FYS3410 - Vår 2011 (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
- Imperfections in crystals: diffusion, point defects, dislocations
- 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 2011

W/19/1/2011:	Introduction and motivation. Periodicity and lattices	1h
M/24/1/2011:	Index system for crystal planes. Crystal structures	2h
W/26/1/2011:	Reciprocal space, Laue condition and Ewald construction	1h
M/31/1/2011:	Brillouin Zones. Interpretation of a diffraction experiment	2h
W/02/2/2011:	Crystal binding, elastic strain and waves	1h
M/07/2/2011:	Elastic waves in cubic crystals; defects in crystals	2h
W/09/2/2011:	Defects in crystals; case study – vacancies; diffusion	2h
M/14/2/2011:	Crystal vibrations and phonons	2h
W/16/2/2011:	Lattice heat capacity: Dulong-Petit and Einstein models	2h
M/21/2/2011:	Phonon density of states (DOS) and Debye model	2h
W/23/2/2011:	General result for DOS; role of anharmonic interactions	2h
M/28/2/2011:	Thermal conductivity and repetition of crystal vibrations	2h
W/02/3/2011:	no lectures	
M/07/3/2011:	no lectures	
W/09/3/2011:	no lectures	
M/14/3/2011:	Free electron Fermi gas in 1D and 3D – ground state	2h
W/17/3/2011:	Density of states, effect of temperature – FD distribution	1h
M/21/3/2011:	Heat capacity of FEFG	2h
W/23/3/2011:	Repetition	1h
M/28/3/2011:	Mid-term exam	

M/04/4/2011:	**Electrical and thermal conductivity in metals**	**2h**
W/06/4/2011:	**Bragg reflection of electron waves at the boundary of BZ**	**2h**
M/11/4/2011:	**Energy bands, Kronig - Penny model**	**2h**
W/13/4/2011:	**Empty lattice approximation; number of orbitals in a band**	**2h**
Påsk uppehåll		
W/27/4/2011	**no lectures**	
M/02/5/2011:	**no lectures**	
W/04/5/2011:	**no lectures**	
M/09/5/2010:	**Semiconductors, effective mass method, intrinsic carriers**	**2h**
W/11/4/2010:	**Impurity states in semiconductors and carrier statistics**	**2h**
M/16/5/2010:	**p-n junctions, Schottky contacts and heterojunctions**	**2h**
W/18/5/2010:	**Metals and Fermi surfaces**	**1h**
M/23/5/2010:	**Repetition**	**2h**
26-27/5/2010:	**Final Exam (sensor:???)**	

Lecture 15: Free electron Fermi gas

- **Free electron Fermi gas (FEFG) – a gas of electrons subject to Pauli principle**
- **One electron system – wave functions – orbits; FEFG in 1D in ground state**
- **FEFG in 3D in ground state**
- **Effect of temperature; Fermi-Dirac distribution**

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Free electron Fermi gas – a gas of electrons subject to Pauli principle

- At low temperature, free mean path of a conduction electron in metal can be as long as 1 cm! Why is it not affected by ion cores or other conduction electrons? (30 seconds discussions)
  - Motion of electrons in crystal (matter wave) is not affected by periodic structure such as ion cores.
  - Electron is scattered infrequently by other conduction electrons due to the Pauli exclusion principle

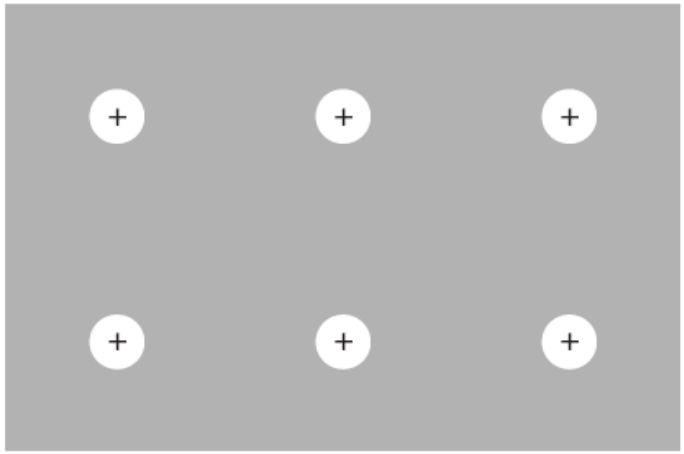

Figure 1 Schematic model of a crystal of sodium metal. The atomic cores are Na^+ ions: they are immersed in a sea of conduction electrons. The conduction electrons are derived from the $3s$ valence electrons of the free atoms. The atomic cores contain 10 electrons in the configuration $1s^2 2s^2 2p^6$. In an alkali metal the atomic cores occupy a relatively small part (~15 percent) of the total volume of the crystal, but in a noble metal (Cu, Ag, Au) the atomic cores are relatively larger and may be in contact with each other. The common crystal structure at room temperature is bcc for the alkali metals and fcc for the noble metals.

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One electron system – wave functions - orbits

- **Neglect electron-electron interaction, infinite potential well, simple QM solution**

$$\psi_n = A \sin\left(\frac{2\pi}{\lambda_n}x\right) ; \qquad \tfrac{1}{2}n\lambda_n = L \ , \qquad \epsilon_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 .$$

Standing wave B. C.
n = 1, 2, …

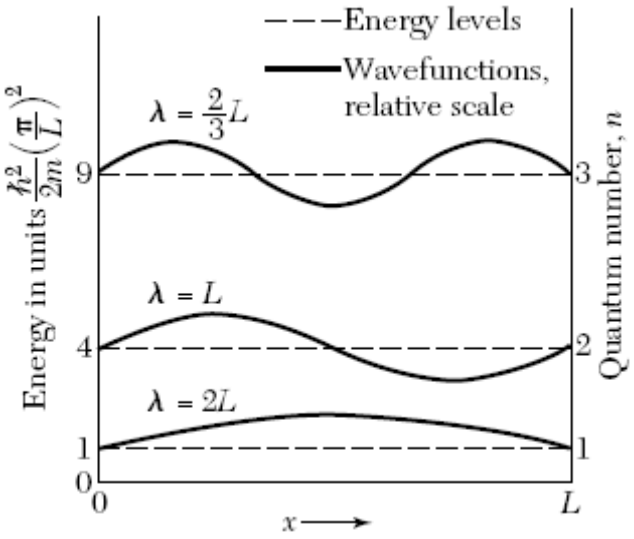

Figure 2 First three energy levels and wavefunctions of a free electron of mass m confined to a line of length L. The energy levels are labeled according to the quantum number n which gives the number of half-wavelengths in the wavefunction. The wavelengths are indicated on the wavefunctions. The energy ϵ_n of the level of quantum number n is equal to $(h^2/2m)(n/2L)^2$.

- The Pauli exclusion principle
– n: quantum number
– m(=1/2 and -1/2): magnetic quantum number
- degeneracy: # of orbitals with the same energy
- Fermi energy (E_F): energy of the topmost filled level in the ground state of the N electron system

In this simple system, every quantum state holds 2 electrons => $n_F = N/2$ ➔ Fermi energy:

$$\epsilon_F = \frac{\hbar^2}{2m}\left(\frac{n_F\pi}{L}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2$$

Great, if we know the electron density, we know the Fermi energy!

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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 instead of the infinite potential wall (standing wave) boundary condition, we get traveling waves as solutions:**

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

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

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

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

$$k=2\pi/\lambda$$

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 $\epsilon_F=\hbar^2k_F^2/2m$ is the energy of an electron having a wavevector k_F.

Only if we know how much space one k point occupies ($\delta k_x \delta k_y \delta k_z = (2\pi/L)^3$)

$$\epsilon_F=\frac{\hbar^2}{2m}k_F^2$$

Due to spin →

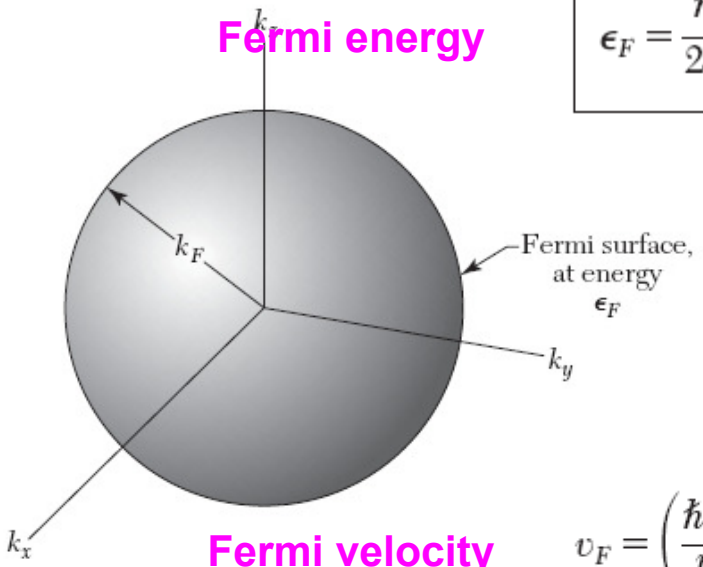
$$2\cdot\frac{4\pi k_F^3/3}{(2\pi/L)^3}=\frac{V}{3\pi^2}k_F^3=N$$

Fermi wave vector

$$k_F=\left(\frac{3\pi^2N}{V}\right)^{1/3}$$

Fermi energy

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



Fermi velocity

$$v_F=\left(\frac{\hbar k_F}{m}\right)=\left(\frac{\hbar}{m}\right)\left(\frac{3\pi^2N}{V}\right)^{1/3}$$

Table 1 Calculated free electron Fermi surface parameters for metals at room temperature

(Except for Na, K, Rb, Cs at 5 K and Li at 78 K)

Valency	Metal	Electron concentration, in cm^{-3}	Radius[a] parameter r_s	Fermi wavevector, in cm^{-1}	Fermi velocity, in $cm\ s^{-1}$	Fermi energy, in eV	Fermi temperature $T_F \equiv \epsilon_F/k_B$, in deg K
1	Li	4.70×10^{22}	3.25	1.11×10^{8}	1.29×10^{8}	4.72	5.48×10^{4}
	Na	2.65	3.93	0.92	1.07	3.23	3.75
	K	1.40	4.86	0.75	0.86	2.12	2.46
	Rb	1.15	5.20	0.70	0.81	1.85	2.15
	Cs	0.91	5.63	0.64	0.75	1.58	1.83
	Cu	8.45	2.67	1.36	1.57	7.00	8.12
	Ag	5.85	3.02	1.20	1.39	5.48	6.36
	Au	5.90	3.01	1.20	1.39	5.51	6.39
2	Be	24.2	1.88	1.93	2.23	14.14	16.41
	Mg	8.60	2.65	1.37	1.58	7.13	8.27
	Ca	4.60	3.27	1.11	1.28	4.68	5.43
	Sr	3.56	3.56	1.02	1.18	3.95	4.58
	Ba	3.20	3.69	0.98	1.13	3.65	4.24
	Zn	13.10	2.31	1.57	1.82	9.39	10.90
	Cd	9.28	2.59	1.40	1.62	7.46	8.66
3	Al	18.06	2.07	1.75	2.02	11.63	13.49
	Ga	15.30	2.19	1.65	1.91	10.35	12.01
	In	11.49	2.41	1.50	1.74	8.60	9.98
4	Pb	13.20	2.30	1.57	1.82	9.37	10.87
	Sn(w)	14.48	2.23	1.62	1.88	10.03	11.64

[a]The dimensionless radius parameter is defined as $r_s = r_0/a_H$, where a_H is the first Bohr radius and r_0 is the radius of a sphere that contains one electron.

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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, $\varepsilon_F = \mu$

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

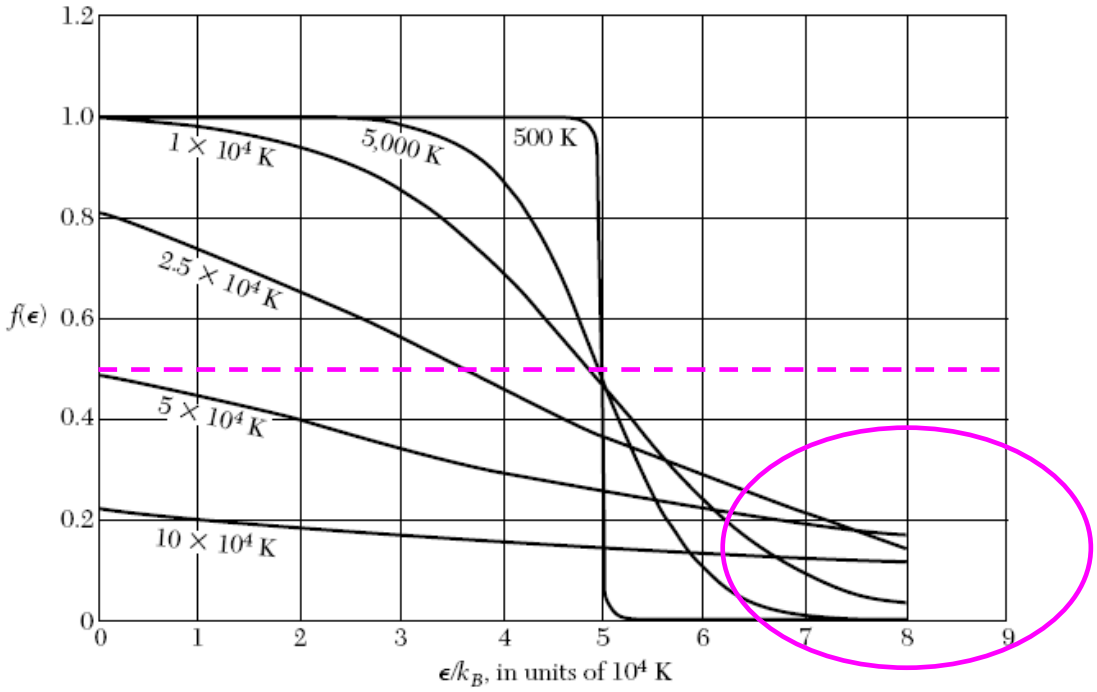


Figure 3 Fermi-Dirac distribution function (5) at the various labelled temperatures, for $T_F \equiv \epsilon_F/k_B = 50{,}000$ K. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature. The chemical potential μ at each temperature may be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

In comparison,

$$f_{Bose-Einstein}(E) = \frac{1}{\exp(\frac{\hbar\omega}{k_B T}) - 1}$$

High energy tail – approximation

$$E - E_F > 3k_B T$$

➔ **Boltzmann-Maxwell distribution**

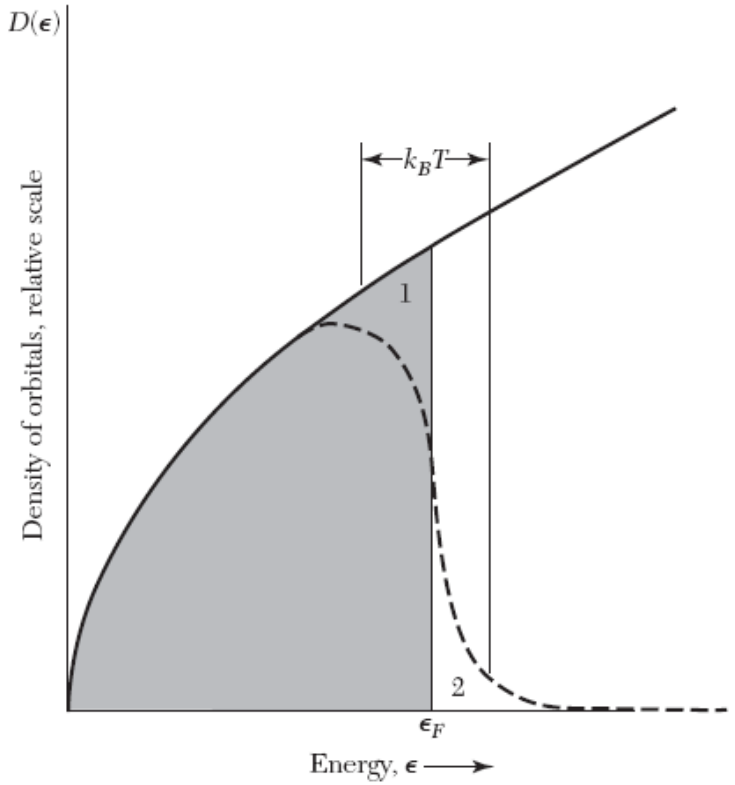
$$f_{Boltzmann-Maxwell}(E) = \exp(-\frac{E - E_F}{k_B T})$$

DOS example: free electrons (parabolic dispersion)

$$3D-DOS(cm^{-3}eV^{-1})$$

$$\frac{d^3k}{(2\pi)^3}=\frac{4\pi k^2dk}{(2\pi)^3}=\frac{4\pi k(E)^2}{(2\pi)^3}\frac{dk}{dE}dE=g_{3D}(E)dE \Rightarrow g_{3D}(E)=2\cdot\frac{4\pi\left(\frac{2mE}{\hbar^2}\right)}{(2\pi)^3}\cdot\sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{E}}=\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}E^{1/2}$$

- **# of states between E and E+dE**



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

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

Note here: $N=N(\varepsilon)$
D(E) has a unit of ev^{-1}.

$$D(\epsilon)\equiv\frac{dN}{d\epsilon}=\frac{V}{2\pi^2}\cdot\left(\frac{2m}{\hbar^2}\right)^{3/2}\cdot\epsilon^{1/2}.$$

Figure 5 Density of single-particle states as a function of energy, for a free electron gas in three dimensions. The dashed curve represents the density $f(\epsilon, T)D(\epsilon)$ of filled orbitals at a finite temperature, but such that k_BT is small in comparison with ϵ_F. The shaded area represents the filled orbitals at absolute zero. The average energy is increased when the temperature is increased from 0 to T, for electrons are thermally excited from region 1 to region 2.