PHYSICS 315

Supplementary Lecture Notes

4.5 Hall Effect

The Hall effect provides important information about the nature of the charge carriers in a conducting material. The setup for a measurement of the effect is illustrated schematically in figure 1 below.

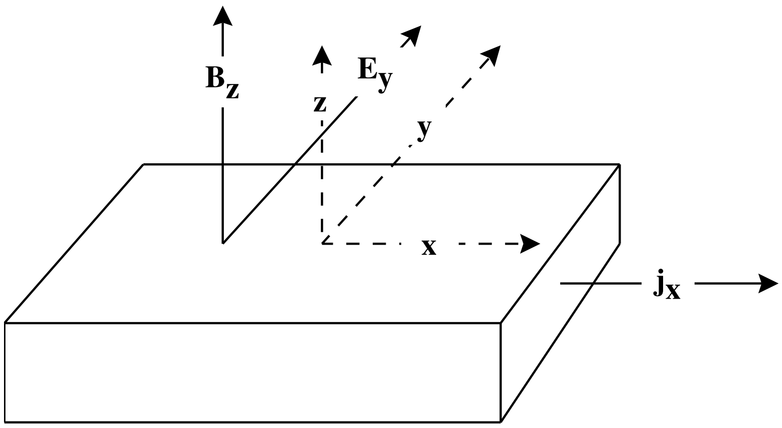

Figure 1: Setup for the Hall effect

An electric current

$$J = j_x A = nev_x A$$

passes through the sample in the $x-$direction. Here j_x is the current density, A the cross-sectional area, n is the carrier density (number of conduction electrons per unit volume), e the carrier charge (negative for electrons), v_x the carrier drift velocity. If there is a constant magnetic induction B_z in the $z-$direction, there will be a force

$$f_y = -eB_z v_x$$

in the $y-$direction. In order to prevent a buildup of elctric charge the force f_y must be compensated by an electric field

$$E_y = B_z v_x = \frac{j_x B_z}{ne}$$

The ratio

$$R_H = \frac{-E_y}{j_x B_z}$$

Table 1: Hall coefficients for some metals

metal	-neR$_H$	metal	-neR$_H$
Li	0.8	Al	-0.3
Na	1.2	Be	-0.4
Rb	1.1	Mg	-0.3
Cs	1.0	Ca	-0.3

is called the *Hall coefficient.* The electric field, the magnetic induction and the current can all be measured, and the resulting Hall coefficient can be compared with the theoretical value $-1/ne$. The results (for high purity samples, at low temeperatures and high field, as quoted in the book by Ashcroft and Mermin), are listed in table 1 for some metals.

The results for the monovalent alkali metals are quite reasonable, but for a number of di- and tri-valent metals not only is the value off by a significant factor, but the sign is wrong, suggesting that that the electrons have positive charge. To resolve this paradox we must go beyond the Drude and Sommerfeld models and consider *electron energy bands in a crystalline solid.*

4.6 Bloch's theorem

The Sommerfeld model discussed previously assumed

1. Electrons move in a constant crystal potential.

2. Dynamical aspects of the interaction among electrons can be neglected.

Our next step is to advance to the *independent elctron model.* This means that we drop assumption 1. above, but keep 2. We do not neglect the electron-electron interaction altogether, but assume that the electrons move in a *self-consistent* potential due to the ions and the other valence electrons. This procedure is otherwise known as *mean field theory*, and is very commonly used in condensed matter physics to obtain theories that give a good overall picture of the phenomena. It should be kept in mind that it is still an approximation, and there are a number of effects that require one to go beyond the independent electron model.Let

$$\vec{L} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

be a lattice vector and $\vec{a}, \vec{b}, \vec{c}$ primitive latice vectors, and

$$\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$$

a reciprocal lattice vector, with $\vec{A}, \vec{B}, \vec{C}$ the primitive ones. The electron wave functions will satisfy a Schrödinger equation where the Hamiltonian must have the periodicity of the lattice.

$$H(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

$$H(\vec{r})\psi(\vec{r} + \vec{L}) = E\psi(\vec{r} + \vec{L})$$

We note that $\psi(\vec{r})$ and $\psi(\vec{r} + \vec{L})$ are solutions to *same differential equation.* From the theory of differential equations we learn that this means that the two solutions can only differ by a constant[1].

$$\psi(\vec{r} + \vec{a}) = c_1\psi(\vec{r})$$

$$\psi(\vec{r} + \vec{b}) = c_2\psi(\vec{r})$$

$$\psi(\vec{r} + \vec{c}) = c_3\psi(\vec{r})$$

$$\psi(\vec{r} + \vec{L}) = (c_1)^{n_1}(c_2)^{n_2}(c_3)^{n_3}\psi(\vec{r})$$

We must next consider the boundary conditions. Assume that the crystal contains N_1 unit cells in the $\vec{a}$ direction, N_2 cells in the $\vec{b}$ direction and N_3 cells in the $\vec{c}$ direction. In a real crystal we would reach a surface when coming to the last cell in any direction. Just as we did in the case of lattice modes, we avoid the added complication of surface states by applying *peridic boundary conditions* (sometimes called Born von Kàrman boundary conditions)

$$\psi(\vec{r} + N_1\vec{a}) = \psi(\vec{r} + N_2\vec{b}) = \psi(\vec{r} + N_2\vec{c}) = \psi(\vec{r})$$

This means that

$$(c_1)^{N_1} = (c_2)^{N_2} = (c_3)^{N_3} = 1$$

with solutions

$$c_i = \exp(\frac{2\pi i\nu_i}{N_i}), \quad with\ i = 1, 2, 3, \quad and\ \nu_i\ \ integer$$

[1]This is strictly speaking only true if the solutions are *non-degenerate*, *i.e*, there is only one spatial state for each energy eigenvalue. This turns out not to be a serious difficulty since one can always find a complete set of solutions for which the statement is true

If we now define the wave vector

$$\vec{q} = \frac{\nu_1}{N_1}\vec{A} + \frac{\nu_2}{N_2}\vec{B} + \frac{\nu_3}{N_3}\vec{C}$$

we see we can label the spatial eigenstates by the wavevector and

$$\psi_{\vec{q}}(\vec{r} + \vec{L}) = e^{i\vec{q}\cdot\vec{L}}\psi_{\vec{q}}(\vec{r})$$

Next we note that since

$$e^{i\vec{G}\vec{L}} = 1$$

for any reciprocal lattice vector $\vec{G}$ and lattice vector $\vec{L}$, we can (just as we did in the case of lattice vibrations) restrict the wavevector $\vec{\mathbf{q}}$ to the first *Brillouin zone*. Let us now define a function

$$u_{\vec{q}}(\vec{r}) = e^{-\vec{q}\cdot\vec{r}}\psi_{\vec{q}}(\vec{r})$$

we find

$$u_{\vec{q}}(\vec{r} + \vec{L}) = e^{-\vec{q}\cdot(\vec{r}+\vec{L})}\psi(\vec{r} + \vec{L}) = e^{-i\vec{q}\cdot\vec{r}}\psi_{\vec{q}}(\vec{r}) = u_{\vec{q}}(\vec{r})$$

i.e. $u_{\vec{q}}(\vec{r})$ has the periodicity of the lattice. The final result that

$$\psi(\vec{r}) = e^{i\vec{q}\cdot\vec{r}}u(\vec{r})$$

with

$$u_{\vec{q}}(\vec{r} + \vec{L}) = u_{\vec{q}}(\vec{r})$$

is called *Bloch's theorem.* Actually, the result was well known to matematicians long before physicists discovered it. In the mathematics literature the result is called *Floquet's theorem.* The theorem plays a fundamental role in condensed matter physics. The solutions to the Schrödinger equation that satisfy Bloch's theorem are called Bloch functions and the eigenstates Bloch states. We can now reformulate the transport theory of the last few sections by saying that the charge carriers are Bloch electrons (or holes) with energy $E_{\vec{q}}$ traveling with the group velocity

$$v_{\vec{q}} = \frac{E_{\vec{q}}}{\hbar\partial\vec{q}}$$

and the Drude model is replaced by the *semiclassical approach* in which Newtons second law becomes[2]

$$\frac{d\vec{p}}{dt} = \hbar\frac{d\vec{q}}{dt} = e(\vec{E} + \vec{v}_{\vec{q}} \times \vec{\mathcal{B}})$$

[2] We use a different font for the magnetic induction $\vec{\mathcal{B}}$ not to confuse it with the reciprocal lattice vector $\vec{B}$.

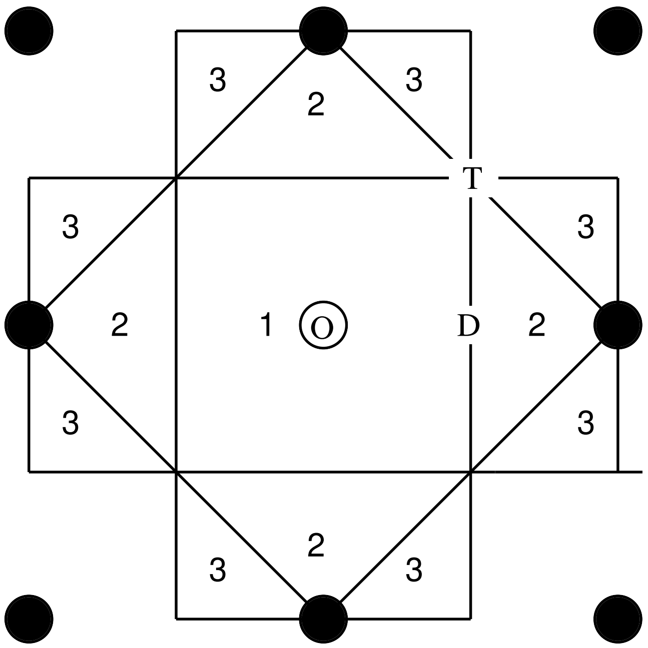

Figure 2: Brillouin zones for the square lattice. Reciprocal lattice points are marked with filled circles. The numbers refer to Brillouin zones.

Although difficult to justify with any kind of rigor, the semiclassical approach is adequate for most applications in condensed matter physics. We note that if $\vec{v}_{\vec{q}}$ and $\vec{q}$ point in opposite directions the magnetic field will act on an electron as if it had a positive charge. This is indeed what happens for some of the bands in di- and trivalent metals.

4.7. Reduced zone scheme.

We next consider the consequences of restricting the wave vectors to the first Brillouin zone, by considering a simple example, the two dimensional square lattice. In the figure 2 shows the construction for this case. The first Brillouin zone consists of the set of points that are closer to the reciprocal lattice vector at the origin than to any other reciprocal lattice vector. Points in the second zone has the origin as their second nearest neighbor while for points in the third zone the origin is the third nearest neighbor and so on. Points in the second and third zone are reduced to the first zone by adding or subtracting a wave vector

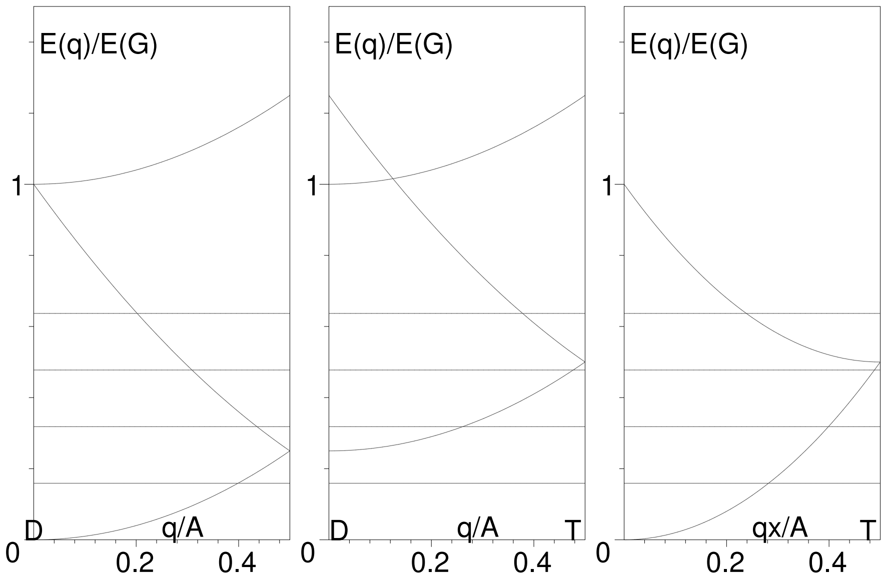

Figure 3: Free electron band structure in the reduced zone scheme for the square lattice, in resectively, the OD,DT and OT directions. Horizontal lines correspond to Fermi energy with valence 1,2,3,4, respectively. The upper energy band in the TO direction is doubly degenerate

$$\vec{G}_1 = \frac{2\pi}{a}\hat{x}, \quad or \quad \vec{G}_2 = \frac{2\pi}{a}\hat{x}$$

In the figure 3 we plot the free electron band structure in the directions OD, DT, OT of the Brillouin zone.

When the crystal potential is included the energy bands change, most strongly where energy levels cross. There are then two main approaches. If one wants to concentrate on having a good description in the regions near the atomic cores one typically chooses to approximate the wave function by linear combinations of atomic orbitals (LCAO-metods). This approach is also called the tight binding method. Alternatively, one concentrates on the interstitial region. In this latter approach one typically expands the Bloch wave function in plane waves and there are then a number of such methods with names such as OPW (orthogonalized plane waves), APW (augmented plane waves) and pseudopotential methods. Finally, one sometimes tries to combine the two approaches such as in the socalled muffin tin approximation.

We will here on briefly describe the simplest of these methods, the tight binding method.