10. ELECTRON DYNAMICS IN ENERGY BANDS.

Aim: This part of the course serves as a general basis for the later lecture on semiconductors. It has also applications in the studies of other substances. In order to study, for example the electrical properties of semiconductors, we need a basic understanding of the motion of electrons in energy bands, i.e. in reciprocal space. This section introduces some important concept related to the dynamic properties of the electrons.

We have earlier treated the equation of motion of an electron within the free electron model. This equation is the same in the present case, but the existence of the reciprocal lattice and Brillouin zones necessitates a more detailed analysis. In particular we study how the electrons move in k-space under the influence of electric and magnetic fields.

1. Equation of motion (K p. 191-194, 230-232).

We concentrate on the behaviour in k-space. The equation of motion is the same as for the free electrons:

$(h/2\pi)\, d\mathbf{k}/dt = -e\,(\mathbf{E} + \mathbf{v}\times\mathbf{B})$.

We consider the motion in a magnetic field. Since the group velocity is $\mathbf{v}=(2\pi/h)\,\nabla_{\mathbf{k}}\varepsilon$, the electrons are moving orthogonal to the applied field and the energy gradient. This means that the electrons move on a surface of constant energy orthogonal to **B**. An electron at the Fermi surface will move in an orbit on the Fermi surface. Three different types of orbits can be defined (K p. 230), namely electronlike (the Fermi surface limits filled states), holelike (the Fermi surface limits a pocket of empty states) and open (the electrons can move on the Fermi surface from zone to zone in non-closed orbits). The latter description refers to the extended zone scheme; in the reduced zone scheme Bragg reflection occurs at the zone boundary and the electron is ”umklapped” to the equivalent position on the other side of the Brillouin zone.

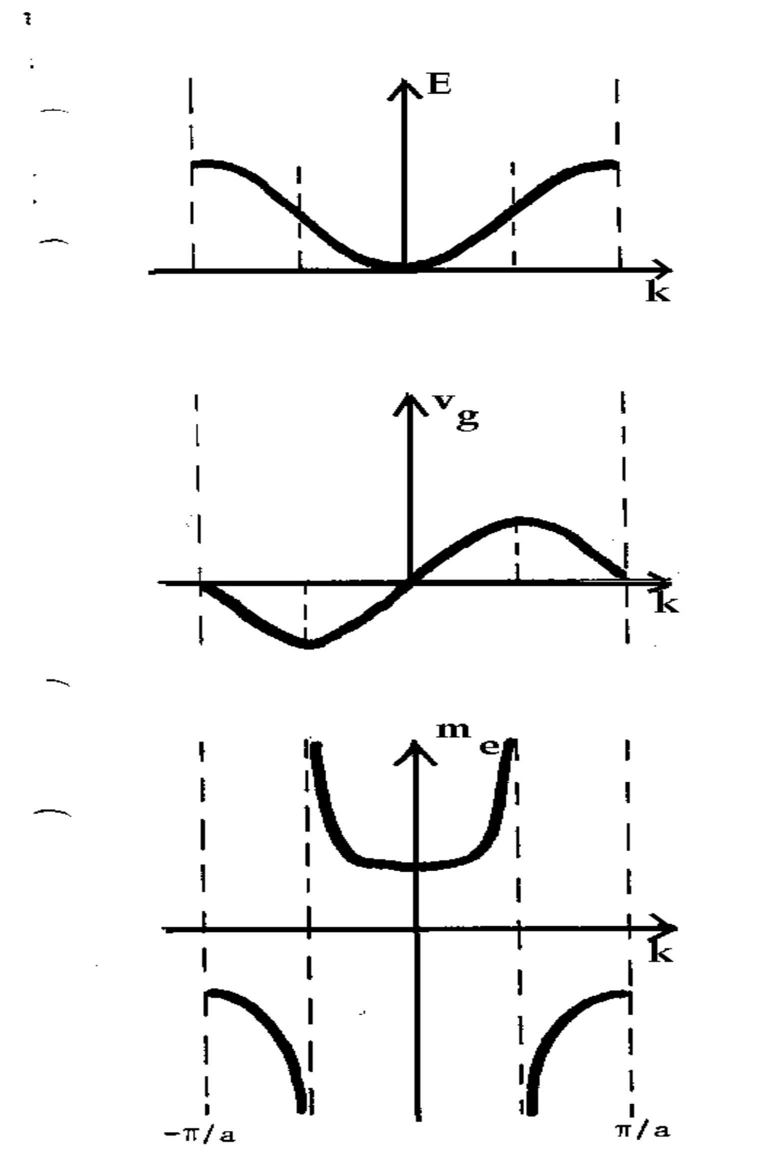
The motion of electrons in orbits in a magnetic field forms the basis of experimental methods for determination of the Fermi surface.

2. Effective mass (K p. 197-200).

We have earlier encountered effective electron masses used to reconcile free electron theory with experiments. Here we find a physical basis of this concept. We determine the relation between the acceleration and force for electron motion in an energy band. The mass of the electron has now to be replaced by an effective mass, eq. (28), K. p.198. For free electrons it reduces to the usual electron mass. The same holds for low k. As k increases the effective mass increases, and becomes negative close to the boundary of the Brillouin zone. Electrons in bonds give rise to narrower energy bands than nearly free electrons, and hence to larger effective electron masses.

The figure below illustrates in one dimension: (a) a typical energy band (b) the velocity of the electron (which is proportional to derivative of energy with respect to k) and (c) the effective mass, which is inversely proportional to the second derivative of energy with respect to k.

The characteristic variation of the effective mass through a nearly-free-electron band is clearly displayed:



3. Holes (K p. 194-197).

Empty orbitals in almost filled bands are called holes. It is much easier to describe the dynamics in a nearly filled band with a small number of holes than by considering a macroscopic number of electrons. A completely filled band cannot give rise to electrical conduction, because there are no vacant states that the electrons can move to. A nearly filled band can however give rise to conduction. We say that it is the holes that are responsible for electrical conduction in this case.

Properties of holes:

1. The sum of all **k**-vectors in a filled band is zero. Now remove one electron from state j. We assign to the hole the sum of the **k**-vectors of the remaining electrons. This is minus the **k** for the vacant state. Hence (h stands for hole and e for electron) $\mathbf{k}_h = -\mathbf{k}_e$.

2. Consider the current density from the nearly filled band,

$$\mathbf{J} = \sum_{i \neq j} (-e\mathbf{v}_i) = e\mathbf{v}_j.$$

The hole is considered to move with the same velocity as an electron in "j" and to have a positive charge.

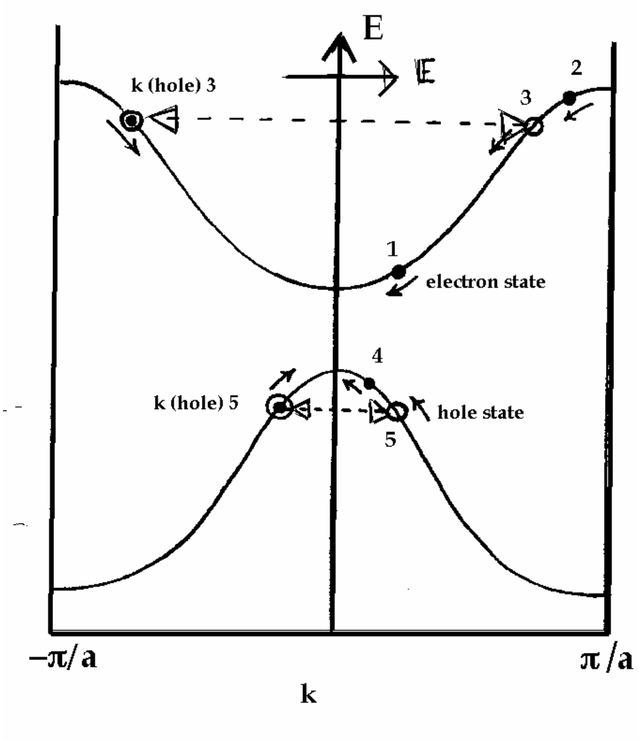
3. This is so, because the equation of motion for $\mathbf{k}_h$ is just like the one above upon substitution of +e for -e. This follows because $\mathbf{k}_h = -\mathbf{k}_e$.

4. The behaviour of the effective mass follows from the equation of motion in real space. Electron and hole velocities are equal and hence also their accelerations. On the force side of the equation the sign is changed, because the charges of electrons and holes have different sign. It follows for the effective masses that $m_h = -m_e$.

In certain cases we have electrons in one band and holes in another one. They give additive contributions to the electrical conductivity of the material. Hence, in real space, electrons and holes move in opposite directions.

How do holes move in k-space? The equation of motion says that electrons move in a k-direction opposite to an applied **E**-field. By the same reasoning, $\mathbf{k}_h$ moves in the direction of the applied field. However, the position of the hole in **k**-space is at $-\mathbf{k}_h$. This meands that **the position of the hole is moving against the applied field, i.e. in the same direction as the electrons**.

The figure below (adapted from Myers) shows a typical energy band for the one-dimensional case. Filled circles denote examples of filled electron states. The empty circles denote empty electron states, while the dots surrounded by a circle denote the corresponding **k**-vectors of the holes.



4. Hall effect (K p.153-156).

By measurements of the Hall coefficient one can determine the sign of the charge carriers in a material, as well as their concentration. As a prerequisite make a repetition of the equation of motion of an electron in electric and magnetic fields in real space.

When a current flows in the x-direction through a long specimen and a magnetic field is applied in the z-direction, the charge carriers are deflected in the negative y-direction. Both positive and negative charge carriers are deflected in the same direction. In steady state a transverse electric field exists in the y-direction. The sign is given by the sign of the carriers. This Hall field is directed as **j**x**B** for negative charge carriers and in the opposite direction for positive ones. The Hall coefficient is defined as

$$R_H = -\mathbf{E}_y / \mathbf{j}\mathrm{x}\mathbf{B} = \pm\ 1/ne,$$

where the + is for positive and the - for negative charges. In addition n is the concentration of charge carriers. We can now understand the positive values of the Hall coefficient that were measured for some metals (K p.155), even for nearly free electron ones like aluminium. For these metals conduction by holes in pockets at the top of partially filled bands is obviously dominating the dynamics.

In the presence of both electrons and holes, the equation above becomes more complicated, see Physics Handbook p. 366.