(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r})$$

Schroedinger equation for an electron in a periodic potential

To be solved in Class (10 minutes)

U(r) = 0

Kronig-Penney model: simple 1D model which considers the non-vanishing potential as a hard-wall potential



Potential far from the nuclei → 0
Potential close to the nuclei → U_0
Range of atomic interaction → a
Atomic periodicity → a+b = P

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+U(x)\,\Psi=E\,\Psi$$ **1D Schroedinger equation**

S.E. solutions:

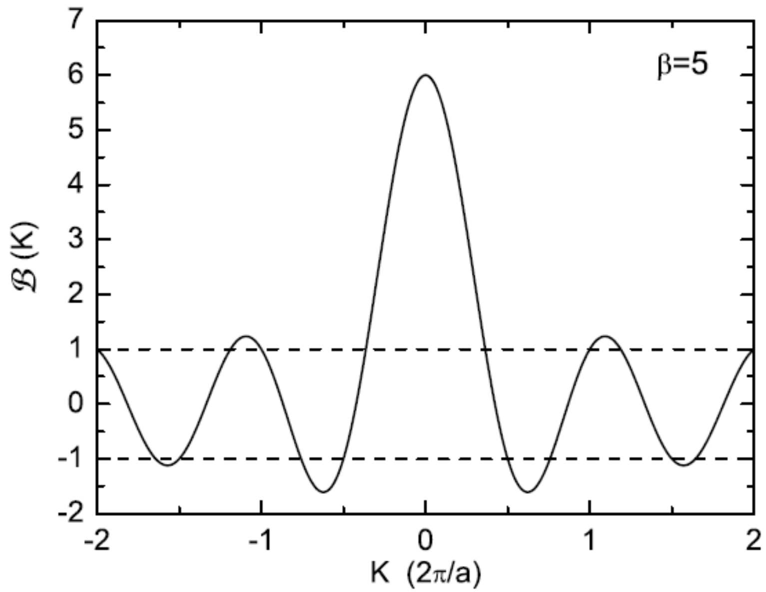
$$\Psi(x)= A\exp(\mathrm{i}Kx)+B\exp(-\mathrm{i}Kx)$$ **in the well**

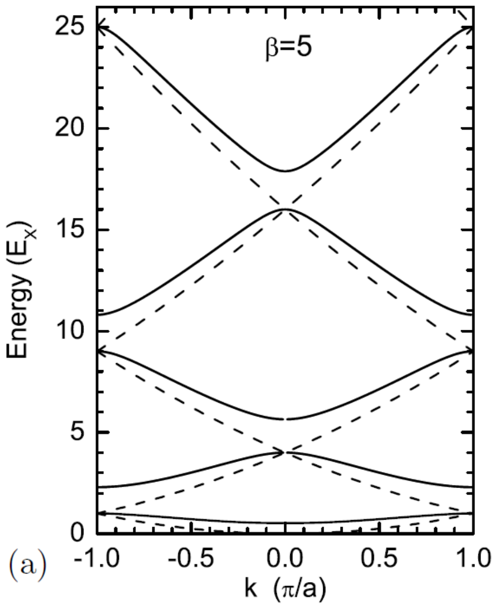
$$\Psi(x)= C\exp(\kappa x)+D\exp(-\kappa x)\ .$$ **in the barrier**

KP solution:

$$\cos(ka)=\beta\,\frac{\sin(Ka)}{Ka}+\cos(Ka)=\mathcal{B}(K)$$

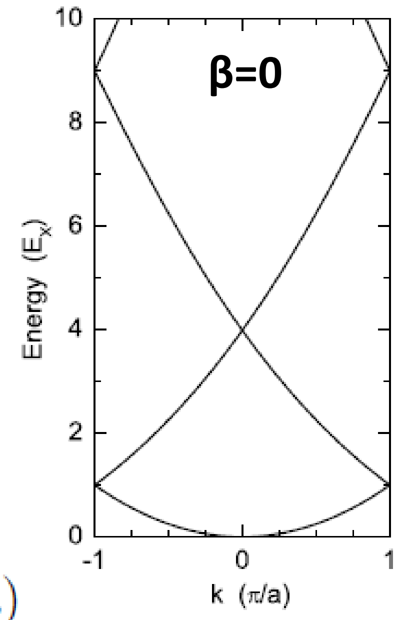
The dimensionless coupling parameter $\beta=\kappa^2 ba/2$ represents the strength of the barrier.



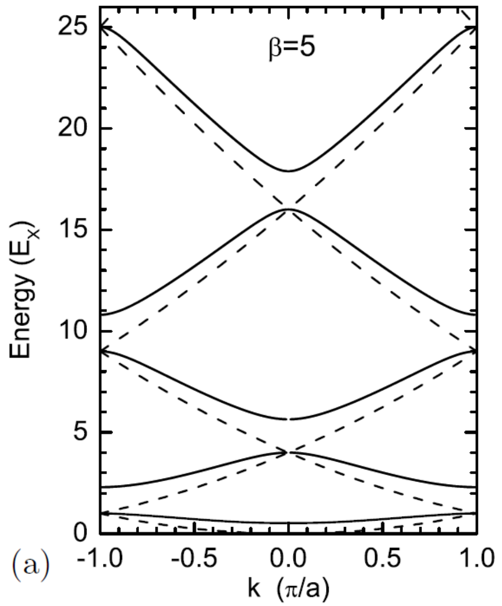


Grundmann Appendix F

Strenght of the barrier



(a)



(a)

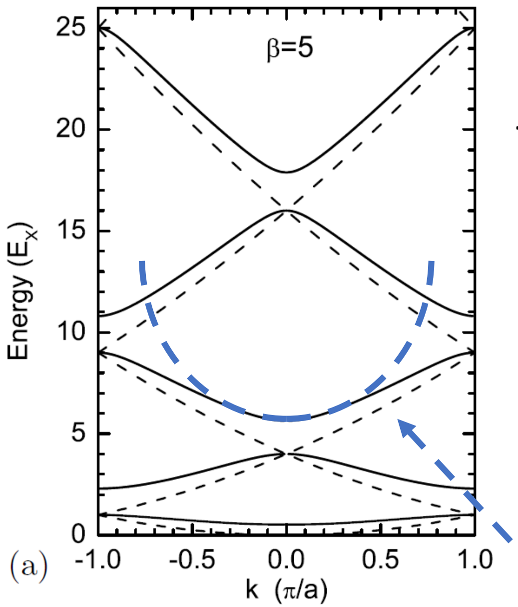
β=20 ?

How does the band structure change when the strength of the barrier increases?

What does it mean that the strength of the barrier increases?

To be discussed in Class (5 minutes)

Parabolic approximation



The curvature of the bands is estimated with a parameter called «effective mass», m^*.

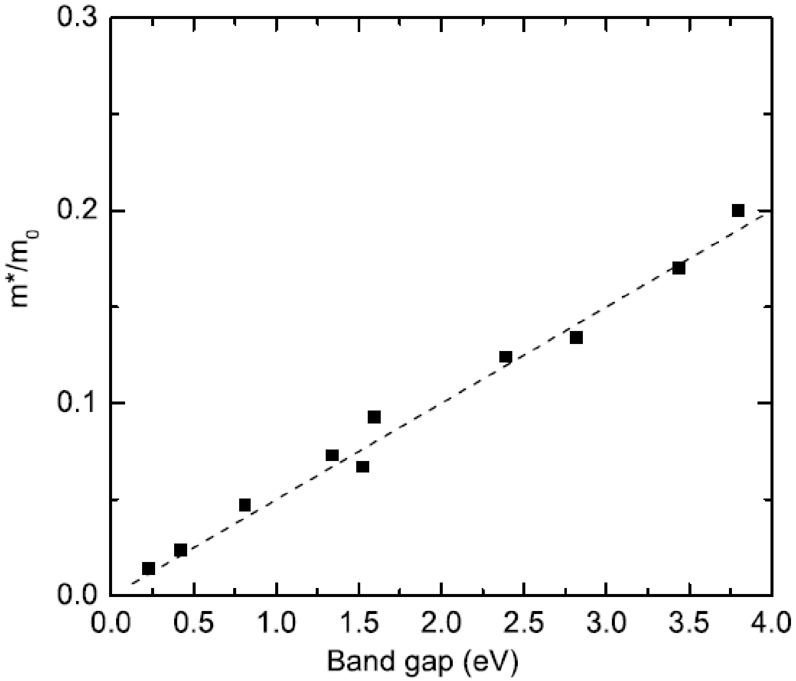
The effective mass is therefore a material parameter which describes in a simple way the dispersion relationship.

$$H\,\Psi(\mathbf{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + U(\mathbf{r})\right]\Psi(\mathbf{r}) = E\,\Psi(\mathbf{r})$$

$$-\frac{\hbar^2}{2m^*}\nabla^2$$

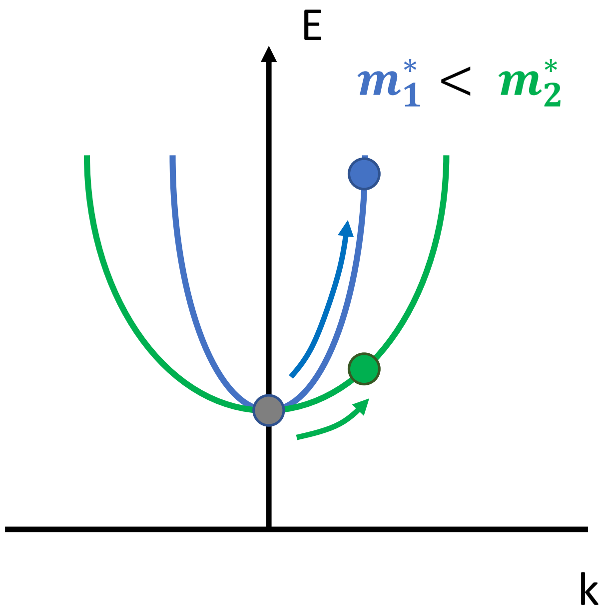
$$E(\mathbf{k}) = \frac{\hbar^2}{2m^*}\mathbf{k}^2$$

The KP model also predicts the increase of effective mass with band gap.
β↑ Eg ↑ and the band flattens (m^* ↑)



Effective mass and functional properties (simplified)

Example 1

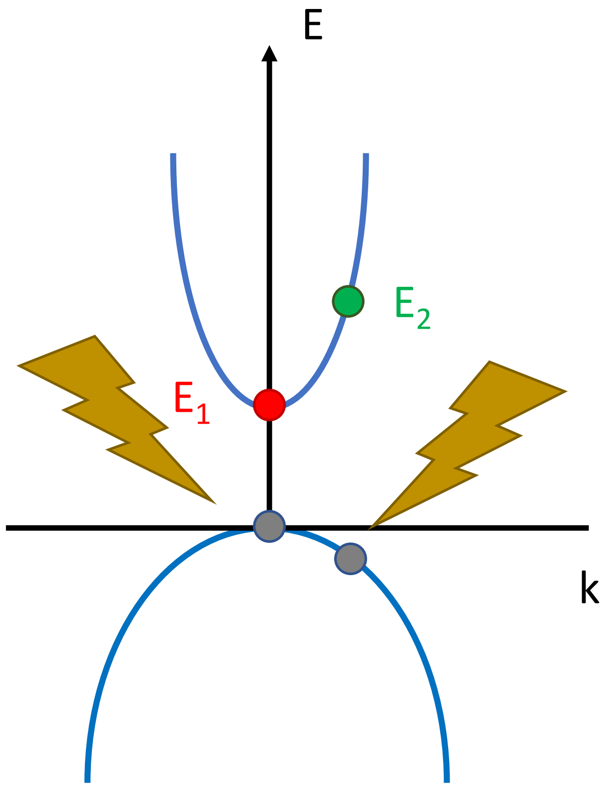


$$e\vec{E} = \vec{F} = \frac{d\vec{p}}{dt} = \frac{\hbar d\vec{k}}{dt}$$

$$\Delta E_1 > \Delta E_2$$

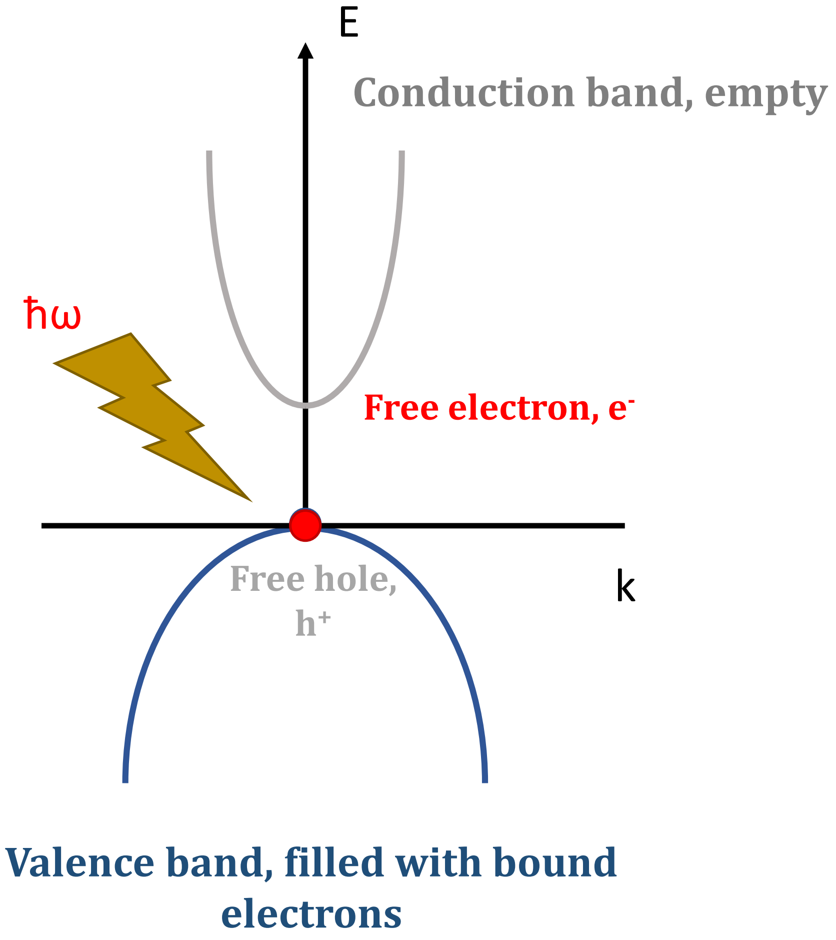
«Light» electrons move «faster»
(see mobility, class07)

Example 2

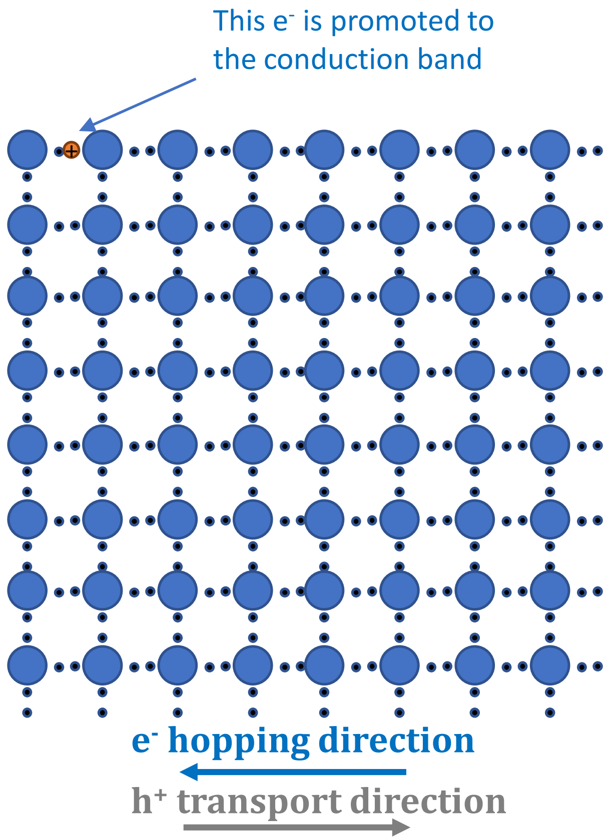


The dispersion relationship defines the photon-assisted interband transitions (see absorption, class08)

Electrons and Holes



T= 0 K



Electrons in the conduction bands have enough energy to overcome the potential barrier so they move freely across the lattice.

The remaining bound electrons can hop to fill the empty state.

Electron hopping correspond to the transport (in opposite direction) of a positively charge particle. This particle is called **hole**.

$$m_e^* < m_h^*$$