

Lecture 13 – Band structure of metals, surface effects

Reading

Ashcroft & Mermin, Ch. 12 (225 - 228), Ch. 14 (264 - 274), 15, 18

Content

- Holes
- Motion of Bloch electrons in magnetic field
- de Haas - van Alphen effect
- Shubnikov - de Haas effect
- Landau levels
- Band structure of selected metals
- The color of a metal
- Work function

Central concepts

- **Holes**

Properties

- 1) Charge $+e$
- 2) $m_h > 0$
- 3) $\mathbf{k}_h = -\mathbf{k}_e$
- 4) $\varepsilon(\mathbf{k}_h) = -\varepsilon(\mathbf{k}_e)$
- 5) $\mathbf{v}_e = \mathbf{v}_h$

- **Motion of Bloch electrons in magnetic field**

Semiclassical approximation

$$\hbar \frac{d\mathbf{k}}{dt} = -e(\mathbf{v}_g \times \mathbf{B})$$

where

$$\mathbf{v}_g = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon$$

This gives $d\mathbf{k}/dt$ parallel with the Fermi surface. *The electron moves along the Fermi surface in a plane perpendicular to the magnetic field (in k -space).*

- **de Haas - van Alphen effect**

Oscillations of magnetization / susceptibility as a function of magnetic field. Periods in $1/B$ depend on presence of extremal cross-section areas A_e of the Fermi surface in the plane normal to the magnetic field.

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar} \cdot \frac{1}{A_e}$$

- **Shubnikov - de Haas effect**

Similar oscillations but in conductivity / resistivity.

- **Landau levels**

The energy of free electrons in magnetic field (along z) is quantized:

$$\varepsilon = \left(n + \frac{1}{2}\right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m}$$

where $n = 0, 1, 2, \dots$ and

$$\omega_c = \frac{eB}{m}$$

is the cyclotron frequency. All levels of certain n are referred to as being in the n th Landau level.

- **Band structure of selected metals**

d-orbitals give 5 narrow d-bands that appear at different locations relative to the Fermi surface for different materials.

The noble metals have ε_F about 2 to 5 eV above the d-bands, to give almost free-electron like Fermi surface.

The transition metals have partially filled d-shells and their d-bands extend through the Fermi surface. Since the d-bands are narrow and contain more levels than free electron bands, the density of states at the Fermi level may become very high.

- **The color of a metal**

A photon may be absorbed and excite an electron from the d-bands to the conduction band, which is the reason for the color of, for instance, Cu and Au.

- **Work function**

$$W = -\varepsilon_F + W_s$$

where

$$W_s = \int e\mathbf{E} \cdot d\mathbf{l}$$