FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/index-eng.xml

Based on Introduction to Solid State Physics by Kittel

Course content

- Periodic structures, understanding of diffraction experiment and reciprocal lattice
- Crystal binding, elastic strain and waves
- Imperfections in crystals: point defects and diffusion
- Crystal vibrations: phonon heat capacity and thermal conductivity
- Free electron Fermi gas: density of states, Fermi level, and electrical conductivity
- **Electrons in periodic potential: energy bands theory classification of metals, semiconductors and insulators**
- Semiconductors: band gap, effective masses, charge carrier distributions, doping, pn-junctions
- Metals: Fermi surfaces, temperature dependence of electrical conductivity

Andrej Kuznetsov, Dept of Physics and Centre for Material Science and Nanothechnology
Postboks 1048 Blindern, 0316 OSLO
Tel: +47-22852870, e-post: andrej.kuznetsov@fys.uio.no
visiting address: MiNaLab, Gaustadaleen 23b

FYS3410 lecture schedule and exams: Spring 2010

M/18/1/2010:	Introduction and motivation. Periodicity and lattices	2h
W/20/1/2010:	Index system for crystal planes. Crystal structures	1h
M/25/1/2010:	Reciprocal space, Laue condition and Ewald construction	2h
W/27/1/2010:	Brillouin Zones. Interpretation of a diffraction experiment	1h
M/01/2/2010:	Crystal binding, elastic strain and waves	2h
W/03/2/2010:	Elastic waves in cubic crystals; defects in crystals	1h
M/08/2/2010:	Defects in crystals; case study - vacancies	2h
W/10/2/2010:	Diffusion	1h
M/15/2/2010:	Crystal vibrations and phonons	2h
W/17/2/2010:	Crystal vibrations and phonons	1h
M/22/2/2010:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
W/24/2/2010:	Phonon density of states (DOS) and Debye model	1h
M/01/3/2010:	General result for DOS; role of anharmonic interactions	2h
W/03/3/2010:	Thermal conductivity	1h
M/08/3/2010:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/10/3/2010:	Density of states, effect of temperature – FD distribution	1h
M/15/3/2010:	Heat capacity and thermal conductivity of FEFG	2h
W/17/3/2010:	Repetition	1h
22/3/2010:	Mid-term exam	

M/12/4/2010:	Drude model and the idea of energy bands	2h
W/14/4/2010:	Nearly free electron model; Kronig - Penny model	2h
M/19/4/2010:	no lectures	
W/21/4/2010:	Empty lattice approximation; number of orbitals in a band	2h
M/26/4/2010:	Semiconductors, effective mass method, intrinsic carriers	2h
W/28/4/2010:	Impurity states in semiconductors and carrier statistics	2h
M/03/5/2010:	p-n junctions and heterojunctions	2h
W/05/5/2010:	surface structure, surface states, Schottky contacts	2h
M/10/5/2010:	Metals and Fermi surfaces	
W/12/5/2010:	no lectures	
W/19/5/2010:	no lectures	2h
W26/5/2010:	Repetition	2h
27-28/5/2010:	Final Exam (sensor: Prof. Arne Nylandsted Larsen at the Aarhus University, Denmark, http://person.au.dk/en/anl@phys.au.dk)	

Lecture 21: Empty lattice approximation; number of orbitals in a band

- **Repetion: periodic potential, nearly free electron model and Kronig-Penney model**
- **Empty lattice approximation**
- **number of orbitals in a band**

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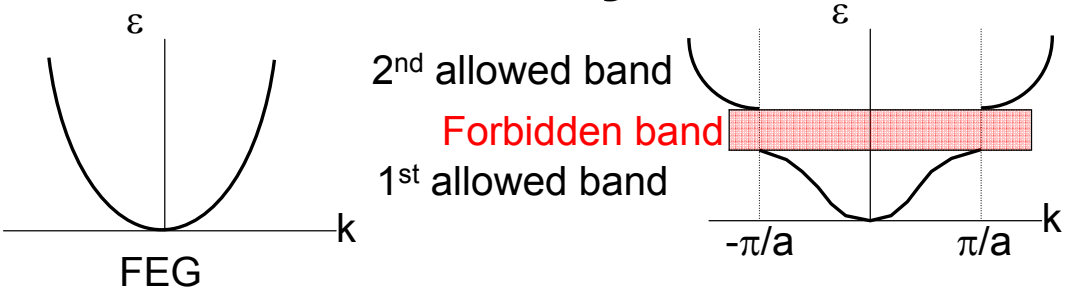
The nearly free e-



FEG

$$\varepsilon_k = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

$$k_x, k_y, k_z = 0; \quad \pm\frac{2\pi}{L}; \quad \pm\frac{4\pi}{L}; \quad \ldots$$

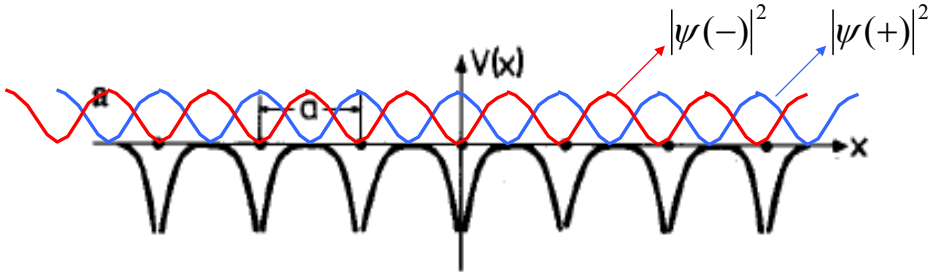
$$\psi_k(r) = \exp(i\vec{k}\cdot\vec{r})$$

What happens at the zone boundary

$$k = \pm\frac{1}{2}G = \pm\frac{n\pi}{a}$$ Bragg condition!!!

The wavefunctions at k=+/- π/a are not the traveling waves exp(iπx/a) or exp(-iπx/a) of free electrons.

$$\psi(+) = \exp(i\pi x/a) + \exp(-i\pi x/a) = 2\cos(\pi x/a) \quad \rho(+) = |\psi(+)|^2 \propto \cos^2(\pi x/a)$$
$$\psi(-) = \exp(i\pi x/a) - \exp(-i\pi x/a) = 2i\sin(\pi x/a) \quad \rho(-) = |\psi(-)|^2 \propto \sin^2(\pi x/a)$$

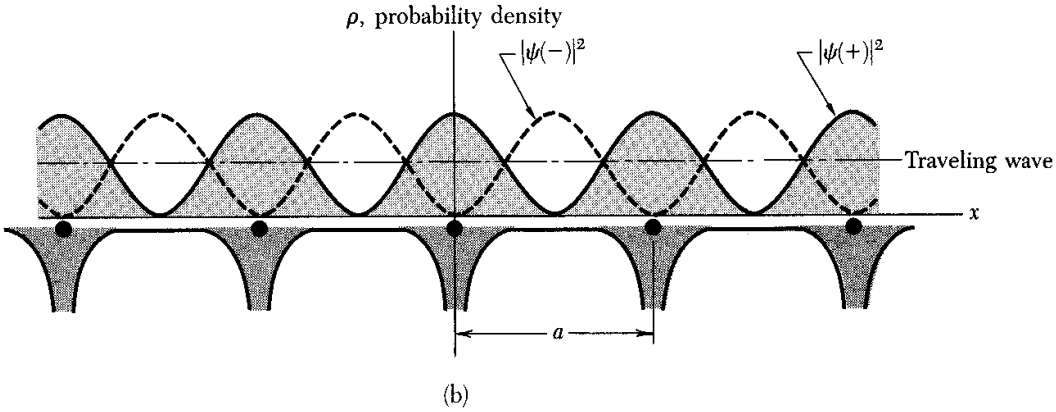


Energy of the two standing waves are different by E_g.

Periodic potential and Bloch functions

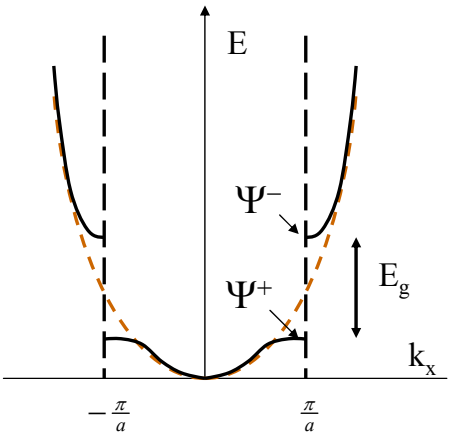
$\Psi^+ \sim 2\ \cos kx$ $\qquad$ $\Psi^- \sim 2i\ \sin kx$

$|\Psi^+|^2 \sim 4\ \cos^2 kx$ $\qquad$ $|\Psi^-|^2 \sim 4\ \sin^2 kx$

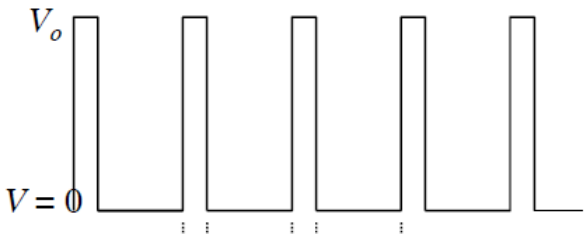


(b)

Periodic potential and Bloch functions

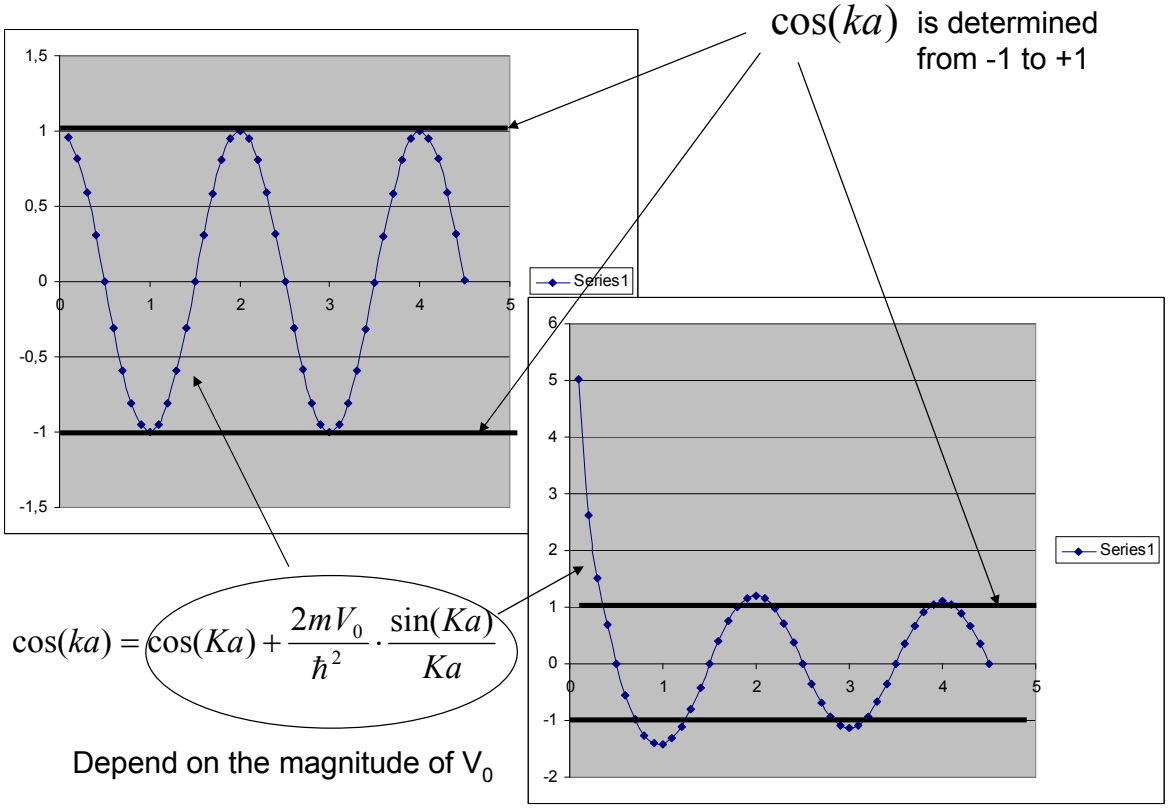


Kronig-Penney model



$$\cos(ka) = \cos(Ka) + \frac{2mV_0}{\hbar^2} \cdot \frac{\sin(Ka)}{Ka}$$

Kronig-Penney model



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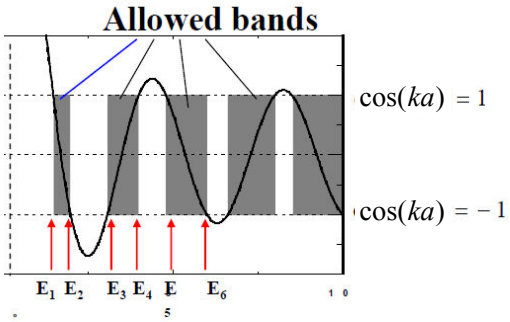
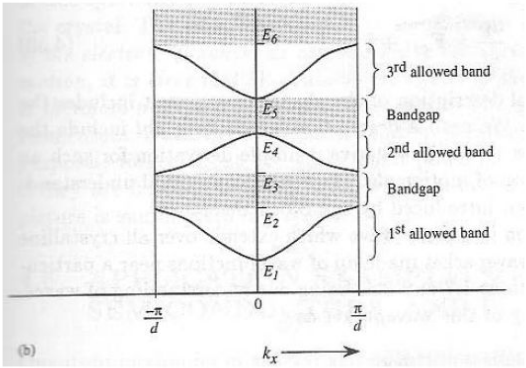
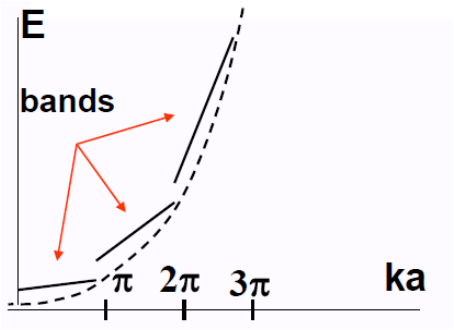


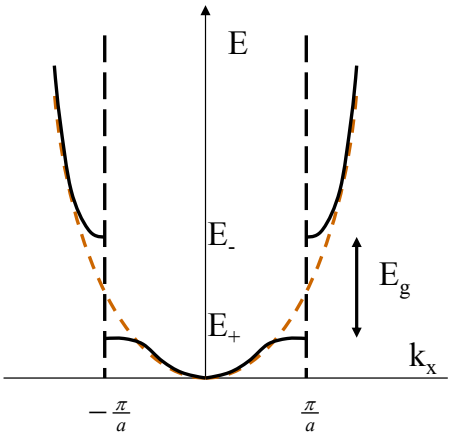
The allowed and forbidden bands are plotted in the E vs. k relation.



Kronig-Penney model

In between the two energies there are no allowed energies; i.e., an energy gap exists. We can sketch these 1-D results schematically:





The periodic potential U(x) splits the free-electron E(k) into "energy bands" separated by gaps at each BZ boundary.

Lecture 21: Empty lattice approximation; number of orbitals in a band

- **Repetion: periodic potential, nearly free electron model and Kronig-Penney model**
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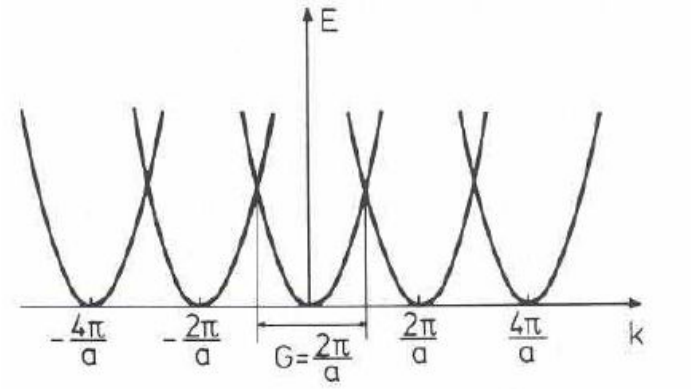
Property of $E(\vec{k}) = E(\vec{k} + \vec{G})$

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

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

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



in 3-dim.

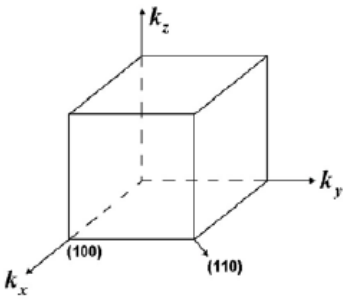
$$E(k_x, k_y, k_z) = \frac{\hbar^2}{2m}(\vec{k} + \vec{G})^2$$

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

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

As an exercise, figure out the free e-band of a simple cubic empty lattice. ie. the low-lying band

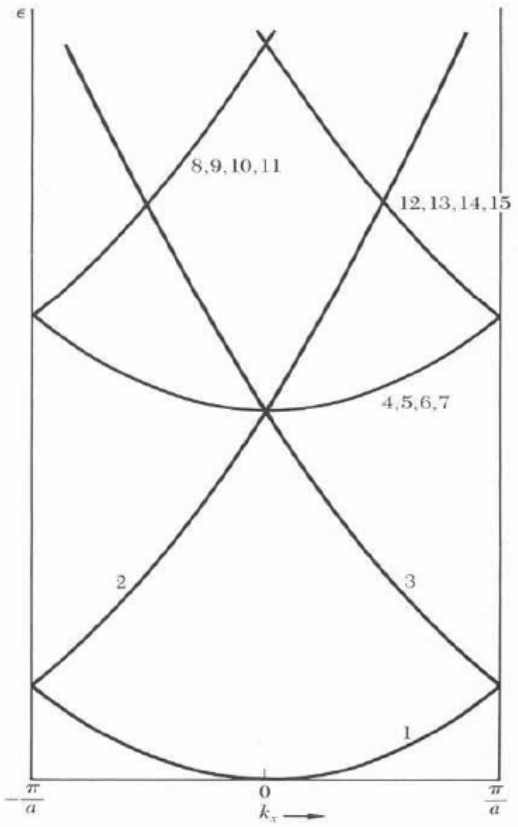
Reciprocal lattice of S.C ⇒S.C



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	$[110]\,[101]$ $[1\bar{1}0]\,[10\bar{1}]$	$2\left(\frac{2\pi}{a}\right)^2$	$\left(k_x^2 + \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2$
⋮	$[\bar{1}10]\,[\bar{1}01]\,[\bar{1}\bar{1}0]\,[\bar{1}0\bar{1}]$		$\left(k_x^2 - \frac{2\pi}{a}\right)^2 + \left(\frac{2\pi}{a}\right)^2$

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.



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The number of states in a band

Independent *k*-states in the first Brillouin zone, i.e. $|k_x| \leq \pi/a$ etc.

Finite crystal: only discrete *k*-states allowed $k_x = \pm\frac{2\pi n_x}{L}, n_x = 0,1,2,....$ etc.

Monatomic simple cubic crystal, lattice constant a, and volume V.

One allowed *k* state per volume $(2\pi)^3/V$ in k-space.

Volume of first BZ is $(2\pi/a)^3$

Total number of allowed k-states in a band is therefore

$$\left(\frac{2\pi}{a}\right)^3 \Big/ \frac{(2\pi)^3}{V} = \frac{V}{a^3} = N$$

Precisely *N* allowed *k*-states i.e. 2N electron states (Pauli) per band

This result is true for any lattice:
each primitive unit cell contributes exactly one *k*-state to each band.

Metals and insulators

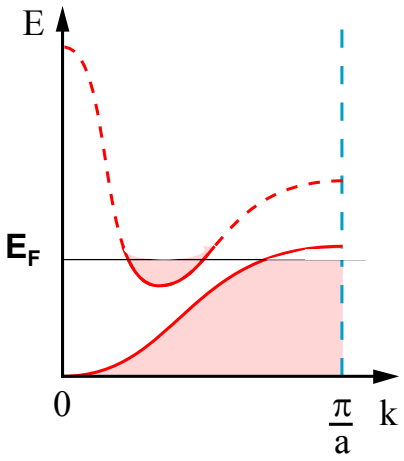
In full band containing 2N electrons all states within the first B. Z. are occupied. The sum of all the k-vectors in the band = 0.

A partially filled band can carry current, a filled band cannot

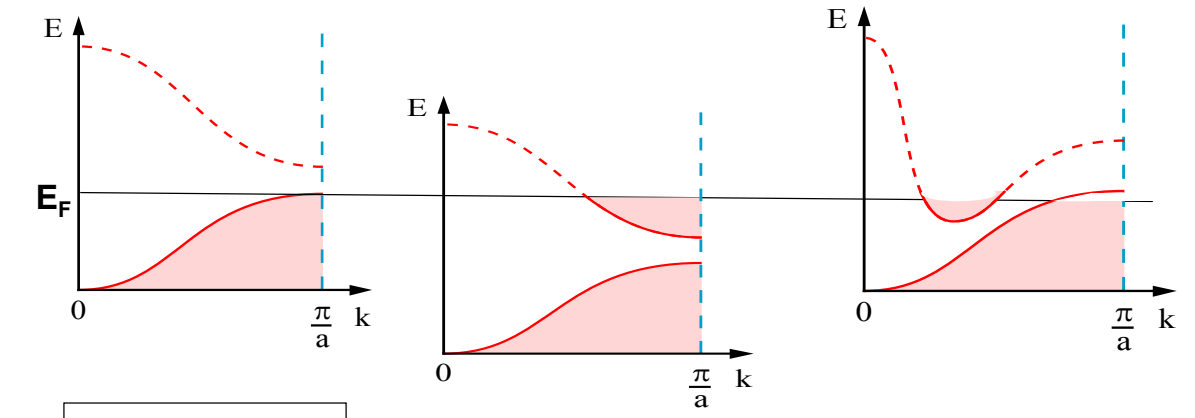
Insulators have an even integer number of electrons per primitive unit cell.

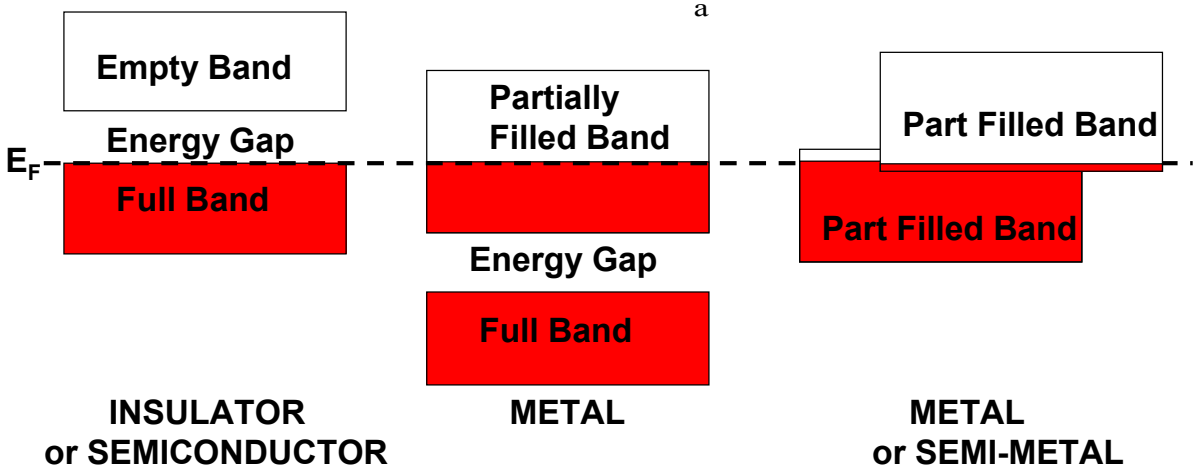
With an even number of electrons per unit cell can still have metallic behaviour due to band overlap.

Overlap in energy need not occur in the same k direction



Metal due to overlapping bands





Insulator -energy band theory