FYS3410 - Vår 2010 (Kondenserte fasers fysikk)

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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

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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:	no lectures	
W/12/5/2010:	no lectures	
W/19/5/2010:	Metals and Fermi surfaces	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 19: Drude model and the idea of energy bands

- **Repetition of FEFG**
- **Basic assumptions of the Drude model**
- **Electrical conductivity and Wiedemann-Franz law**
- **Hall effect**
- **Shortcomings of the Drude model**
- **Idea of energy bands**

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FEFG in 3D

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}}\,\psi_{\mathbf{k}}(\mathbf{r})$$

- **Invoking periodic boundary condition we get traveling waves as solutions:**

$$\psi(x+L, y, z) = \psi(x, y, z)$$

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) = \exp\,(i\mathbf{k}\cdot\mathbf{r})\ ,}$$

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

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)$$

$$\boxed{\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}\ .}$$

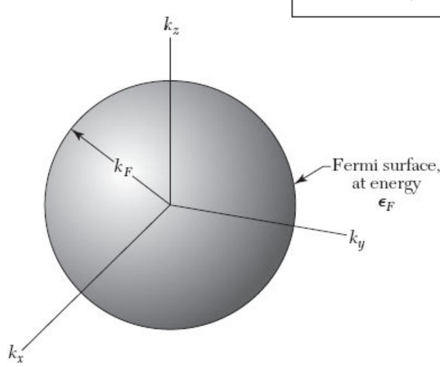

Figure 4 In the ground state of a system of N free electrons the occupied orbitals of the system fill a sphere of radius k_F, where $\epsilon_F = \hbar^2 k_F^2/2m$ is the energy of an electron having a wavevector k_F.

Effect of temperature; Fermi-Dirac distribution

- Describes the probability that an orbit at energy E will be occupied in an ideal electron gas under thermal equilibrium
- μ is chemical potential, f($\varepsilon = \mu$)=0.5; at 0K, $\varepsilon_F = \mu$

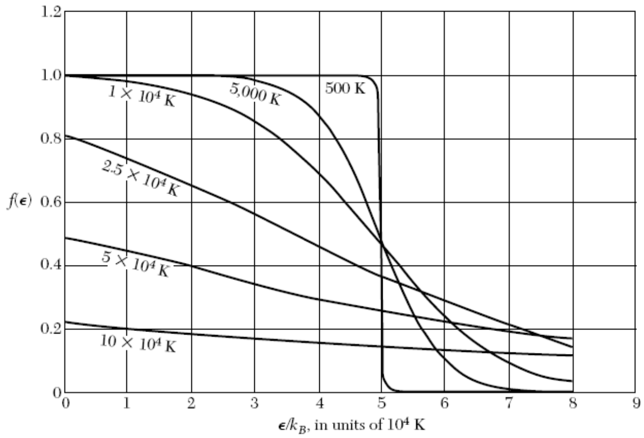

Figure 3 Fermi-Dirac distribution function (5) at the various labelled temperatures, for $T_F \equiv \epsilon_F/k_B = 50{,}000$ K. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature. The chemical potential μ at each temperature may be read off the graph as the energy at which $f = 0.5$.

$$f(\epsilon) = \frac{1}{\exp[(\epsilon - \mu)/k_BT] + 1} .$$

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Basic assumptions of the Drude model

Combining ideas of an electron as a “charge” carrier and kinetic gas theory

• no collisions between electrons - independent electron approximation;

• positive charge is located at the immobile ion cores and electronc can collide with the ion cores canging their velocity – however in between collisions no interaction is taking place – free lectron approximation;

• electrons reach thermal equilibrium with the lattice participating in the collisions so that the mean kinetic energy is $1/2\ (mv_t^2) = 3/2(k_B T)$

• τ - is a time in between collisions and $\lambda = v_t\ \tau$ - is a mean free path

• number of electrons participating in, e.g. conduction, is equivalent to the number of electrons on the outer shell of the atom providing concentrations in the range of $5x10^{22}$ electrons/cm^3

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m_e	k_B	T	v_t^2	v_t
9,10E-31	1,38E-23	300	1,36E+10	1,17E+05
9,10E-31	1,38E-23	273	1,24E+10	1,11E+05
9,10E-31	1,38E-23	77	3,50E+09	5,92E+04
9,10E-31	1,38E-23	15	6,82E+08	2,61E+04

Lambda	tau	q	n	conductivity
1,00E-09	8,56E-15	1,60E-19	5,00E+28	1,20E+07
1,00E-09	8,97E-15	1,60E-19	5,00E+28	1,26E+07
1,00E-09	1,69E-14	1,60E-19	5,00E+28	2,38E+07
1,00E-09	3,83E-14	1,60E-19	5,00E+28	5,38E+07

Here we have a problem: the calculated conductivity has increased but the actual experimental increase is significantly bigger.

However, one otfthe most convincing pieces of evidence of the Drude theory in his time used to be a qualitatively correct description of the Widemann-Fraz law – the ratio of teermal and electrical conductivity is a constant for all metals at a given temperature: $\kappa/\sigma = LT$.

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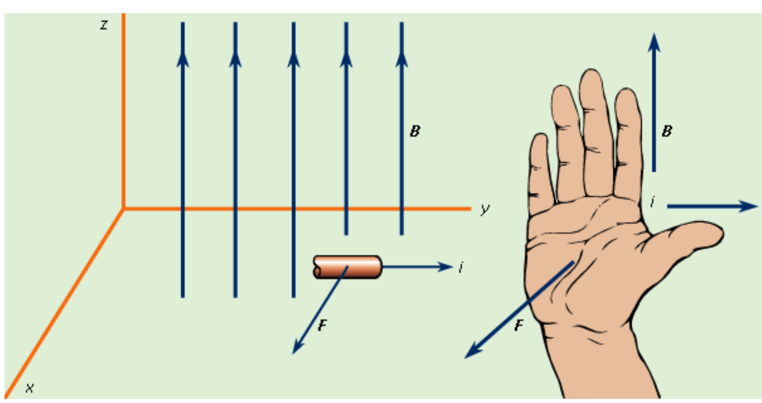
magnetic force: right-hand rules



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- temperature dependence of the electrical conductivity even for pure metals – because of unclear of the magnitude of the mean free path
- Scattering of R_H-values in terms of the sign and magnitudes
- alloying of very small amount of material (doping) may incease the conductivity by several orders of magnitude
- nearly no contribution to the specific heat from electrons at room temperature – contrudiction to the 3R-value by Dulong-Petit.
- …

!!! FEFG concept explains the last shortcoming. Indeed, only a small fraction of electrons – of the order of kT in the DOS-plot – have to be taken into consideration when calculating the heat capacity related to the electrons.

Bur FEFG can not explain the alloying or Hall effects…

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Adding the the potential created by the rest of the particles around

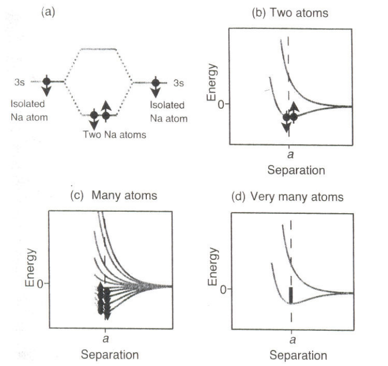


Figure 6.1 The formation of energy bands in solids. (a) Bonding and antibonding energy levels and their occupation for a molecule constructed from two Na atoms. The black dots and arrows symbolize the electrons with their spin. (b) The molecule's energy levels as a function of interatomic separation. (c) The energy levels for a cluster of many Na atoms as a function of their separation. (d) For very many energy levels there is a quasicontinuum between the lowest and highest energy levels. The band is half-filled with electrons as illustrated by the bar.

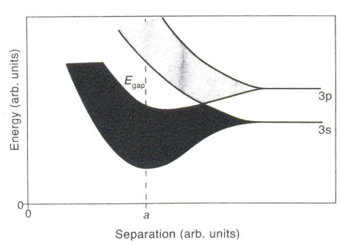
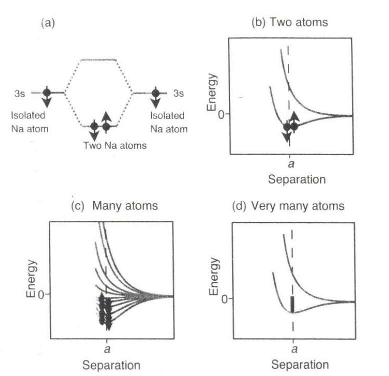


Figure 6.2 Band formation in Si. The lower band corresponds to the sp^3 states and is completely filled.



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