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)

Energy bands in solids

- **Bloch theorem**
- **Kronig-Penney model**
- **Empty lattice approximation**
- **Number of states in a band and filing of the bands**

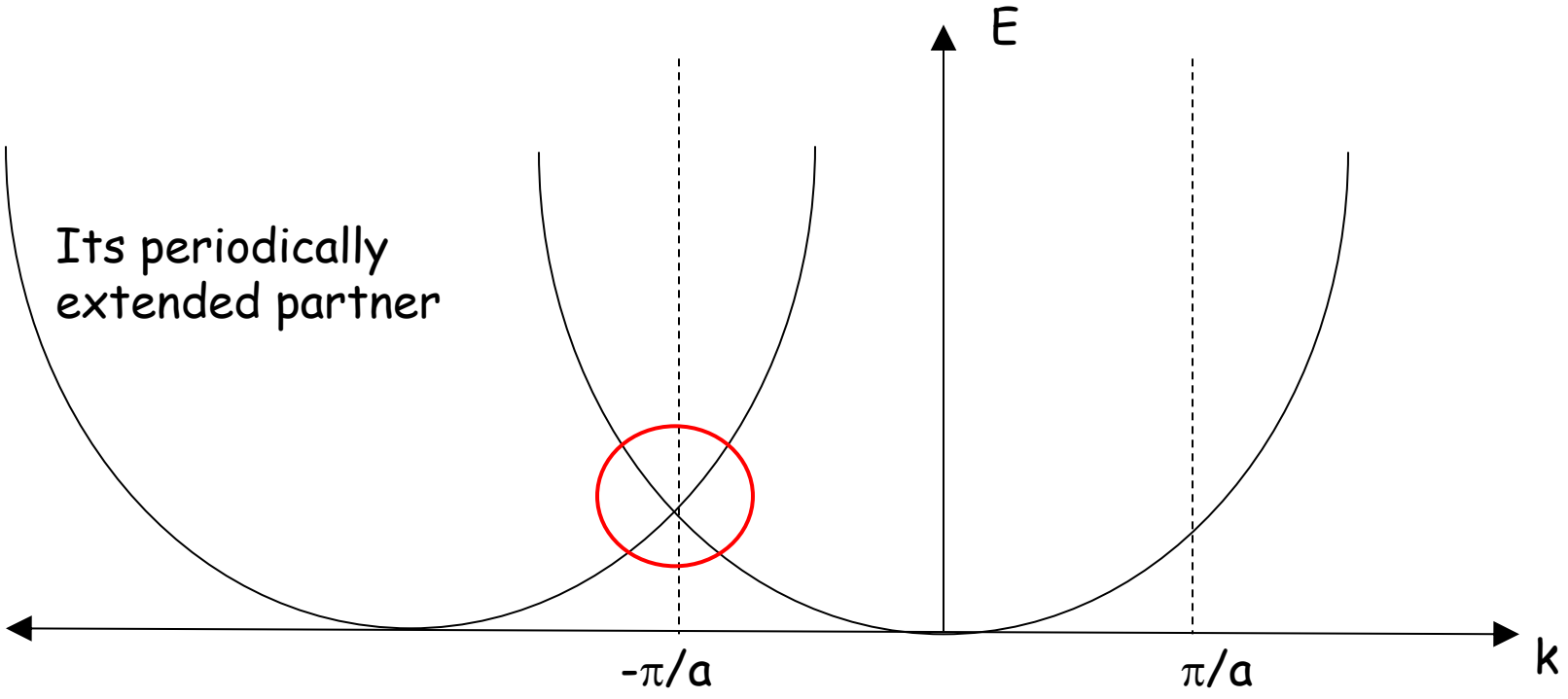
Lecture 18: Energy bands in solids

- **Origin of the band gap and Bloch theorem**
- **Kronig-Penney model**
- **Empty lattice approximation**
- **Number of states in a band and filing of the bands**

Why do we get a gap?

Let us start with a free electron in a periodic crystal,
but ignore the atomic potentials for now

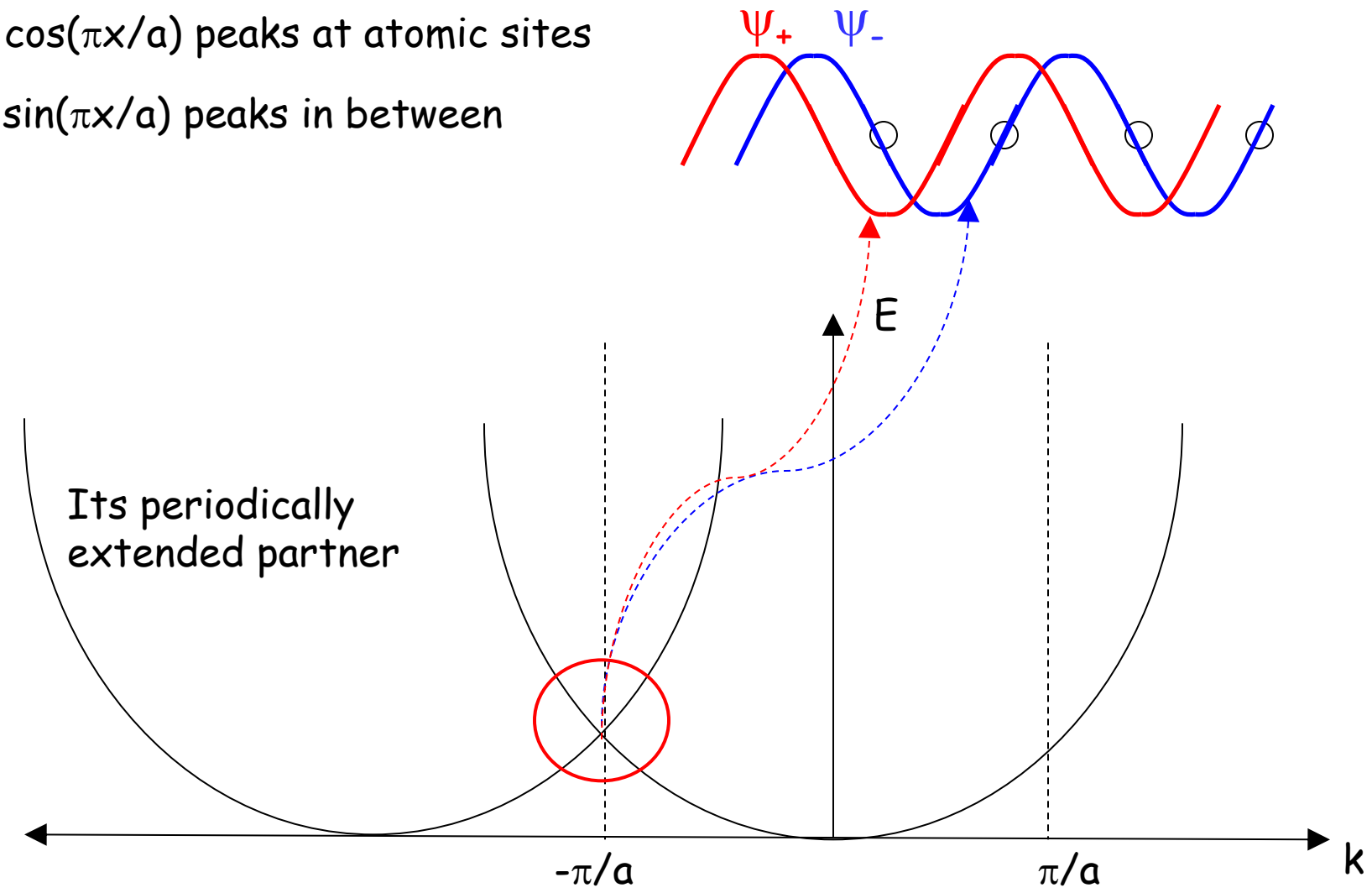
At the interface (BZ), we have two counter-propagating waves $e^{\pm ikx}$,
with $k = \pi/a$, that Bragg reflect and form standing waves $\psi_{\pm}$



Why do we get a gap?

ψ_+ ~ cos(πx/a) peaks at atomic sites

ψ_- ~ sin(πx/a) peaks in between



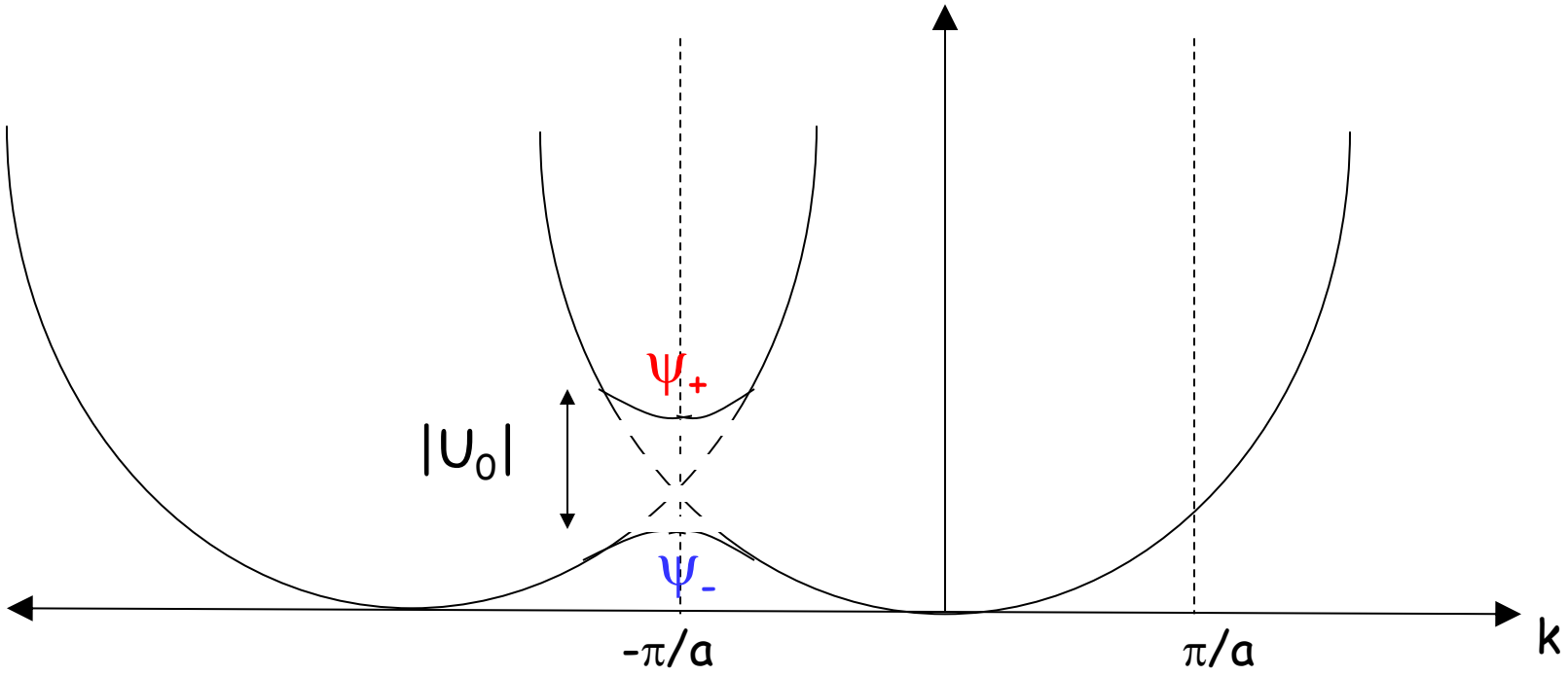
Let's now turn on the atomic potential

The ψ_+ solution sees the atomic potential and increases its energy

The ψ_- solution does not see this potential (as it lies between atoms)

Thus their energies separate and a gap appears at the BZ

This happens only at the BZ where we have standing waves



Bloch theorem

If V(r) is periodic with the periodicity of the lattice, then the solutions of the one-electron Schrödinger eq.

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$$

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}}$$

Where $u_k(r)$ is periodic with the periodicity of the direct lattice.

$u_k(\mathbf{r}) = u_k(\mathbf{r}+\mathbf{T})$; **T** is the translation vector of lattice.

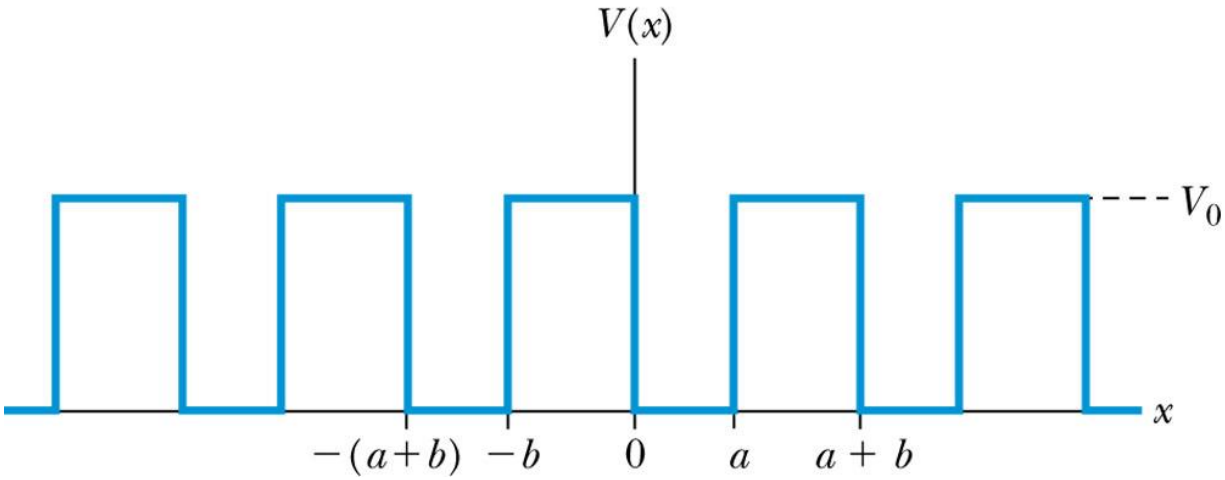
" The eigenfunctions of the wave equation for a periodic potential are the product of a plane wave $\exp(i\mathbf{k}\cdot\mathbf{r})$ times a function $u_k(\mathbf{r})$ with the periodicity of the crystal lattice."

Energy bands in solids

- Origin of the band gap and Bloch theorem
- **Kronig-Penney model**
- Empty lattice approximation
- Number of states in a band and filing of the bands

Kronig-Penney Model

- Kronig and Penney assumed that an electron experiences an infinite one-dimensional array of finite potential wells.
- Each potential well models attraction to an atom in the lattice, so the size of the wells must correspond roughly to the lattice spacing.



Kronig-Penney Model

- An effective way to understand the energy gap in semiconductors is to model the interaction between the electrons and the lattice of atoms.

- **R. de L. Kronig** and **W. G. Penney** developed a useful one-dimensional model of the electron lattice interaction in 1931.

Kronig-Penney Model

- Since the electrons are not free their energies are less than the height V_0 of each of the potentials, but the electron is essentially free in the gap $0 < x < a$, where it has a wave function of the form

$$\psi = Ae^{ikx} + Be^{-ikx}$$

where the wave number k is given by the usual relation:

$$k^2 = 2mE / \hbar^2$$

Kronig-Penney Model

- In the region between $a < x < a + b$ the electron can tunnel through and the wave function loses its oscillatory solution and becomes exponential:

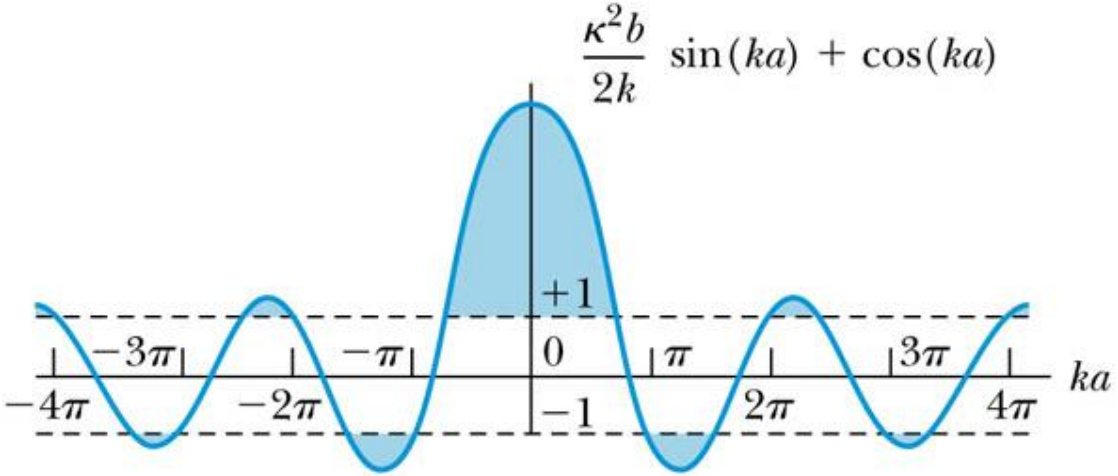
$$\psi = Ce^{\kappa x} + De^{-\kappa x}$$

$$\kappa^2 = 2m(V_0 - E)/\hbar^2$$

Kronig-Penney Model

$$\frac{\kappa^2 b}{2k}\sin(ka) + \cos(ka) = \cos(Ka)$$

- The left-hand side is limited to values between +1 and −1 for all values of K.
- Plotting this it is observed there exist restricted (shaded) **forbidden zones** for solutions.



Kronig-Penney Model

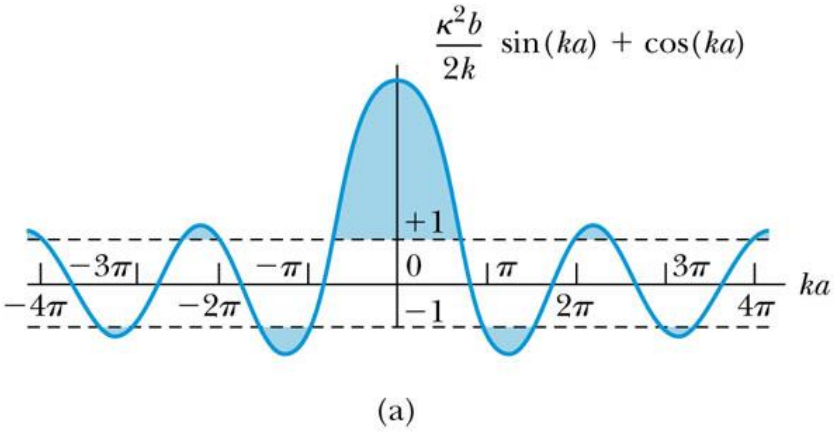
- Matching solutions at the boundary, Kronig and Penney find

$$\frac{\kappa^2 b}{2k}\sin(ka)+\cos(ka)=\cos(Ka)$$

Here *K* is another wave number. Let's label the equation above as KPE – Kronig-Penney equation

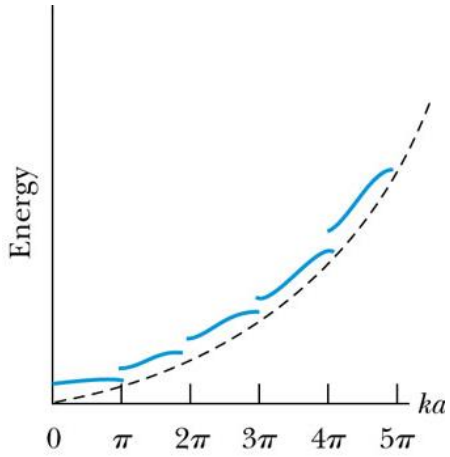
Kronig-Penney Model

(a) Plot of the left side of Equation (KPE) versus *ka* for $\kappa^2 ba / 2 = 3\pi / 2$. Allowed energy values must correspond to the values of *k* for $k = \sqrt{2mE/\hbar^2}$ for which the plotted function lies between -1 and +1. Forbidden values are shaded in light blue.



(a)

(b) The corresponding plot of energy versus *ka* for $\kappa^2 ba / 2 = 3\pi / 2$, showing the forbidden energy zones (gaps).



(b)

Energy bands in solids

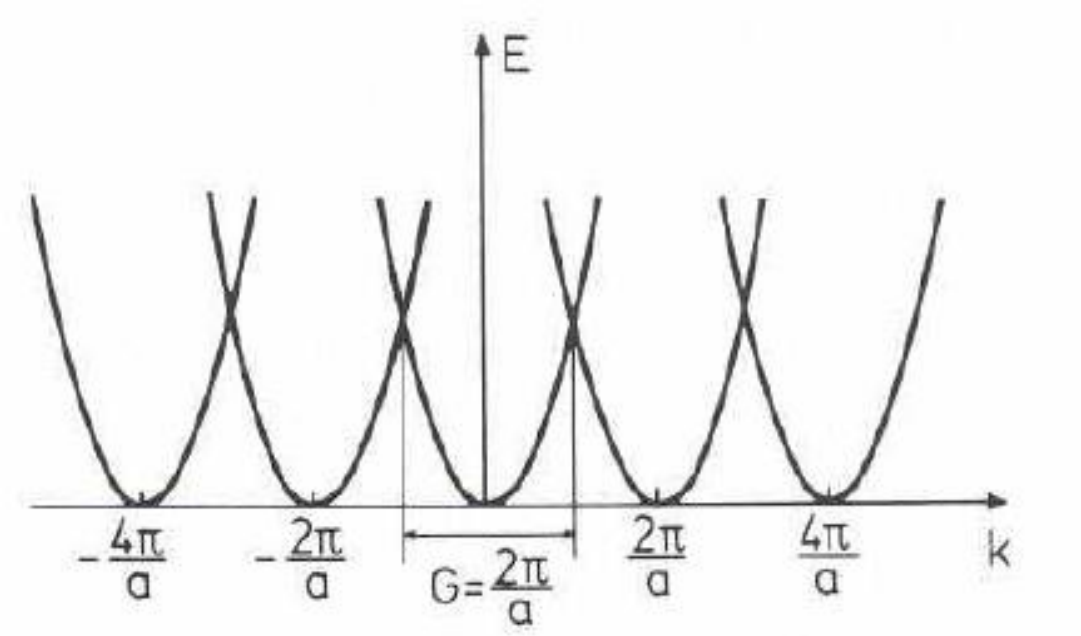
- Origin of the band gap and Bloch theorem
- Kronig-Penney model
- **Empty lattice approximation**
- Number of states in a band and filing of the bands

Empty lattice approximation

Suppose that we have empty lattice where the periodic V(x)=0. Then the e-s in the lattice are free, so that

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

$$E(k) = E(k+G) \quad \Rightarrow \quad E = \frac{\hbar^2}{2m}\left(k + \frac{2\pi}{a}n\right)^2$$



Empty lattice approximation

in 3-dim.

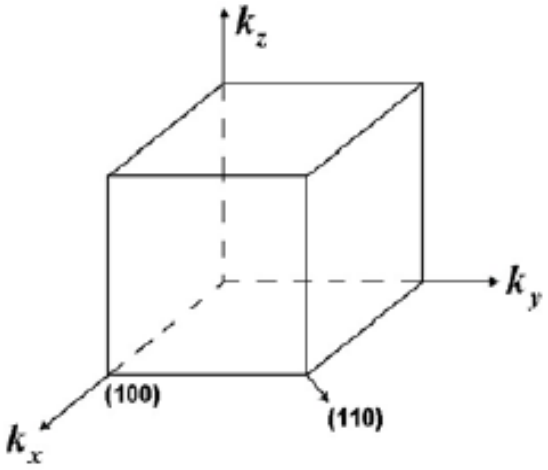
$$E(k_x, k_y, k_z) = \frac{\hbar^2}{2m}(\vec{k} + \vec{G})^2$$

$$= \frac{\hbar^2}{2m}\left[(k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2\right]$$

$$= \frac{\hbar^2}{2m}\left[(k_x + \frac{2\pi}{a}n_x)^2 + (k_y + \frac{2\pi}{a}n_y)^2 + (k_z + \frac{2\pi}{a}n_z)^2\right]$$

Empty lattice approximation

In simple cubic (SC) empty lattice

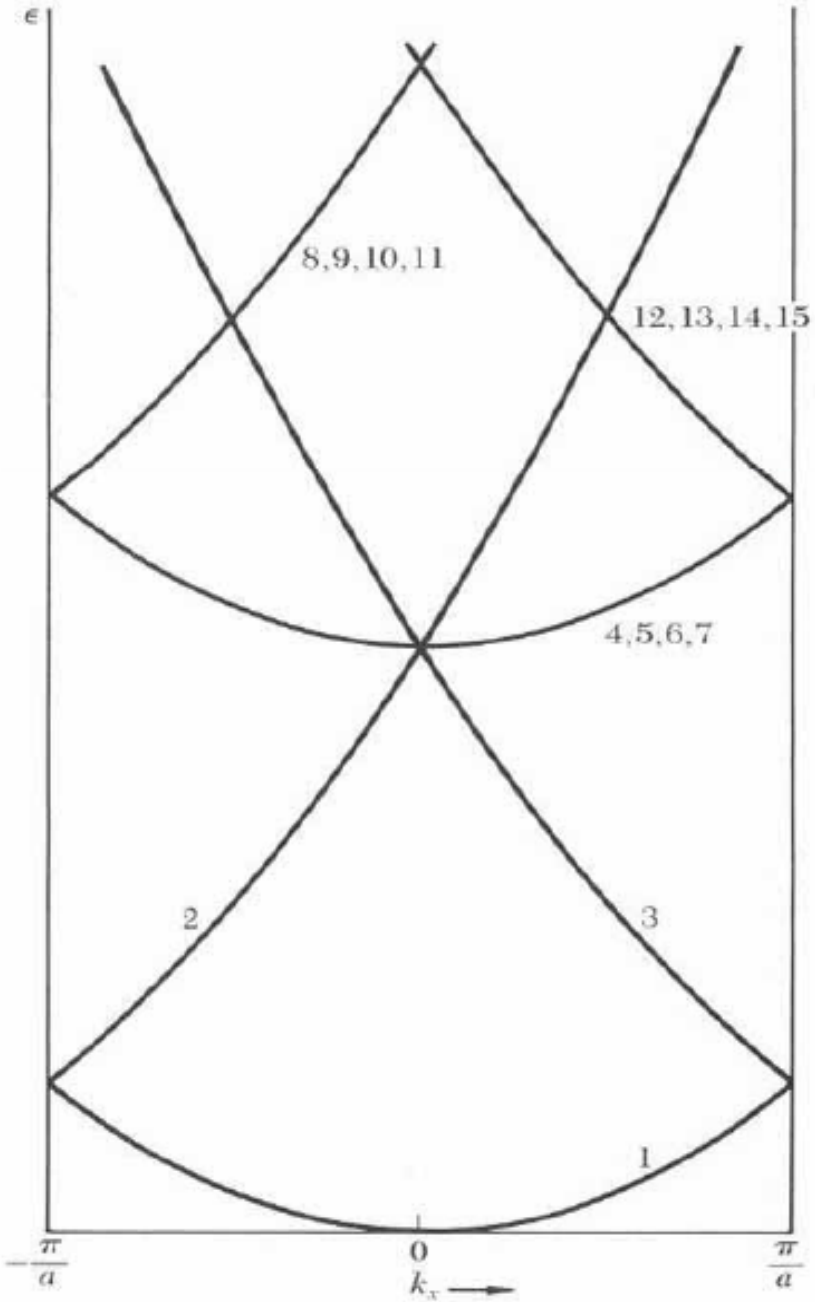


Band	$G\left[\frac{2\pi}{a}\right]$	$E(000)$	$E(k_x 00)\left[\frac{\hbar^2}{2m}\right]$
1	$[000]$	0	k_x^2
2, 3	$[100]$ $[\bar{1}00]$	$\left(\frac{2\pi}{a}\right)^2$	$\left(k_x \pm \frac{2\pi}{a}\right)^2$
4, 5 6, 7	$[010]\,[0\bar{1}0]$ $[001]\,[00\bar{1}]$	$\left(\frac{2\pi}{a}\right)^2$	$k_x^2 + \left(\frac{2\pi}{a}\right)^2$
8, 9 10, 11	$[110]\,[101]$ $[1\bar{1}0]\,[10\bar{1}]$	$2\left(\frac{2\pi}{a}\right)^2$	$\left(k_x^2 + \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2$
⋮	$[\bar{1}10]\,[\bar{1}01]\,[\bar{1}\bar{1}0]\,[\bar{1}0\bar{1}]$		$\left(k_x^2 - \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2$

Empty lattice approximation

Band	$E(k_x 00)\left[\frac{\hbar^2}{2m}\right]$
1	k_x^2
2, 3	$\left(k_x \pm \frac{2\pi}{a}\right)^2$
4, 5 6, 7	$k_x^2 + \left(\frac{2\pi}{a}\right)^2$
8, 9 10, 11	$\left(k_x^2 + \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2$
⋮	$\left(k_x^2 - \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2$

Everything can be described within the 1st B.Z.



Lecture 18: Energy bands in solids

- Origin of the band gap and Bloch theorem
- Kronig-Penney model
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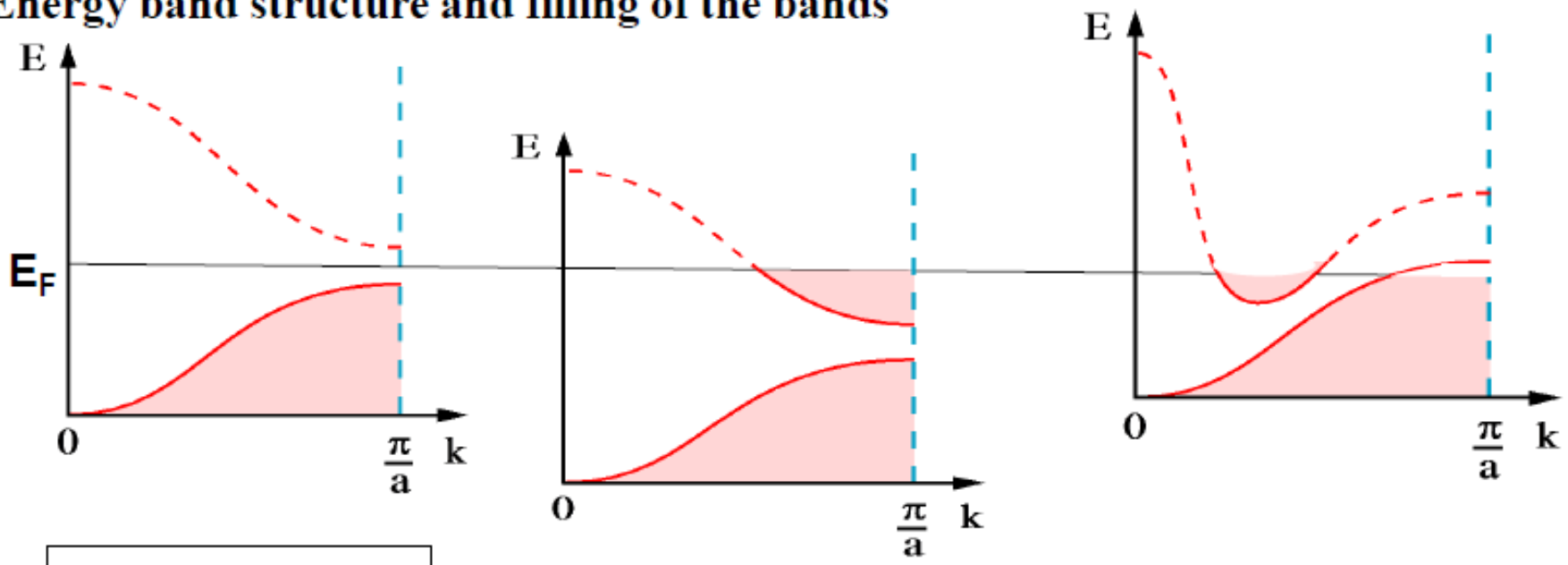
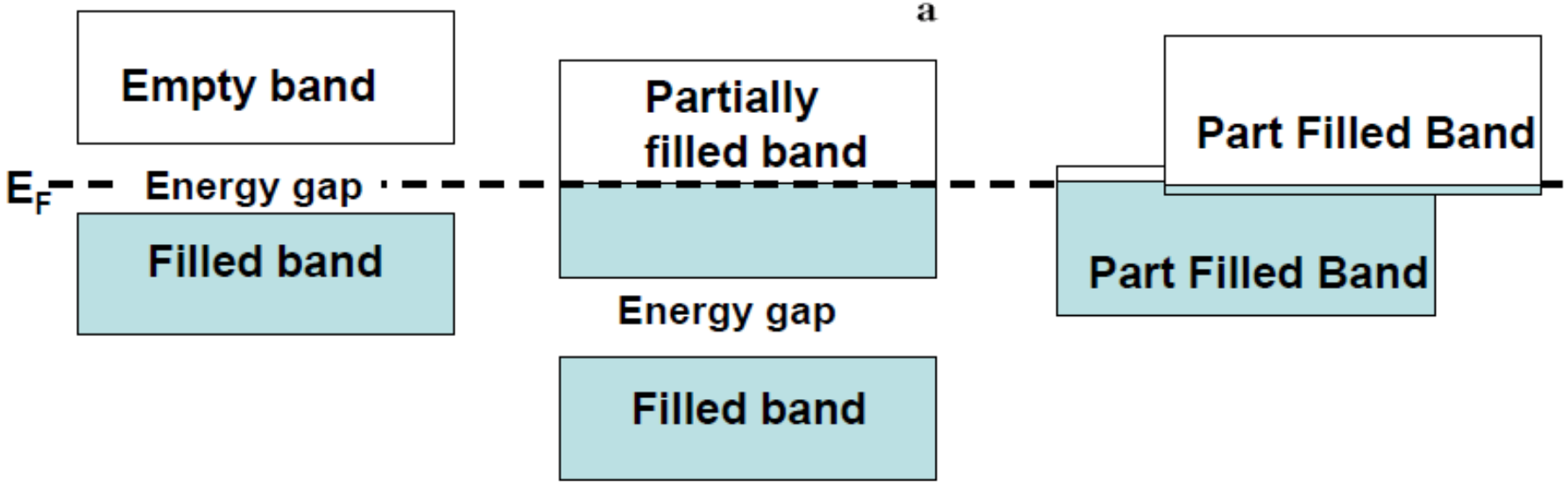
- **Number of states in a band and filing of the bands**

Energy band structure and filling of the bands





INSULATOR or SEMICONDUCTOR

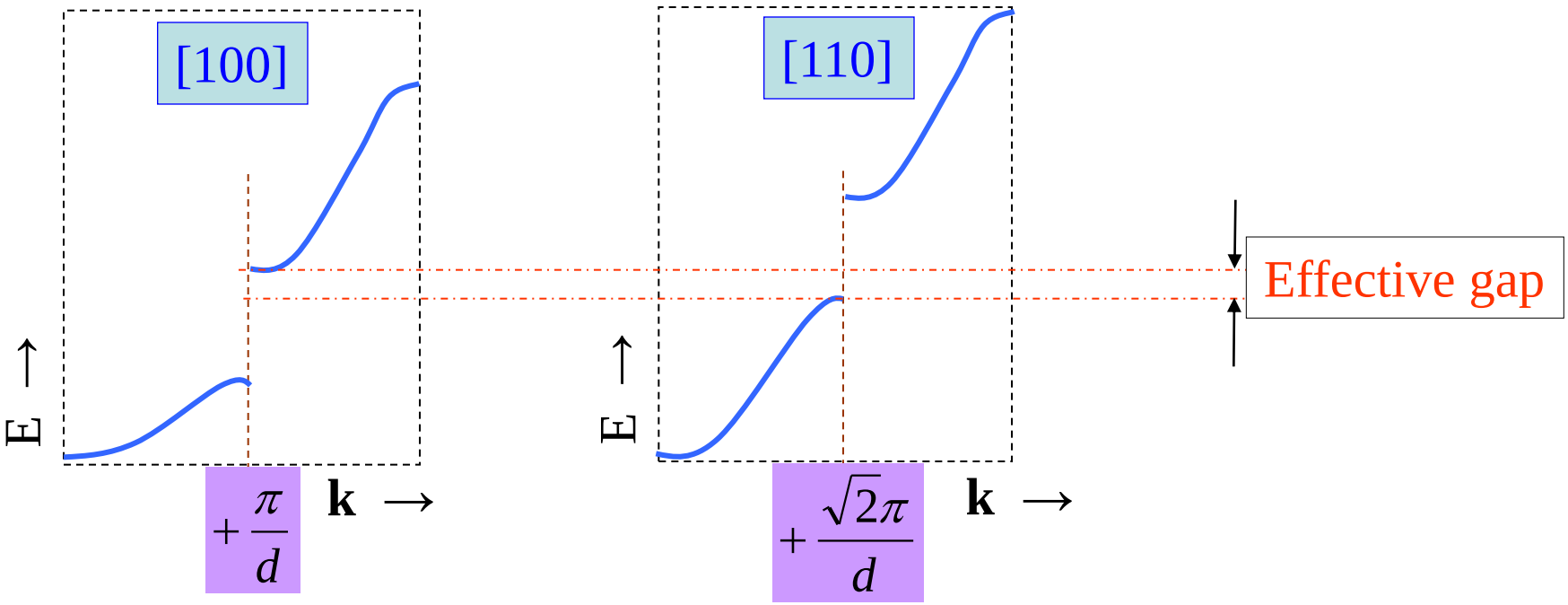
METAL

METAL or SEMI-METAL

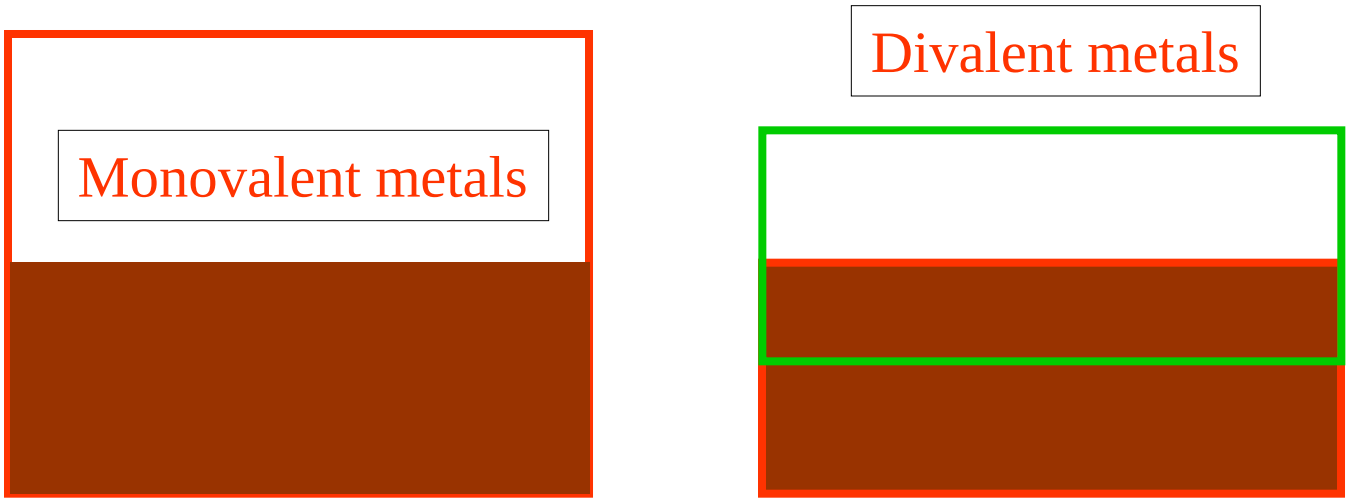
Number of states in a band

$$k = \frac{n\pi}{d \sin\theta}$$

$$k = \frac{\pi}{d \sin 90^{o}} \qquad k = \frac{\pi}{d \sin 45^{o}}$$

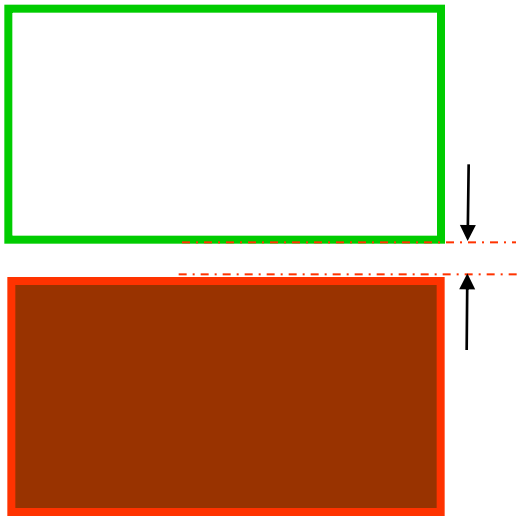


Filing of the bands



- Monovalent metals: Ag, Cu, Au → 1 e^- in the outermost orbital
  ⇒ outermost energy band is only half filled
- Divalent metals: Mg, Be → overlapping conduction and valence bands
  ⇒ they conduct even if the valence band is full
- Trivalent metals: Al → similar to monovalent metals!!!
  ⇒ outermost energy band is only half filled !!!

Filing of the bands



SEMICONDUCTORS and ISOLATORS

Band gap

- Elements of the 4th column (C, Si, Ge, Sn, Pb) → valence band full but no overlap of valence and conduction bands
- Diamond → PE as strong function of the position in the crystal
  ⇨ Band gap is 5.4 eV
- Down the 4th column the outermost orbital is farther away from the nucleus and less bound ⇒ the electron is less strong a function of the position in the crystal ▶ reducing band gap down the column