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Problems for *Physik der Materie III*

Due by June 19, 2019

Series 8: Electron energy bands and Fermi surface

8.1 Free electrons in square and cubic lattices

(a) Calculate the ratio $E_{\bar{X}}/E_{\bar{M}}$ of the energies of a free electron at a corner of the first Brillouin zone ($\bar{X}$-point) of a two-dimensional square lattice and at the midpoint of a side face ($\bar{M}$-point).

(b) What is the corresponding ratio for a three-dimensional simple cubic lattice, i. e. for the R- and X-points (Fig. 1)?

(c) The electronic band structure of crystalline solids is usually presented by plotting the energy E versus the wave vector $\boldsymbol{k}$ along particular straight lines in $\boldsymbol{k}$-space. Such $E(\boldsymbol{k})$ curves are shown in the reduced zone scheme along directions of high symmetry.
For free electrons in a two-dimensional square lattice, make a simple sketch of the lowest energy band along two lines in the first Brillouin zone joining the points $\bar{\Gamma}(\boldsymbol{k}=0)$ and $\bar{M}$ as well as the points $\bar{\Gamma}$ and $\bar{X}$. Take into account the different energies at the Brillouin zone boundaries determined in (a).

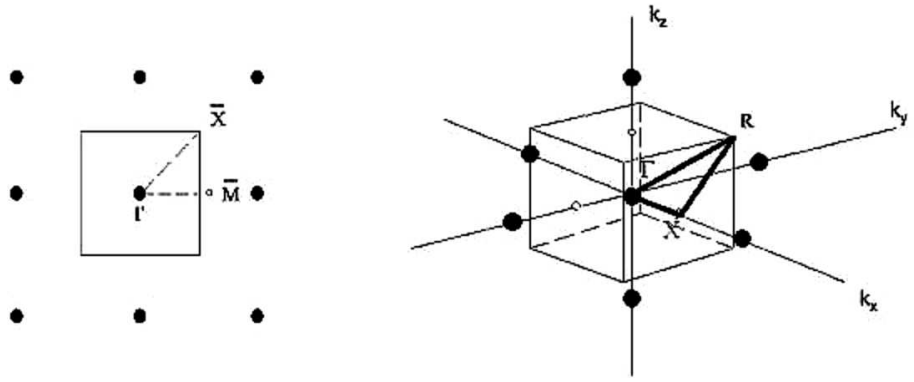

Figure 1: Brillouin zones of a two-dimensional square lattice (left) and a three-dimensional simple cubic lattice (right). Points of high symmetry are denoted $\Gamma, X, R, \bar{\Gamma}, \bar{M}, \bar{X}$.

8.2 Fermi surface of a rectangular lattice

A two-dimensional metal has one atom of valency one in a simple rectangular primitive cell with constants $a_1 = 2$ Å and $a_2 = 4$ Å. The metal is assumed to behave like a free electron Fermi gas.

(a) Calculate the dimensions of the first Brillouin zone in cm^{-1}.

(b) Calculate the radius k_F of the free electron Fermi "sphere" in cm^{-1}.
Use the number of states $N(k)$ of a free electron gas in two dimensions and express k_F in terms of the electron density n_{el}.

(c) Draw the Fermi "sphere" to scale on a drawing of the first Brillouin zone.

(d) Sketch the first two Brillouin zones in the extended zone scheme.

(e) Sketch the Fermi "sphere" in the reduced zone scheme. Occupied electron states should be marked by shaded areas.

(f) Sketch the Fermi "sphere" in the extended zone scheme and discuss the changes that occur for nearly free electrons, i. e. for electrons in a rectangular lattice with a weak periodic potential.

(g) Make simple sketches of the lowest two energy bands $E(\boldsymbol{k})$ along a line in the first Brillouin zone joining the points $\boldsymbol{k} = (0, 0)$ ($\bar{\Gamma}$-point) and $\boldsymbol{k} = (\pi/a_1, 0)$ ($\bar{M}$-point) for free and nearly free electrons. Use the reduced zone scheme and mark the occupied and unoccupied energy states.