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Wrocław University of Technology

## Nanoengineering

Leszek Bryja, Joanna Jadczak, Krzysztof Ryczko

# MATTER – RADIATION INTERACTION Theory of Condensed Matter II

Wrocław 2011

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#### 1. Lambert–Beer law

The Lambert-Beer law is fundamental law describing interaction of light with a matter in the linear matter response approximation. It states that there is a logarithmic dependence between the transmission T, of light through a substance and the product of the absorption coefficient of the substance,  $\eta$ , and the distance l the light travels through the material:

$$T = \frac{I}{I_0} = e^{-\eta l} , \qquad (1.1)$$

where  $I_0$  and I are the intensity of the incident light and the transmitted light, respectively.

This is general law for a gas, liquid and solid state when the excitation light intensity is not too high. The equation follows so called linear response of the matter.

The derivation of this law is not difficult. Let us divide the sample into infinitesimally thin slices dl perpendicular to the beam of an absorbed light. The light passing through a slice is slightly less intense than the light that entered since some of the photons are absorbed. The difference of the intensity dI due to the absorption is equal to:

$$dI = -I\eta dl \tag{1.2}$$

The solution to this simple differential equation is obtained by integrating both sides to obtain the intensity of light at the exit from matter I as a function of its width l:

$$\ln(I) - \ln(I_0) = -\eta \ . \tag{1.3}$$

Rearranging and exponentiating yields to equation 3.1.

In the case of liquids the relation for the transition of light through the matter is expressed in a form with 10 as a base of the exponential function:

$$T = \frac{I}{I_0} = 10^{-\eta' l}.$$
 (1.4)

The base 10 and base e conventions must not be confused because they give different values for the absorption coefficient:

$$\eta^* \neq \eta \,. \tag{1.5}$$

However, it is easy to convert one to the other, using

$$\eta = \eta^* \ln(10) \approx 2.303 \eta^*. \tag{1.6}$$

The transmission (or transmissivity) is expressed in terms of an absorbance which, for liquids, is defined as:

$$A^* = -\log\left(\frac{I}{I_0}\right) \tag{1.7}$$

whereas, for other materials (a solid state and a gas), it is usually defined as

$$A = -\ln\left(\frac{I}{I_0}\right). \tag{1.8}$$

#### 2. Maxwell's equations

Maxwell's equations are four equations describing how the electric and magnetic fields develop in space and time in relation to sources, charge density and current density. They are presented in two forms: differential and integral they are of basic importance for the physics and together with the Lorentz force law, form the foundation of classical electrodynamics. The equations are named after the Scottish physicist and mathematician James Clerk Maxwell who first published them in 1861. It is worth to recall the name of Heinrich Rudolf Hertz who clarified and expanded the electromagnetic theory of light that had been put forth by Maxwell. The equation in their present elegant and short form was written by Hertz. Equations derived by Maxwell were very complicated. Unfortunately we remember now Hertz only as the first scientist who satisfactorily demonstrate the existence of electromagnetic waves by building an apparatus to produce and detect radio waves. Individually, the equations are known as Faraday's law of induction, Ampere's law with Maxwell's correction, Gauss's law and Gauss's law for magnetism.

In the Gaussian units, the equations take the following form:

$$c \ rot\overline{E} = -\frac{\partial\overline{B}}{\partial t}$$
(2.1)

$$c \ rot\overline{\mathrm{H}} = \frac{\partial\overline{\mathrm{D}}}{\partial \mathrm{t}} + 4\pi\overline{\mathrm{j}},$$
 (2.2)

$$div\,\overline{D} = 4\pi \acute{n} \,, \tag{2.3}$$

$$div B = 0 \tag{2.4}$$

Where  $\overline{E}$  is an electric field also called the electric field intensity,

 $\overline{B}$  is a magnetic field also called the magnetic induction or the magnetic field density or the magnetic flux density,

 $\overline{\mathbf{D}}$  is an electric displacement field also called the electric induction or the electric flux density,

 $\overline{H}$  is a magnetizing field also called auxiliary magnetic field or magnetic field intensity or magnetic field.

The relations between above field vectors are as follows:

$$\overline{B} = \mu \overline{H}, \qquad \overline{j} = \sigma \overline{E}, \qquad \overline{D} = (1 + 4\pi\alpha)\overline{E},$$
 (2.5)

where  $\sigma$  is conductivity and  $\alpha$  is an electric polarisability.

#### 3. Wave equation. Complex refractive index

#### Wave equation

In the case of non-magnetic materials and no electric field sources, when

$$\mu = 1 \quad and \quad \rho = 0 \tag{3.1}$$

we can simplify above equation to:

$$c \ rot \,\overline{\mathbf{E}} = -\frac{\partial \,\overline{\mathbf{H}}}{\partial \mathbf{t}} , \qquad (3.2)$$

$$c \ rot \,\overline{\mathbf{H}} = \frac{\partial \overline{\mathbf{E}}}{\partial t} + 4\pi\alpha \frac{\partial \overline{\mathbf{E}}}{\partial t} + 4\pi\sigma \,\overline{\mathbf{E}} , \qquad (3.3)$$

$$div\,\overline{H} = div\,\overline{E} = 0 \ . \tag{3.4}$$

Differentiating over time equation (1.8) we get:

$$\frac{\partial}{\partial t} \left( c \ rot \,\overline{H} \right) = \frac{\partial}{\partial t} \left( \frac{\partial \overline{E}}{\partial t} + 4\pi\alpha \frac{\partial \overline{E}}{\partial t} + 4\pi\sigma \overline{E} \right) = \left( \frac{\partial^2 \overline{E}}{\partial t^2} + 4\pi\alpha \frac{\partial^2 \overline{E}}{\partial t^2} + 4\pi\sigma \frac{\partial \overline{E}}{\partial t} \right) \quad (3.5)$$

and assuming than time and space variables are independent and use equation (1.7) we get:

$$\frac{\partial}{\partial t} \left( c \ rot \,\overline{H} \right) = c \ rot \frac{\partial \overline{H}}{\partial t} = -c^2 rot \ rot \overline{E} . \tag{3.6}$$

With use of identity:

$$rot \, rot = grad \, div - \Delta \tag{3.7}$$

we finally have electromagnetic wave equation:

$$c^{2} \Delta \overline{E} = \frac{\partial^{2} \overline{E}}{\partial t^{2}} + 4\pi \alpha \frac{\partial^{2} \overline{E}}{\partial t^{2}} + 4\pi \sigma \frac{\partial \overline{E}}{\partial t}.$$
 (3.8)

#### Complex refractive index

We are looking for the solution as sinusoidal plane-wave:

$$\overline{E} = \overline{\varepsilon}_{o} e^{i(\omega t - \overline{k}\overline{r})} = \overline{\varepsilon}_{o} e^{i\omega(t - \frac{\overline{N} r}{c})}, \qquad (3.9)$$

where

$$\omega = \frac{2\pi}{T}, \quad k = \frac{2\pi}{\lambda} \overline{E}, \quad \overline{N} = n\overline{u}. \tag{3.10}$$

We will solve equation in three different cases.

#### 1. Vacuum

In the vacuum case the conductivity and polarisibility vanish:

$$\sigma = 0 \quad and \quad \alpha = 0 \tag{3.11}$$

so that equation (1.13) simplifies to:

$$c^2 \ \Delta \overline{\mathbf{E}} = \frac{\partial^2 \overline{\mathbf{E}}}{\partial t^2} \tag{3.12}$$

and inserting function (1.14) into (1.17) one obtains:

$$-\frac{\omega^2}{c^2}N^2c^2\,\overline{E} = -\omega^2\overline{E}, \qquad N^2 = 1.$$
(3.13)

#### 2. Dielectric

In the dielectric case the conductivity is still equal to zero but we have non vanishing polarisibility:

$$\sigma = 0 \quad and \quad \alpha \neq 0 \tag{3.14}$$

so equation (1.13) takes a following form:

$$c^{2} \Delta \overline{E} = \frac{\partial^{2} E}{\partial t^{2}} (1 + 4\pi\alpha)$$
(3.15)

and we obtain the solution well known from optics:

$$-\frac{\omega^2}{c^2}N^2c^2\,\overline{E} = -\omega^2\overline{E}(1+4\pi\alpha), \qquad N^2 = 1+4\pi\alpha \,\,, \tag{3.16}$$

what we can write in a following form:

$$N^{2} = \varepsilon_{o} = 1 + 4\pi\alpha, \quad \overline{N} = n\overline{u}, \quad n = \sqrt{\varepsilon_{o}}, \quad (3.17)$$

where n is a refractive index and  $\varepsilon_0$  is a permittivity also called electric constant.

#### 3. Metals and semiconductors

In the metal and semiconductor case we have both not vanishing conductivity and polarisibility:

$$\sigma \neq 0 \quad and \quad \alpha \neq 0 \tag{3.18}$$

and the solution is:

$$-\frac{\omega^2}{c^2}N^2c^2\,\overline{E} = \left(-\omega^2\varepsilon_o + 4\pi\sigma i\omega\right)\overline{E}\,,\tag{3.19}$$

which gives:

$$N^2 = \varepsilon_o - i \frac{4\pi\sigma}{\omega} \tag{3.20}$$

so we have to introduce a complex refractive index:

$$\overline{N} = (n - ik)\overline{u} . \tag{3.21}$$

Where n is a refractive index and k is called extinction. Inserting above equation into (1.25) we get:

$$(n-ik)^2 = \varepsilon_o - i\frac{4\pi\sigma}{\omega}, \qquad (3.22)$$

what yields formulas for:

$$n^2 - k^2 = \varepsilon_o \tag{3.23}$$

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and

$$2nk = \frac{4\pi\sigma}{\omega}.$$
(3.24)

The last formula can be also written in a form:

$$nk = \frac{\sigma}{v}.$$
(3.25)

The physical sense of a complex refractive index

When we insert complex refractive index (1.26) into the wave function in a form (1.14) we get:

$$E = \varepsilon_o e^{i\omega(t - \frac{1}{c}(n - ik)z)} = E = \varepsilon_o e^{-k\frac{\omega}{c}z} e^{i\omega(t - \frac{n}{c}z)}.$$
(3.26)

Constant value of:

$$\omega\left(t - \frac{n}{c}z\right) = const \tag{3.27}$$

gives well known phase velocity:

$$u_f = \frac{dz}{dt} = \frac{c}{n},\tag{3.28}$$

hence  $\mathbf{n}$  describe the normal real refractive index.

The power density of the electromagnetic field, meaning the intensity of light passing through the matter is:

$$I \sim \overline{E^2} \tag{3.29}$$

so we have:

$$I = I_o e^{-\frac{2k\omega}{c}z} = I_o e^{-\eta z}.$$
 (3.30)

Above equations describes relation between the absorption coefficient  $\eta$  and the extinction k:

$$\eta = \frac{2k\omega}{c} = \frac{4\pi}{\lambda}k$$
(3.31)

and so it describes the absorption properties of matter.

#### 4. Boltzmann equation

In this and further chapters we will consider behavior of electrons in crystals under the external fields. We will start from stationary Boltzmann equation. Although this equation is related to transport in solid state definition and terms introduced to describe transport phenomena are commonly used in optical studies of solid state.

Transport of electrons and holes in crystals can be described by a semi-classical Boltzmann equation, derived by Ludwig Boltzmann to describe the statistical distribution of a particle in a fluid. Originally this equation was proposed to describe transport in gas but it is also valid for a solid state. The Boltzmann equation is an equation for the time evolution of the distribution function  $f(\bar{r}, \bar{p})$  in phase space, where  $\bar{r}$  and  $\bar{p}$  are position and momentum, respectively. This equation describes a particle in steady or slowly varying external fields, so the total change of  $f(\bar{r}, \bar{p})$  is equal to zero:

$$\frac{df}{dt} = 0. \tag{4.1}$$

The distribution function is not much different Fermi-Dirac thermal distribution function:

$$f_0 = \frac{1}{\exp((E - E_F) / kT) + 1}.$$
(4.2)

Boltzmann divided time evolution of  $f(\overline{r}, \overline{p})$  into two parts: one connected with the drift of particle in 6 dimension phase space and second due to the collisions. In the case of solid states collisions are scatterings on imperfections in the crystal lattice. So the time evolution of electron or hole can be expressed in a form:

$$\frac{df}{dt} = \left(\frac{df}{dt}\right)_{drift} + \left(\frac{df}{dt}\right)_{scatt} = 0.$$
(4.3)

#### Drift term

Let us consider a small cube in phase space  $f(\overline{r}, \overline{p})$  (see fig. 4.1). The variation of number of states in time  $\Delta t$  can be expressed as:

$$\Delta f = f(x - x\Delta t, y - y\Delta t, z - z\Delta t, k_1 - k_1\Delta t, k_2 - k_2\Delta t, k_3 - k_3\Delta t) - (4.4)$$

$$f(x, y, z, k_1, k_2, k_3).$$

So the derivative is equal to:

$$\left(\frac{df}{dt}\right)_{drift} = \lim_{\Delta t \to 0} \frac{\Delta f}{\Delta t} =$$

$$-\frac{\partial f}{\partial x} \dot{x} - \frac{\partial f}{\partial y} \dot{y} - \frac{\partial f}{\partial z} \dot{z} - \frac{\partial f}{\partial k_1} \dot{k}_1 - \frac{\partial f}{\partial k_2} \dot{k}_2 - \frac{\partial f}{\partial k_3} \dot{k}_3 = -\dot{r} \nabla_r f - \dot{k} \nabla_k f.$$

$$(4.5)$$

$$k_3$$

$$k_4$$

$$k_4$$

$$k_4$$

Fig. 4.1 The cube of a side equal to  $\Delta k$  in a phase space  $\langle \overline{r}, \overline{p} \rangle$ .

Since external force change the wave vector according to the formula:

$$\hbar \dot{\overline{k}} = \overline{F} \tag{4.6}$$

we can rewrite the drift term in a form:

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = -\overline{v}\nabla_r f - \frac{\overline{F}}{\hbar}\nabla_k f \,. \tag{4.7}$$

#### Scattering term

This scattering term can be expressed in a following form:

$$\left(\frac{df}{dt}\right)_{scatt} = \int_{BZ} P(\overline{k}', \overline{k})[1 - f(\overline{k}')]\rho(\overline{k}')f(\overline{k}')d^{3}\overline{k}' - \int_{BZ} P(\overline{k}, \overline{k}')[1 - f(\overline{k}')]\rho(\overline{k}')f(\overline{k})d^{3}k',$$
(4.8)

where

$$\int_{BZ} P(\overline{k}, \overline{k}')[1 - f(\overline{k}')]\rho(\overline{k}')f(\overline{k})d^3k'$$
(4.9)

is an integral over the Brillouine zone describing the number of scatterings in time unit which transfer an electron with wave vector  $\overline{k}$  into any state of wave vector  $\overline{k}'$ , and

$$\int_{BZ} P(\overline{k'}, \overline{k}) [1 - f(\overline{k'})] \rho(\overline{k'}) f(\overline{k'}) d^3k'$$
(4.10)

is an integral describing the opposite process i.a. transferring due to scattering processes electrons with arbitrary wave vector  $\overline{k}'$  into the state with wave vector  $\overline{k}$ . Term  $P(\overline{k}, \overline{k}')$ describes transfer probability from state  $\overline{k}$  to state  $\overline{k}'$ , term  $\rho(\overline{k}')$  describes the density of state in  $\overline{k}$  space, and terms  $[1 - f(\overline{k}')]$  and  $f(\overline{k})$  describe number of free places in a finite and an initial state respectively.

So, finally the Boltzmann equation can be written in a form:

$$-\overline{v}\nabla_{r}f - \frac{\overline{F}}{\hbar}\nabla_{k}f + \int_{BZ} P(\overline{k}',\overline{k})[1 - f(\overline{k}')]\rho(\overline{k}')f(\overline{k}')d^{3}k'$$
  
$$-\int_{BZ} P(\overline{k},\overline{k}')[1 - f(\overline{k}')]\rho(\overline{k}')f(\overline{k})d^{3}k' = 0.$$
(4.11)

The Boltzmann equation refers to stationary case when scattering of electrons are much faster than variations of external fields. Unfortunately it is deferential-integral non-linear

equation practically impossible to solve. In further consideration we will linearize it transforming it into solvable form.

#### 5. Relaxation time

In order to simplify the collision term we have to make a few simplifying assumptions:

1. The electron energy is parabolic and isotropic on wave vector, it is we have one effective mass in all directions:

$$E = \frac{\hbar^2 k^2}{2m^*}.$$
 (5.1)

2. The electron energy is not changed during scatterings, justifying the equality:

$$\left|\overline{k}'\right| = \left|\overline{k}\right|. \tag{5.2}$$

This is not true but since the actual change of the energy in one scattering process is very small this assumption is acceptable and what is important it allows to linearize the Boltzmann equation.

3. The probability of an electron transfer from the state with wave vector  $\overline{k}$  to the state with wave vector  $\overline{k'}$  is the same as the transfer in opposite direction:

$$P(\overline{k}, \overline{k}') = P(\overline{k}', \overline{k}).$$
(5.3)

3. The distribution f is not much different from the thermal equilibrium distribution  $f_o$  and is equal to:

$$f = f_o + f_1. (5.4)$$

4.  $f_1$  is treated as a small perturbation:

$$f_o = f_1. \tag{5.5}$$

5.  $f_1$  can be described by a special function which is a product of two vectors:

$$f_1 = \overline{\nu} \cdot \overline{\chi}(E) \,. \tag{5.6}$$

The last assumption can be interpreted as a linear term in Taylor's expansion of f:

$$f(\overline{k}) = f_o(\overline{k} - \overline{\delta}) \approx f_o(\overline{k}) - \frac{\partial f_o}{\partial E} \nabla_k E \cdot \overline{\delta} =$$

$$f_o(\overline{k}) + \frac{1}{\hbar} \nabla_k E \cdot \left( -\frac{\partial f_o}{\partial E} \hbar \overline{\delta} \right) = f_o(\overline{k}) + \overline{\nu} \cdot \overline{\chi}(E),$$
(5.7)

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since

$$\frac{1}{\hbar}\nabla_k E = \overline{\nu} . \tag{5.8}$$

Inserting (5.3) into (4.8) we obtain a simple formula for scattering term:

$$\left(\frac{df}{dt}\right)_{scatt} = \int_{BZ} P(\overline{k}, \overline{k}') [f(\overline{k}) - f(\overline{k}')] \rho(\overline{k}') d^3k'.$$
(5.9)

Further, using formulas (5.2) and (5.6) we have:

$$\left(\frac{df}{dt}\right)_{scatt} = \int_{BZ} P(\overline{k}, \overline{k}') \overline{\chi}(E) [\overline{\nu}(\overline{k}') - \overline{\nu}(\overline{k})] \rho(\overline{k}') f(\overline{k}) d^3k'$$
(5.10)

and since for isotropic and parabolic bands (eq. 5.1) the translational velocity is equal to:

$$\overline{\nu} = \frac{1}{\hbar} \nabla_k E = \frac{\hbar}{m^*} \overline{k} . \tag{5.11}$$

The scattering term takes a form:

$$\left(\frac{df}{dt}\right)_{scatt} = \frac{\hbar}{4\pi^3 m^*} \int_{BZ} P(\overline{k}, \overline{k}') \overline{\chi}(E) \left(\overline{k}' - \overline{k}\right) d^3k'.$$
(5.12)

Since we assumed the conservation of the energy in scattering processes, which is equivalent to the conservation of the length of wave vector and isotropy of the crystal we can take a transfer probability function in a form:

$$W(\overline{k},\overline{k}') = \delta(\overline{k}-\overline{k}')\theta(k,\mathcal{G}), \qquad (5.13)$$

where  $\delta(\overline{k} - \overline{k'})$  is Dirac delta function and function  $\theta(k, \mathcal{G})$  reflects the fact that transfer probability depends only on the length of wave vector  $\overline{k}$  and the angle  $\mathcal{G}$  between initial and final vectors  $\overline{k}$  and  $\overline{k'}$ .

To perform the integration we use spherical coordinates with the distinguished axis along wave vector  $\overline{k}$ . As it is seen from the Fig. 5.1 the component of the vector  $\overline{k'}$  along the

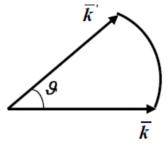


Fig. 5.1. The configuration of the spherical coordinates.

vector  $\overline{k}$  is equal to:

$$k = \overline{k'} - \overline{k} = (\cos \vartheta - 1)\overline{k} \tag{5.14}$$

so the integration over the Brillouine zone gives:

$$\left(\frac{df}{dt}\right)_{scatt} = \frac{\hbar}{4\pi^{3}m^{*}}\int_{0}^{2\pi}d\varphi\int_{0}^{k_{m}}dk\int_{0}^{\pi}\delta(\overline{k}-\overline{k}')\theta(k,\theta)\overline{\chi}(E)\left[\overline{k}_{\perp}'+\left(\overline{k}'-\overline{k}\right)\right]\left(\overline{k}'\right)^{2}\sin\theta d\theta = (5.15)$$

$$\frac{\hbar}{4\pi^{3}m^{*}}\int_{0}^{\pi}\theta(k,\theta)\overline{k}\overline{\chi}(E)(\cos\theta-1)k^{2}\sin\theta d\theta,$$

since the integration over the component  $\overline{k'_{\perp}}$  perpendicular to distinguished vector  $\overline{k}$  is equal to zero. We also made the approximation  $k_m \to \infty$  which is acceptable in semiconductors since probability of occupations of states with high wave vectors  $\overline{k}$  is very small. The term  $\overline{k}\overline{\chi}(E)$  is not dependent on  $\mathcal{G}$  and can be put on in front of integral and since

$$\frac{\hbar}{m^*} \overline{k} \overline{\chi}(E) = \overline{v} \overline{\chi}(E) = f_1$$
(5.16)

we finally get the scattering part of time derivative of the distribution function in a form:

$$\left(\frac{df}{dt}\right)_{scatt} = -\frac{f_1}{2\pi^2} \int_0^{\pi} (1 - \cos\theta) k^2 \sin\theta d\theta.$$
(5.17)

The term

$$\frac{1}{\tau} = \frac{1}{2\pi^2} \int_0^{\pi} (1 - \cos \theta) k^2 \sin \theta d\theta$$
 (5.18)

is called the relaxation time.

The reason for such name is simple. When the external perturbation is removed, it is

$$\left(\frac{df}{dt}\right)_{drift} = 0.$$
 (5.19)

The total derivative of the distribution function is not equal to zero:

$$\left(\frac{df}{dt}\right) \neq 0 \tag{5.20}$$

and the distribution function return to their thermal equilibrium state according to the equation:

$$\frac{df}{dt} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{scatt} = 0 + \left(\frac{df}{dt}\right)_{scatt} = -\frac{f - f_0}{\tau} = -\frac{f_1}{\tau}.$$
(5.21)

So we have the simple equation for  $f_1$  to solve:

$$\frac{df_1}{dt} = -\frac{f_1}{\tau}.$$
(5.22)

The solution is the exponential return of the system to thermal equilibrium with characteristic time  $\tau$ :

$$f_1 = f_1^0 e^{-\frac{l}{\tau}}.$$
 (5.23)

In most cases for different scattering mechanism the relaxation time is can be described by a simple power function of energy:

$$\tau(E) = A E^{\left(p - \frac{1}{2}\right)}.$$
(5.24)

For acoustic phonons p = 0, for optical phonons p = 1, for neutral impurities p = 1/2and for ionized impurities p = 2. Temperature dependence of the relaxation time is more complicated and can be found in advanced theoretical textbooks. Knowing the relaxation time one has to calculate the mean free path of a particle  $\lambda$ :

$$\lambda = v\tau . \tag{5.25}$$

Since

$$v \sim E^{\frac{1}{2}}$$
 (5.26)

we have that:

$$\lambda \sim E^{\frac{1}{2}} E^{(p-\frac{1}{2})} = E^{p} .$$
(5.27)

#### 6. Ohm's law. Microscopic conductivity

In the relaxation time approximation the stationary Boltzmann equation can be written in a form:

$$\nabla_r f \cdot \overline{\nu} + \frac{1}{\hbar} \nabla_k f \cdot \overline{F} + \frac{f_1}{\tau} = 0.$$
(6.1)

The form of the function  $f_1$  depends on external fields and properties of a matter (crystal). Let us consider the situation when the distribution function is isotropic in a real 3 dimensional space at  $\overline{r}$ :

$$\nabla_r f$$
 (6.2)

and only constant electric field  $\overline{\varepsilon}$  is applied. Than the force acting on a particle with the charge q is equal to:

$$\overline{F} = q\overline{\varepsilon} . \tag{6.3}$$

Than the Boltzmann equations takes a form:

$$\frac{q}{\hbar}\nabla_k f \cdot \overline{\varepsilon} + \frac{f_1}{\tau} = 0.$$
(6.4)

In the dependence  $f = f_o + f_1$  the equilibrium term  $f_o$  depends on  $\overline{k}$  only via energy so we may write:

$$\nabla_k f = \frac{\partial f_o}{\partial E} \nabla_k E + \nabla_k f_1.$$
(6.5)

When we limit above dependence only to linear terms in the perturbation we can neglect the  $\nabla_k f_1$  term as it is perturbation of a perturbation. So the eq. 6.4 can be written in a form:

$$q\frac{\partial f_o}{\partial E}\overline{\nu}\cdot\overline{\varepsilon} + \frac{\overline{\nu}\cdot\overline{\chi}}{\tau} = \overline{\nu}\left(q\frac{\partial f_o}{\partial E}\cdot\overline{\varepsilon} + \frac{\overline{\chi}}{\tau}\right) = 0, \qquad (6.6)$$

where we use dependence  $f_1 = \overline{v} \cdot \overline{\chi}$ .

Since the velocity  $\overline{\chi}$  can have an arbitrary direction the eq. 6.6 is fulfilled only when:

$$q\frac{\partial f_o}{\partial E} \cdot \overline{\varepsilon} + \frac{\overline{\chi}}{\tau},\tag{6.7}$$

which gives the formula for  $\overline{\chi}$ :

$$\overline{\chi} = q\tau \left(-\frac{\partial f_o}{\partial E}\right)\overline{\varepsilon} \tag{6.8}$$

and for perturbation term of the distribution function  $f_1$ :

$$f_1 = q\tau \left(-\frac{\partial f_o}{\partial E}\right) \overline{v} \overline{\mathcal{E}} .$$
(6.9)

Using above dependence we can calculate the density of current which is the sum over all electrons in the band:

$$\overline{j} = \sum q \overline{\nu} \,. \tag{6.10}$$

When the sum is substitute by an integral we have to introduce the occupation function fand density of states  $\rho(\overline{k})$ :

$$\overline{j} = q \int_{BZ} v f \rho(\overline{k}) d^3 k \,. \tag{6.11}$$

Since the distribution function is a sum of two terms  $f = f_o + f_1$  the integral can be divided in two parts:

$$\overline{j} = q \int_{BZ} \overline{v} f_o \rho d^3 k + q \int_{BZ} \overline{v} f_1 \rho d^3 k .$$
(6.12)

The first term is equal to zero as in the thermal equilibrium  $f_o$  the integral contain an asymmetric arguments. Physically for an electron moving with velocity  $\overline{v}$  there is another one moving opposite  $-\overline{v}$  resulting in zero net current.

Inserting (6.9) into (6.12) and employing the equation  $e^2 = q^2$  we have:

$$\overline{j} = \frac{e^2}{4\pi^3} \int_{BZ} \overline{\nu} \tau \left(-\frac{\partial f_o}{\partial E}\right) (\overline{\nu} \cdot \overline{\varepsilon}) d^3 k .$$
(6.13)

As the electric field is the only distinguished axe the integration can be performed in a spherical coordinates with angle  $\mathcal{G}$  between wave vector  $\overline{k}$  of an electron and electric field  $\overline{\varepsilon}$ . The integral takes the form:

$$\overline{j} = \frac{e^2}{4\pi^3} \int_0^{\infty} d\varphi \int_0^{\infty} dk \int_0^{\pi} (\overline{v}_{\perp} + \overline{v}_{\parallel}) \tau \left(-\frac{\partial f_o}{\partial E}\right) v \varepsilon \cos \vartheta k^2 \sin \vartheta dk d\vartheta, \qquad (6.14)$$

where assuming  $k_m \to \infty$  as the derivative  $-\frac{\partial f_o}{\partial E}$  rapidly decrease aside of Brillouine zone.

The integral over the angle  $\varphi$  of a vector component perpendicular to the electric field  $\overline{v}_{\perp}$  is equal to zero and the component parallel to field can be written in a form:

$$\overline{v}_{\parallel} = \frac{\overline{\varepsilon}}{\varepsilon} v \cos \vartheta \tag{6.15}$$

so the integral (6.14) takes a form:

$$\overline{j} = \frac{e^2}{4\pi^3} \overline{\varepsilon} \int_{0}^{\pi} \int_{0}^{\infty} \tau \left( -\frac{\partial f_o}{\partial E} \right) v^2 k^2 \cos^2 \vartheta \sin \vartheta dk d\vartheta.$$
(6.16)

The integration over the angle  $\mathcal{G}$  is equal to:

$$\int_{0}^{\pi} \cos^2 \vartheta \sin \vartheta d\vartheta = \frac{2}{3}.$$
(6.17)

Using parabolic energy dependence on the wave vector

$$E = \frac{\hbar^2 k^2}{2m^*}$$
(6.18)

we can substitute the velocity in eq. 6.16 according to the formula:

$$\overline{v}^2 = \frac{1}{\hbar} \nabla_k E = \frac{\hbar^2}{m^{*2}} \overline{k}^2$$
(6.19)

and taking energy as a integration variable we finally obtain the expression for the current in a form:

$$\overline{j} = \frac{e^2}{3\pi^2} \overline{\varepsilon} \int_0^\infty \tau \left( -\frac{\partial f_o}{\partial E} \right) k^3 dE \,.$$
(6.20)

The above integral frequently occurs in the transport theory so it is advisable to introduce a special term:

$$\langle X \rangle = \frac{1}{3\pi^2} \int_0^\infty X(E) \left( -\frac{\partial f_o}{\partial E} \right) k^3(E) dE,$$
 (6.21)

where X denote an arbitrary physical quantity.

So we can write down the current in a form:

$$\overline{j} = \frac{e^2}{m^*} \langle \tau \rangle \overline{\varepsilon} .$$
(6.22)

This dependence is reminiscence of the classical electrodynamics dependence:

$$\overline{j} = \sigma \overline{\varepsilon} \tag{6.23}$$

from which we can write down the conductivity as:

$$\sigma = \frac{e^2}{m^*} \langle \tau \rangle. \tag{6.24}$$

The equation expresses macroscopic physical quantity  $\sigma$  in terms of microscopic properties of the crystal: an effective mass  $m^*$  and relaxation time  $\tau$ .

The physical meaning of an integral  $\langle X \rangle$  can be interpreted when we perform a simple calculation. Let us consider what we obtain when we 1 into this term. After integration by parts we obtain:

$$\langle 1 \rangle = \frac{1}{3\pi^2} \int_0^\infty \left( -\frac{\partial f_o}{\partial E} \right) k^3 dE = -\frac{f_o k^3}{3\pi^2} \bigg|_0^\infty + \frac{1}{\pi^2} \int_0^\infty f_o k^2 \frac{dk}{dE} dE =$$

$$\int_0^\infty f_o \frac{1}{4\pi^3} 4\pi k^2 dk = \int f_o \rho(k) d_3 k = n$$
(6.25)

so the  $\langle X \rangle$  denote the concentration of electrons and  $\langle X \rangle$  is an average value of the quantity X over the entire band. The term  $-\frac{f_o k^2}{3\pi^2}k^3$  is equal to zero in given limits which is obvious for k = 0 and since  $f_o$  vanishes at  $\infty$ .

The term:

$$\tilde{X} := \frac{\langle X \rangle}{\langle 1 \rangle} \tag{6.26}$$

corresponds to the mean value of quantity X for one electron.

The conduction can be also expressed in a form:

$$\sigma = \frac{e^2}{m^*} < 1 > \tilde{\tau} = en \frac{e}{m^*} \tilde{\tau} .$$
(6.27)

From the other hand the conductivity is expressed by mobility as:

$$\sigma = en\mu. \tag{6.28}$$

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Comparison of both equations give macroscopic description of mobility:

$$\mu = \frac{e}{m^*} \tilde{\tau} . \tag{6.29}$$

We obtain an important results that mobility is proportional to relaxation time of an electron and inverse proportional to an effective mass.

#### Metals

Let us consider the strongly degenerated electron gas. This case is important for metals and strongly doped semiconductors when function  $-\frac{\partial f_o}{\partial E}$  can be approximated by the Dirac  $\delta$  function:

$$-\frac{\partial f_o}{\partial E} \approx \delta(E - E_F).$$
(6.30)

Than the integral  $\langle X \rangle$  is equal to the value of physical quantity X at the Fermi level:

$$\left\langle X \right\rangle = \frac{1}{3\pi^2} \int X \left( -\frac{\partial f_o}{\partial E} \right) k^3 dE = \frac{1}{3\pi^2} X(E_F) k^3(E_F)$$
(6.31)

and the average value of X is equal to:

$$\tilde{X} = \frac{\langle X \rangle}{\langle 1 \rangle} = X(E_F).$$
(6.32)

So in the formula for mobility of electrons in metals relaxation time is that on Fermi level:

$$\mu = \frac{e}{m^*} \tau(E) \,. \tag{6.33}$$

When the current is conducted by electrons and holes from many bands and valleys one has to sum over them:

$$\overline{j} = \sum_{i} \frac{e^2}{m_i^*} < \tau >_i \overline{\mathcal{E}} .$$
(6.34)

The index i denotes bands and valleys.

Hence the formula for conductivity is than expressed in a form:

$$\sigma = \sum_{i} \frac{e^2}{m_i^*} \langle \tau \rangle_i \,. \tag{6.35}$$

#### 7. Boltzmann equation in electric and magnetic fields

The transport in magnetic field is a one of the central problems in the solid state physics. The study of transport in magnetic field embraces many aspects of galvano-magnetics phenomena and deliver most information about matter. The electron subjected to electric and magnetic field is driven by Lorentz force:

$$\overline{F} = q \left( \overline{\varepsilon} + \frac{1}{c} \overline{v} \times \overline{B} \right).$$
(7.1)

In Boltzmann equation the scattering term remain unchanged. Only the drift term should be modified by substituting electric field by both electric and magnetic fields (see. eq. 6.4):

$$\frac{q}{\hbar}\nabla_{k}f\cdot\left(\overline{\varepsilon}+\overline{\nu}\times\overline{B}\right)+\frac{f_{1}}{\tau}=0.$$
(7.2)

In the case of electric and magnetic fields we cannot assume as in the case of electric field that:

$$\nabla_k f_1 = 0 \tag{7.3}$$

in extension of the distribution f function on  $f_o$  and  $f_1$ 

$$\nabla_k f = \nabla_k f_o + \nabla_k f_1 = \frac{\partial f_o}{\partial E} \overline{\nu} \hbar + \nabla_k f_1, \qquad (7.4)$$

since it immediately removes the magnetic field from the Boltzmann equation as a scalar product of velocity by vector product of velocity and magnetic field is equal to zero:

$$q\frac{\partial f_o}{\partial E}\overline{\nu} \cdot \left(\overline{\varepsilon} + \overline{\nu} \times \overline{B}\right) + \frac{f_1}{\tau} = 0.$$
(7.5)

In magnetic and electric field case we have to substitute the vector function  $\overline{\chi}^0$  in expression:

$$f_1 = \overline{\nu} \cdot \overline{\chi}^0 \tag{7.6}$$

for perturbation of distribution function by a new function  $\overline{\chi}$  related to  $\overline{\chi}^0$  but including information about the magnetic field. It can be shown after long and complicated calculation that it can be done by a formula:

$$\overline{\chi} = \overline{\overline{T}} \overline{\chi}^0, \qquad (7.7)$$

where  $\overline{\overline{T}}$  is a tensor and  $\overline{\chi}^0$  is the same as in the case of the electric field only:

$$\overline{\chi}^{0} = q\tau(-\frac{\partial f_{o}}{\partial E})\overline{\varepsilon}.$$
(7.8)

There is no general solution if the angle between electric and magnetic fields is arbitrary. The analytical solutions are only in two cases:

- 1. When fields are parallel  $\overline{B}$   $\overline{\varepsilon}$
- 2. When fields are perpendicular  $\overline{B} \perp \overline{\varepsilon}$

The second case covers many physical phenomena and so begin our consideration from it. When electric field is along the x axis and magnetic field along z axis:

$$\overline{\varepsilon} = (\varepsilon, 0, 0)$$

$$\overline{B} = (0, 0, B)$$
(7.8)

and bands are spherical and parabolic the  $\overline{\overline{T}}$  tensor takes a form:

$$\overline{\overline{T}} = \begin{pmatrix} \frac{1}{1+\varsigma^2} & \frac{\varsigma}{1+\varsigma^2} & 0\\ -\frac{\varsigma}{1+\varsigma^2} & \frac{1}{1+\varsigma^2} & 0\\ 0 & 0 & 1 \end{pmatrix},$$
(7.9)

where  $\varsigma$  parameter is described by a formula:

$$\varsigma = \omega_c \tau \tag{7.10}$$

and

$$\omega_c = \frac{qB}{m^* c} \tag{7.12}$$

is an electron cyclotron frequency.

The parameter  $\varsigma$  is equal to the mean angle path of an electron around the magnetic field.

The perturbation of the distribution function  $f_1$  is now equal to:

$$f_1 = q\tau \left(-\frac{\partial f_o}{\partial E}\right) \overline{\overline{T}} \overline{\varepsilon} \overline{\overline{\nu}} .$$
(7.13)

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The density of current is calculated in the same way as for electric field case (see eq. 6.13):

$$\overline{j} = \frac{e^2}{4\pi^3} \int_{BZ} \overline{v} \tau \left(-\frac{\partial f_o}{\partial E}\right) \overline{\overline{T}} \overline{\varepsilon} \cdot \overline{v} d^3 k \,. \tag{7.14}$$

The only difference is that instead of  $\overline{\varepsilon}$  we have  $\overline{\overline{T}}\overline{\varepsilon}$ . All calculation are the same and as can be easily shown we finally get equation similar to eq.6.22:

$$\overline{j} = \frac{e^2}{m^*} \left\langle \overline{\overline{T}} \tau \right\rangle \overline{\varepsilon} . \tag{7.15}$$

The  $\overline{\overline{T}}$  tensor cannot be taken out in front of the integral since it is energy dependent. The conductivity now is a tensor:

$$\overline{\overline{\sigma}} = \frac{e^2}{m^*} \left\langle \overline{\overline{T}} \tau \right\rangle. \tag{7.16}$$

Putting (7.9) into (7.16) we obtain the exact formula for conductivity tensor:

$$\overline{\overline{\sigma}} = \frac{e^2}{m^*} \begin{pmatrix} \left\langle \frac{\tau}{1+\varsigma^2} \right\rangle & \left\langle \frac{\varsigma\tau}{1+\varsigma^2} \right\rangle & 0 \\ -\left\langle \frac{\varsigma\tau}{1+\varsigma^2} \right\rangle & \left\langle \frac{\tau}{1+\varsigma^2} \right\rangle & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$
(7.17)

#### 8. Hall effect

The conductivity components are not explicitly determine in experiments since actually we measure only the current and the potential. The most spectacular effects in which magnetic field influences the behaviour of electrons are Hall effect and magneto-resistance. The scheme of Hall effect is illustrated in Fig. 8.1.

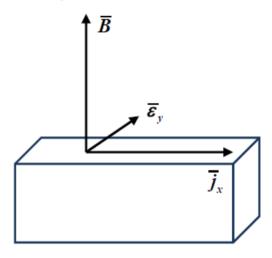


Fig. 1 The configuration of the Hall effect experiment.

The current passes in the x axis direction. When magnetic field is subjected along z direction electrons are deviated in the y axis direction resulting a voltage difference (the Hall voltage  $U_H$ ) across the sample.

Since current pass only in the *x* axis direction we have:

$$j_{v} = \sigma_{21}\varepsilon_{x} + \sigma_{22}\varepsilon_{v} = 0 \tag{8.1}$$

and from that:

$$\varepsilon_x = -\frac{\sigma_{22}}{\sigma_{21}}\varepsilon_y = \frac{\sigma_{11}}{\sigma_{12}}\varepsilon_y. \tag{8.2}$$

Using this equality we can eliminate  $\mathcal{E}_x$  from the dependence on  $j_x$ :

$$j_x = \sigma_{11}\varepsilon_x + \sigma_{12}\varepsilon_y \tag{8.3}$$

we have:

$$j_{x} = \left(\frac{\sigma_{11}^{2}}{\sigma_{12}} + \sigma_{12}\right) \mathcal{E}_{y} = \left(\frac{\sigma_{11}^{2} + \sigma_{12}^{2}}{\sigma_{12}}\right) \mathcal{E}_{y}.$$
(8.4)

Originally Hall expressed above dependence in a form:

$$U_H = \pm \frac{1}{nec} BI_x, \tag{8.5}$$

where  $I_x$  is the current in the x axis direction and n is the electron concentration. He found that the voltage caused by perpendicular magnetic field is proportional to this field and to the current. He also found that the sign of  $U_H$  is determined by the sign of current charges.

In our case since we used in our calculations an electric field  $\varepsilon$  and a current density j the equations equivalent to those obtained by Hall can be written in a form:

$$\varepsilon_{v} = RBj_{x}, \tag{8.6}$$

where R is so called the Hall constant.

From eq. (8.4) and (8.6) R can be expressed as a function of the magnetic field B and a conductivity tensor  $\sigma_{xy}$ :

$$R = \frac{\varepsilon_y}{Bj_x} = \frac{1}{B} \left( \frac{\sigma_{12}}{\sigma_{11}^2 + \sigma_{12}^2} \right).$$
(8.7)

Using the explicit form of the conductivity tensor  $\sigma_{xy}$  form eq. 7.17 we can expressed the Hall constant *R* by microscopic quantities of a crystal. Let us consider the case of a weak magnetic field when

$$\varsigma = \omega_c \tau \quad 1. \tag{8.8}$$

In this case we has to limit in a expansion of R to linear terms:

$$R = \frac{1}{B} \left( \frac{\frac{e^2}{m^*} \left\langle \frac{\varsigma \tau}{1+\varsigma^2} \right\rangle}{\frac{e^4}{m^{*2}} \left( \left\langle \frac{\tau}{1+\varsigma^2} \right\rangle^2 + \left\langle \frac{\varsigma \tau}{1+\varsigma^2} \right\rangle^2 \right)} \right) = \frac{1}{B} \frac{\langle \varsigma \tau \rangle}{\frac{e^2}{m^*} \langle \tau \rangle^2} = \frac{1}{B} \frac{\left\langle \frac{eB}{mc} \tau^2 \right\rangle}{\frac{e^2}{m^*} \langle \tau \rangle^2} = \frac{1}{B} \frac{\left\langle \frac{eB}{mc} \tau^2 \right\rangle}{\frac{e^2}{m^*} \langle \tau \rangle^2} = \pm \frac{1}{nec} \frac{\langle \tau^2 \rangle \langle 1 \rangle}{\langle \tau \rangle^2},$$
(8.9)

where we use equality  $\langle 1 \rangle = n$ .

The term:

$$r = \frac{\left\langle \tau^2 \right\rangle \langle 1 \rangle}{\left\langle \tau \right\rangle^2} \tag{8.10}$$

is called the Hall scattering coefficient.

So the Hall constant R can be now expressed in a form:

$$R = \pm \frac{r}{nec}.$$
(8.11)

When r and R are known than the current concentration can be determined. When the conductivity is additionally measured than using the simplified expression:

$$\sigma = en\mu, \qquad (8.12)$$

the mobility can be also determined from the equation:

$$\left|R\sigma\right| = \frac{r\mu}{c} \to \mu = \frac{\left|R\sigma\right|c}{r}.$$
 (8.13)

The value of the Hall scattering coefficient r can be easily calculated in the case of metals. In this case in expression for relaxation time:

$$\langle \tau \rangle = \frac{1}{3\pi^2} \int \tau \left( -\frac{\partial f_o}{\partial E} \right) k^3 dE$$
 (8.14)

we can put:

$$-\frac{\partial f_o}{\partial E} \approx \delta(E - E_F), \qquad (8.15)$$

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which gives:

$$\left\langle \tau \right\rangle = \frac{1}{3\pi^2} \tau(E_F) k^3(E_F) \,. \tag{8.16}$$

In the same way we obtain that:

$$\left\langle \tau^2 \right\rangle = \frac{1}{3\pi^2} \tau^2(E_F) k^3(E_F) \tag{8.17}$$

and

$$\langle \tau \rangle^{2} = \left( \frac{1}{3\pi^{2}} \tau(E_{F}) k^{3}(E_{F}) \right) \cdot \left( \frac{1}{3\pi^{2}} \tau(E_{F}) k^{3}(E_{F}) \right) =$$

$$\left( \frac{1}{3\pi^{2}} \tau^{2}(E_{F}) k^{3}(E_{F}) \right) \frac{1}{3\pi^{2}} k^{3}(E_{F}).$$

$$(8.18)$$

The electron concentration n is equal to the number of states in the Fermi sphere:

$$\langle 1 \rangle = n = \frac{\frac{4}{3}\pi k^3(E_F)}{4\pi^3} = \frac{1}{3\pi^2}k^3(E_F).$$
 (8.19)

Inserting eq. (8.17)- (8.19) into eq. (8.10) one can easily obtain:

$$r = 1$$
 (8.20)

for the case of electrons in metals. This results is in agreement with those obtained by Hall. In semiconductors calculations of the value of the Hall scattering coefficient r are more complicated. In most cases this value is:

$$1 \le r \le 2. \tag{8.21}$$

#### 9. Magneto-resistance

Magneto-resistance is measured in the configuration presented in the Fig. 9.1. The magnetic field is perpendicular to the current flow.

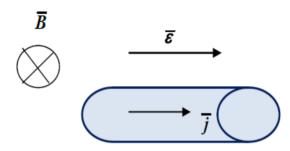


Fig. 9.1. The configuration of magneto-resistance experiments.

In the week magnetic field regime one can express the equality between the relative change of resistivity and conductivity in a simple form:

$$\frac{\Delta\rho}{\rho} = -\frac{\Delta\sigma}{\sigma} = \frac{\sigma(0) - \sigma(H)}{\sigma(0)}.$$
(9.1)

The current does not flow in the y axis direction:

$$j_y = \sigma_{21}\varepsilon_x + \sigma_{22}\varepsilon_y = 0 \tag{9.2}$$

so we can express the  $\mathcal{E}_{y}$  component by  $\mathcal{E}_{x}$  component:

$$\varepsilon_{y} = -\frac{\sigma_{21}}{\sigma_{22}} \varepsilon_{x} = \frac{\sigma_{12}}{\sigma_{11}} \varepsilon_{x}, \qquad (9.3)$$

where we used equalities:

$$\sigma_{11} = \sigma_{22} \quad and \quad \sigma_{21} = -\sigma_{12}.$$
 (9.4)

Putting above expression to the  $j_x$  equation:

$$j_x = \sigma_{11}\varepsilon_x + \sigma_{12}\varepsilon_y \tag{9.5}$$

we get:

$$j_{x} = \frac{\sigma_{11}^{2} + \sigma_{12}^{2}}{\sigma_{11}} \varepsilon_{x}.$$
(9.6)

In this configuration we simply measure conductivity in the x axis direction as a function of the magnetic field:

$$\sigma(H) = \frac{\sigma_{11}^{2} + \sigma_{12}^{2}}{\sigma_{11}}.$$
(9.7)

When we insert above dependence to eq. 9.1 we get:

$$\frac{\Delta\rho}{\rho} = \frac{\sigma(0)\sigma_{11} - \sigma_{11}^2 - \sigma_{12}^2}{\sigma(0)\sigma_{11}}.$$
(9.8)

Terms in above equation are described by formulas (see eq. 7.17):

$$\sigma_{11} = \frac{e^2}{m^*} \left\langle \frac{\tau}{1+\varsigma^2} \right\rangle \tag{9.9}$$

$$\sigma_{12} = \frac{e^2}{m^*} \left\langle \frac{\tau\varsigma}{1+\varsigma^2} \right\rangle, \tag{9.10}$$

$$\sigma(0) = \frac{e^2}{m^*} \langle \tau \rangle. \tag{9.11}$$

Since the  $\frac{e^2}{m^*}$  term in eq. 9.8 both in numerator and denominator occur in the same power

we can evaluate above expressions without it:

$$\sigma_{11} \sim \left\langle \frac{\tau}{1+\varsigma^2} \right\rangle \cong \left\langle \tau \right\rangle - \left\langle \varsigma^2 \tau \right\rangle, \tag{9.12}$$

$$\sigma_{12} \sim \langle \tau \rangle^2 - 2 \langle \tau \rangle \langle \varsigma^2 \tau \rangle, \qquad (9.13)$$

$$\sigma_{12} \sim \left\langle \tau \varsigma \right\rangle^2. \tag{9.14}$$

Inserting above dependences to eq. 9.8 and limiting the expansion up to  $\zeta^2$  terms one may obtain:

$$\frac{\Delta\rho}{\rho} = \frac{\langle \tau \rangle^2 - 2\langle \tau \rangle \langle \varsigma^2 \tau \rangle - \langle \tau \rangle^2 + 2\langle \tau \rangle \langle \varsigma^2 \tau \rangle - \langle \varsigma \tau \rangle^2}{\langle \tau \rangle^2}.$$
(9.15)

After a simple calculation we have:

$$\frac{\Delta\rho}{\rho} = \frac{\left\langle \varsigma^2 \tau \right\rangle}{\left\langle \tau \right\rangle} - \frac{\left\langle \varsigma \tau \right\rangle^2}{\left\langle \tau \right\rangle^2}.$$
(9.16)

Since

$$\varsigma = \omega_c \tau \quad and \quad \sigma = en\mu$$
 (9.17)

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we obtain the final expression for the magnetic field variation of the resistivity:

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$$\frac{\Delta\rho}{\rho} = \frac{\mu^2 B^2}{c^2} \left[ \frac{\langle \tau^3 \rangle \langle 1 \rangle^2}{\langle \tau \rangle^3} - \frac{\langle \tau^4 \rangle \langle 1 \rangle^2}{\langle \tau \rangle^4} \right].$$
(9.18)

As the Hall voltage is linearly dependent on the magnetic field the magneto-resistant is a quadratic function of the magnetic field. Namely the Hall effect is a first range effect whereas the magneto-resistant is the second order effect similarly like the current density and the Joule heat are when the electric field is concerned.

#### 10. Boltzmann equation for alternating fields. Complex conductivity

In the case of alternating fields with a period comparable to the relaxation time the equation (4.1) referring to Boltzmann stationary equation is no longer valid. Suppose we have a quickly varying electromagnetic field:

$$\overline{E} = \overline{\varepsilon}_{o} e^{i(\omega t - \overline{k}\overline{r})}$$
(10.1)

We cannot assume that:

$$f_1 = 0$$
, (10.2)

since  $f_1$  is now varying with the electromagnetic frequency field:

$$f_1 = f_1^{(0)} e^{i\omega t} \,. \tag{10.3}$$

So that:

$$\frac{d(f_0 + f_1)}{dt} = \frac{df_1}{dt} = i\omega f_1^{(0)} e^{i\omega t} = i\omega f_1,$$
(10.4)

since

$$\frac{df_0}{dt} = 0. \tag{10.5}$$

In the case of steady or slowly varying fields we get an equation:

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = \frac{f_1}{\tau},\tag{10.6}$$

which for quickly changing fields due to equation (2.12) has to be replacing by equation:

$$\left(\frac{\partial f}{\partial t}\right)_{drift} = \frac{f_1}{\tau} + i\omega f_1 + f_1 \left(\frac{1}{\tau} + i\omega\right).$$
(10.7)

Let us introduce the complex conductivity by redefinition of relaxation time:

$$\sigma = \frac{e^2 \langle \tau \rangle}{m^*} \to \sigma^*(\omega) = \frac{e^2}{m^*} \left\langle \frac{\tau}{1 + i\omega} \right\rangle.$$
(10.8)

We can express the complex conductivity in a following form:

$$\sigma^*(\omega) = \sigma_1 + i\sigma_2 = \frac{e^2}{m^*} \left\langle \frac{\tau}{1 + \omega^2 \tau^2} \right\rangle - i\omega \frac{e^2}{m^*} \left\langle \frac{\tau}{1 + \omega^2 \tau^2} \right\rangle.$$
(10.9)

Since the current density is proportional to the electric field we have:

$$\overline{j} = \sigma^* \overline{E} = (\sigma_1 + i\sigma_2) \overline{\varepsilon}_o e^{i\omega t} = \sigma_1 \overline{\varepsilon}_o e^{i\omega t} + \sigma_2 \overline{\varepsilon}_o e^{i\left(\omega t - \frac{\pi}{2}\right)}, \quad (10.10)$$

where

$$\sigma_{2o}\,\overline{\varepsilon}_{o}\,e^{i\left(\omega t-\frac{\pi}{2}\right)} \tag{10.11}$$

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is a so called Maxwell correction.

The meaning of the imaginary term of the complex conductivity can be easily interpreted when we consider Ampere's circular law with the Maxwell's correction:

$$c \operatorname{rot} \overline{H} = \frac{\partial \overline{D}}{\partial t} + 4\pi \,\overline{j} = \frac{\partial}{\partial t} \left(\overline{\varepsilon} + 4\pi \,\overline{P}\right) + 4\pi \,\overline{j} \,. \tag{10.12}$$

Since polarization is proportional to the electric field

$$\overline{P} = \alpha \,\overline{\varepsilon} \,. \tag{10.13}$$

we get:

$$c \operatorname{rot} \overline{H} = (1 + 4\pi\alpha) \frac{\partial \overline{\varepsilon}}{\partial t} + 4\pi\sigma \overline{\varepsilon} = \frac{\partial \overline{\varepsilon}}{\partial t} + 4\pi(\sigma + i\omega\alpha)$$
(10.14)

so complex conductivity can be expressed in a form:

$$\sigma^* = \sigma + i\omega\alpha \,. \tag{10.15}$$

Following equation (2.17) we get a formula for the real and imaginary term of the complex conductivity in a form:

$$\sigma(\omega) = \frac{e^2}{m^*} \left\langle \frac{\tau}{1 + \omega^2 \tau^2} \right\rangle, \tag{10.16}$$

$$\alpha(\omega) = -\frac{e^2}{m^*} \left\langle \frac{\tau^2}{1 + \omega^2 \tau^2} \right\rangle.$$
(10.17)

The quantities described in above equations correspond to quantities measured in experiments, it is conductivity  $\sigma(\omega)$  and polarisibility  $\alpha(\omega)$ . Please, notice that polarisibility includes only electrons but not the lattice. The latter case will be considered in further paragraphs. Hence the imaginary part in equation (10.17) contains only polarizibility of free carriers the polarisibility is negative. This reflects the Lentz rule that electrons rotate contrariwise to the change of an external fields (a diamagnetic case).

# 11. Metallic reflectivity

In this chapter we will study interaction of light with a matter in a frame of Maxwell's and Boltzmann equations. Consider a limit condition, when (see equation3.24):

$$2nk = \frac{4\pi\sigma}{\omega} \to 0. \tag{11.1}$$

It occurs in two cases when :

$$k \Longrightarrow 0 \quad it \quad n = \sqrt{\varepsilon_0} \tag{11.2}$$

or when:

$$n \Longrightarrow 0 \quad it \quad k = \sqrt{-\varepsilon_0}$$
 (11.3)

In the first case we simply have transparent material with refractive index n. The second case is connected with metallic reflection.

Reflection coefficient is given by a following formula:

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}.$$
(11.4)

In the first case we than get:

$$R = \frac{(n-1)^2}{(n+1)^2}.$$
 (11.5)

In the second case we get:

$$R = \frac{k^2}{k^2} = 1. \tag{11.6}$$

This is so called metallic reflectivity which we will consider in more details in a next chapter.

#### 12. Plasma frequency in metals and semiconductors

Let us consider above dependences in more details for metals and strongly doped semiconductors with high concentration  $n_e$  of electrons. For semiconductors we should also consider a case with holes giving the same results. In the case of metals formulas (10.16) and (10.17) can be written in a following form:

$$\sigma(\omega) = \frac{e^2}{m^*} n_e \frac{\tau}{1 + \omega^2 \tau^2}, \qquad (12.1)$$

$$\alpha(\omega) = -\frac{e^2}{m^*} n_e \frac{\tau^2}{1+\omega^2 \tau^2}.$$
(12.2)

When we include polarization of atoms in a crystal lattice the formula for permittivity (3.17) takes a form:

$$\varepsilon_o = 1 + 4\pi\alpha \rightarrow \varepsilon_o = \varepsilon_l + 4\pi\alpha$$
, (12.3)

where  $\varepsilon_l$  is a polarisibility of a lattice. Inserting above equation into formulas (3.23) and (3.24) we get:

$$n^{2} - k^{2} = \varepsilon_{s} - \frac{4\pi e^{2}}{m^{*}} n_{e} \frac{\tau^{2}}{1 + \omega^{2} \tau^{2}}$$
(12.4)

and

$$2nk = \frac{4\pi e^2}{m^*} n_e \frac{\tau / \omega}{1 + \omega^2 \tau^2}.$$
 (12.5)

Let us introduce two quantities:

$$\gamma = \frac{1}{\tau} \quad and \quad \omega_p^2 = \frac{4\pi e^2 n_e}{\varepsilon_s m^*}, \tag{12.6}$$

where  $\omega_p$  is cold plasma frequency. It is connected with free particles in crystals (electron or holes). Gamma is the invert of relaxation time and is of the range of  $10^9-10^{12}$ s<sup>-1</sup>, which corresponds to frequencies from microwave to far infrared. Dependences for n and k now take a form:

$$n^{2} - k^{2} = \varepsilon_{s} \left( 1 - \frac{\omega_{p}^{2}}{\gamma^{2} + \omega^{2}} \right)$$
(12.7)

and

$$2nk = \varepsilon_s \frac{\gamma}{\omega} \frac{\omega_p^2}{\gamma^2 + \omega^2}.$$
 (12.8)

In metals  $\omega_p$  is in the range of:

$$\omega_p = 10^{16} \, s^{-1}. \tag{12.9}$$

Hence plasma frequency is in ultraviolet. When we perform experiments in visible region we can assume that:

$$\gamma \qquad \omega < \omega_p. \tag{12.10}$$

In the optical region so called visible (VIS) we have:

$$n^{2} - k^{2} = \varepsilon_{s} \left( 1 - \frac{\omega_{p}^{2}}{\omega^{2}} \right)$$
(12.11)

and

$$2nk = \varepsilon_s \frac{\gamma \omega_p^2}{\omega^3}.$$
 (12.12)

So in the whole visible region we have  $n^2 - k^2 < 0$  and  $nk \to 0$  which, as was discussed above, results in reflection coefficient equals to one. It is so called metallic reflection. When we however cross with frequencies the plasma frequency  $\omega_p$  than we have  $n^2 - k^2 > 0$  and still  $nk \to 0$  and reflection coefficient gradually decreases which means that metals are transparent in ultraviolet.

# 13. Free electron absorption

For the frequencies above the plasma frequency  $\omega_p$  the material is partly transparent and we can measure the absorption coefficient  $\eta$  when the width of the sample *d* is not to high, it is the intensity of light coming through the samples:

$$I == I_o e^{-\eta d} \tag{13.1}$$

is measurable.

In experiments it is usually required width not higher than:

$$d < \frac{8}{\eta}.$$
 (13.2)

From equations (12.26) and (12.43) we evaluate that in ultraviolet the absorption coefficient for metals is equal to:

$$\eta = \frac{2k\omega}{c} = \frac{\varepsilon_s \gamma \omega_p^2}{cn\omega^2},$$
(13.3)

which means that is proportional to square of wave length. This is so called an absorption on free electrons. In reality this dependence is not exactly quadratic.

#### 14. Damped oscillators -classical approximation

In the study of matter-radiation interaction in some cases the simple model of damped oscillators are introduced. Especially when interaction of matter with waves from micro- and infrared ranges are investigated.

Let us consider an electron oscillating in one dimension x in an electric field. The second Newton principle in this case reads:

$$m\ddot{x} = -kx - b\dot{x} - e\varepsilon_0 e^{i\omega t}, \qquad (14.1)$$

where

-kx is the harmonic force

 $-b\dot{x}$  is the damped force

 $-e\varepsilon_0 e^{i\omega t}$  is the external electric force.

It is convenient to express above terms in a form:

$$kx = m\omega_0^2 x, \qquad (14.2)$$

where  $\omega_0$  is a normal mode of a system, it is the undamped angular frequency

$$b\dot{x} = m\gamma \dot{x}, \qquad (14.3)$$

where  $\gamma$  is a damping constant. The eq. 19.1 can be now written in a form:

$$m\ddot{x} + m\gamma\dot{x} + m\omega_0^2 x = -e\varepsilon_0 e^{i\omega t}.$$
 (14.4)

Putting

$$x = x_0 e^{i\omega t} \tag{14.5}$$

and dividing both sides by m we get an equation for the amplitude of frequency  $x_0$ :

$$\left(-\omega^2 + i\omega\gamma + \omega_o^2\right)x_0 = -\frac{e}{m}\varepsilon_o.$$
 (14.6)

The solution of eq.19.4 can be finally written in a form:

$$x = \frac{-\frac{e}{m}}{\omega_o^2 - \omega^2 + i\omega\gamma} \varepsilon_o e^{i\omega t}.$$
 (14.7)

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When we have n indentical oscillators in a unit volume than the density of current given by such oscillators equals to:

$$j = -ne\dot{x} \,. \tag{14.8}$$

Differentiating eq. 19.7 and putting it into eq. 19.8 we get a current density in a form:

$$j = n \frac{e^2}{m} \frac{i\omega}{\omega_o^2 - \omega^2 + i\omega\gamma} \varepsilon_o e^{i\omega t}$$
(14.9)

and from that the equation for the complex conductivity, which is more interesting since is independent on the external field and is simply characteristic for the crystal:

$$\sigma^* = \frac{j}{\varepsilon} = \frac{ne^2}{m} \frac{i\omega}{\omega_o^2 - \omega^2 + i\omega\gamma}.$$
 (14.10)

Since complex conductivity  $\sigma^*$  is expressed by real conductivity  $\sigma$  and polarisibility  $\alpha$  (see also chapter 3):

$$\sigma^* = \sigma + i\omega\alpha \,. \tag{14.11}$$

Then by separation the real and imaginary part we obtain expression for physical quantities measured in experiments; the conductivity:

$$\sigma = n \frac{e^2}{m} \frac{\omega^2 \gamma}{\left(\omega_o^2 - \omega^2\right)^2 + \omega^2 \gamma^2}$$
(14.12)

and the polarisability:

$$\alpha = -n \frac{e^2}{m} \frac{\omega_o^2 - \omega^2}{\left(\omega_o^2 - \omega^2\right)^2 + \omega^2 \gamma^2}.$$
(14.13)

The polarizability is negative as according to Lentz rule electrons rotate contrariwise to the change of an external fields (a diamagnetic case). The conductivity and the polarizability change resonantly in the vicinity of  $\omega_o$ . Let consider this variation. When we denote the difference between  $\omega$  and  $\omega_o$  as:

$$\Delta \omega = \omega - \omega_o, \qquad (14.14)$$

then we can make a simple approximation:

$$\omega_o^2 - \omega^2 \approx -2\omega\Delta\omega \,. \tag{14.15}$$

Putting above dependence into equation 19.11 we get an expression for conductivity in a form:

$$\sigma = n \frac{e^2}{m} \frac{\gamma}{\left(\Delta\omega\right)^2 + \left(\frac{\gamma}{2}\right)^2}.$$
(14.16)

The absorption coefficient  $\eta$  is expressed by the conductivity  $\sigma$  in a form (see also chapter 3):

$$\eta = \frac{4\pi\sigma}{cn_r},\tag{14.17}$$

where  $n_r$  is a refractive index (we added index r in order not to mix refractive index with an electron concentration n). Putting expression we obtain an approximate formula for the change of  $\eta$  in the vicinity of  $\omega_o$  in a form:

$$\eta \approx \frac{\pi n e^2}{c n_r m} \frac{\gamma}{\left(\Delta \omega\right)^2 + \left(\frac{\gamma}{2}\right)^2}.$$
(14.18)

This dependence is presented in a Fig. 19.1. As it is seen it is a resonant line with a Full Width at Half Maximum (FWHM) equal to  $\gamma$ .

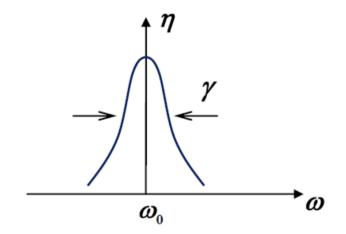


Fig. 19.1. The variation of the polarisibility in vicinity of normal angular frequency mode of a system  $\omega_o$ .

Using the approximation 19.15 we can also evaluate the polarisibility  $\alpha$  in vicinity of  $\omega_o$  and we obtain a formula:

$$\alpha \approx -n \frac{e^2}{2m\omega_o} \frac{\Delta\omega}{\left(\Delta\omega\right)^2 + \left(\frac{\gamma}{2}\right)^2}.$$
(14.19)

Further we get a formula describing the difference between squares of real  $n_r$  and imaginary k part of an refractive index (see also chapter 3):

$$n_r^2 - k^2 = 1 + 4\pi\alpha = 1 - \frac{2\pi ne^2}{m\omega_o} \frac{\Delta\omega}{\left(\Delta\omega\right)^2 + \left(\frac{\gamma}{2}\right)^2}.$$
 (14.20)

Above dependence is presented in a Fig. 19.2.

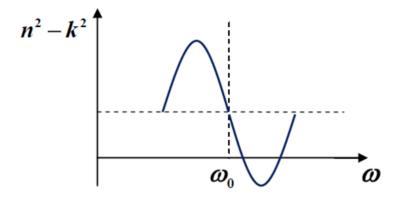


Fig. 19.2. The variation of  $n_r^2 - k^2$  in vicinity of normal angular frequency mode of a system  $\omega_o$ .

When the absolute value of the polarisibility  $\alpha$  is high enough, it is higher than 1 we get:

$$n_r^2 - k < 0. (14.21)$$

It is the case of total reflectance of a matter, so called metallic reflection (see chapter 11). Since  $n_r^2 - k^2$  depends on concentration we can always take enough electrons to obey above condition. The electrons in a crystal can be treated as oscillators with normal frequency  $\omega_o$  equal to zero:

$$\omega_a = 0. \tag{14.22}$$

When we put above value to eq. (19.12) and (19.1) we get following expressions for conductivity:

$$\sigma = \frac{Ne^2}{m} \frac{\gamma}{\omega^2 + \gamma^2}$$
(14.23)

and polarisibility

$$\alpha = -\frac{Ne^2}{m} \frac{1}{\omega^2 + \gamma^2} \,. \tag{14.24}$$

This expressions are similar to those obtained from Boltzmann equation but of course is much more simplified since in Boltzmann equation relaxation time  $\tau = 1/\gamma$  depends on energy. In simple cases the model of damped oscillators works, e.g. In the case of electrons in metals when all electrons from the Fermii sphere have the same property.

#### 15. Oscillator strength - quantum mechanical approximation

... In the previous paragraph we have introduced the a semi-classical interpretation of electrons in crystals. In this paragraph we will briefly present a quantum mechanical description of the interaction of an electron with a electromagnetic wave.

The full Hamiltonian of electrons in crystals under interaction of electromagnetic wave has a form:

$$\hat{H} = \hat{H}_{cr} + \hat{H}_{R} + \hat{H}_{int}, \qquad (15.1)$$

where

 $\hat{H}_{cr}$  is the Hamiltonian of an electron in a crystal,

 $\hat{H}_{R}$  is the Hamiltonian of radiation,

 $\hat{H}_{int}$  is the Hamiltonian of electron – radiation interaction.

terms in Hamiltonian  $\hat{H}$  describe an electron in a crystal, radiation and interaction of electron with radiation respectively. Interaction of an electron with radiation in quantum mechanics is introduced via a general momentum and a vector potential  $\overline{A}$  of an electromagnetic field in the following way. Let us consider the electromagnetic wave characterised by angular frequency  $\omega$  and propagation vector  $\overline{q}$ :

$$\overline{\varepsilon} = \overline{\varepsilon}_0 \cos\left(\omega t \pm \overline{qr}\right), \tag{15.2}$$

where  $\overline{\mathcal{E}}_0$  is the polarisation vector.

Instead of using electric field  $\overline{\varepsilon}$  associated with an electric potential  $\Phi$  we can use a gauge with a vector potential  $\overline{A}$  defined as:

$$\overline{\varepsilon} = -\frac{1}{c} \frac{\partial \overline{A}}{\partial t}.$$
(15.3)

As in a classical mechanic we can introduce a vector potential  $\overline{A}$  into an electron momentum  $\overline{p}$  and transfer to general momentum description of an electromagnetic field but now as an operator:

$$\hat{p} \rightarrow \left(\hat{p} + \frac{e}{c}\hat{A}\right).$$
 (15.4)

In one electron effective mass approximation the Hamiltonian will take a form:

$$\hat{H} = \frac{1}{2m^*} \left( \hat{p} + \frac{e}{c} \hat{A} \right)^2,$$
(15.5)

which can be written down as:

$$\hat{H} = \frac{1}{2m^*}\hat{p}^2 + \frac{e}{2m^*c}\left(\hat{p}\hat{A} + \hat{A}\hat{p}\right) + \frac{e^2}{2m^*c^2}\hat{A}^2.$$
(15.6)

When the field is week the last term can be neglected and we can write Hamiltonian in a form:

$$\hat{H} = \hat{H}_{cr} + \frac{e}{2m^{*}c} \left( \hat{p}\hat{A} + \hat{A}\hat{p} \right),$$
(15.7)

where

$$\hat{H}_{cr} = \frac{1}{2m^*} \hat{p}^2.$$
(15.8)

As this is weak we can treat the second term in eq. 15.7 describing interaction of an electron with an electromagnetic wave as a perturbation and according to quantum mechanics rules express it in a form:

$$\hat{H}_{int} = \frac{e}{mc} \hat{p} \hat{A}.$$
(15.9)

As the electromagnetic wave is time dependent the perturbation (15.9) will induce transitions between the initial states  $|i\rangle$  and final states  $|f\rangle$ . The term  $|\alpha\rangle$  denotes an eigenstate of Hamiltonian of an electron in a crystal  $\hat{H}_{cr}$  with energy  $E_{\alpha}$ .

According to the Fermi Golden Rule the transition probability per time unit from the initial state  $|i\rangle$  to the final state  $|f\rangle$  under the action of interaction Hamiltonian  $\hat{H}_{int}$  is described by a formula:

$$P_{fi} = \frac{2\pi}{\hbar} \frac{e}{mc} \left| \hat{A} \left\langle f \left| \hat{p} \right| \right| i \right\rangle \right|^2 \delta \left( E_f - E_i - \hbar \omega \right).$$
(15.10)

In optical transition a dimensionless quantity called the oscillator strength is introduced. The oscillator strength express the strength of the transition and is given in a form:

$$f_{fi} = \frac{2|\langle f | \hat{p} | i \rangle|^2}{m(E_f - E_i)}.$$
(15.11)

We can perform a following transition from classical mechanic to quantum mechanics. When we assign to all transitions between the initial state  $|i\rangle$  and final state  $|f\rangle$  the oscillator strength  $f_{fi}$  we can rewrite the classical expression for the conductivity  $\sigma$  (eq.14.16) and the polarsibility  $\alpha$  (eq.14.19) in a form:

$$\sigma = \sum_{f=1}^{N} f_{if} \frac{e^2}{4m} \frac{\gamma_{if}}{\left(\omega_{if}^2 - \omega^2\right)^2 + \left(\frac{\gamma_{if}}{2}\right)^2},$$
(15.12)

$$\alpha = \sum_{f=1}^{N} f_{if} \frac{e^2}{2m\omega_{if}} \frac{\omega_{if} - \omega}{\left(\omega_{if}^2 - \omega^2\right)^2 + \left(\frac{\gamma_{if}}{2}\right)^2},$$
(15.13)

where

$$\omega_0 = \omega_{if} = \frac{\left|E_f - E_i\right|}{\hbar} \tag{15.14}$$

and  $\gamma_{if}$  is a line width in a sense of Full Width at Half Maximum.

According to quantum mechanics rules the sum over all transitions from the given initial state  $|i\rangle$  to all possible final states  $|f\rangle$  is equal to one:

$$\sum_{f=1}^{N} f_{if} = 1.$$
(15.15)

The oscillator strength  $f_{if}$  can be both positive and negative. All transitions from the ground state to excited states are positive. In the case of energy separated transitions the intensity of a line observed in experiment is proportional to the oscillator strength  $f_{if}$ . There are also many additional rules concerning an optical transition. As the an angular momentum of photon can be equal to  $\pm 1$  or 0 the total angular momentum of an electron can be changed only by this values, it is:

$$\Delta l = \pm 1, 0. \tag{15.16}$$

The sum (15.12) and (15.13) are used in a case of optical transitions in atoms, whereas in metals and semiconductors above sums are replaced by integrals.

# 16. Cyclotron resonance - semi-classical approximation

In this paragraph we will use approximations of electrons as oscillators with zero normal frequency to solve the cyclotron resonance problem.

Let us consider the case when two external fields are applied to the crystal:

 $1^{\circ}$  The constant magnetic field  $\overline{B}$  applied in the z axis direction

$$B = (0, 0, B). \tag{16.1}$$

 $2^0$  The alternating electromagnetic field with the angular frequency  $\omega$  applied in a the xy plane

$$\overline{E} = \left(E_x, E_x, 0\right). \tag{16.2}$$

The classical equation of motion with the Lorentz force:

$$\overline{F}_{L} = -\left(\overline{E} + \frac{e}{c}\overline{v} \times \overline{B}\right)$$
(16.3)

and the damped force:

$$\overline{F}_d = -m\overline{\nu}\gamma \tag{16.4}$$

can be expressed in a form:

$$m\ddot{x} = -m\gamma\dot{x} - \frac{e}{c}\dot{y}B - eE_{x}e^{i\omega t},$$

$$m\ddot{y} = -m\gamma\dot{y} - \frac{e}{c}\dot{x}B - eE_{y}e^{i\omega t}.$$
(16.5)

The above equations can be separated by introducing new variables:

$$x + iy \quad and \quad x - iy. \tag{16.6}$$

After a simple but long calculations we get equations in a more convenient form:

$$(x \pm iy)'' + \gamma (x \pm iy)' \mp i\omega_c (x \pm iy)' = -\frac{e}{c} (E_x \pm iE_y) e^{i\omega t}, \qquad (16.7)$$

where

$$\omega_c = \frac{eB}{mc} \tag{16.8}$$

is a the cyclotron frequency.

According to the symmetry of the equation (16.7) we are looking for the solution in a form:

$$x \pm iy = A_{\pm}e^{i\omega t} \,. \tag{16.9}$$

Putting function (16.9) into equation (16.9) we get:

$$\left(-\omega^{2} + i\omega\gamma \pm \omega\omega_{c}\right)A_{\pm} = -\frac{e}{m}\left(E_{x} \pm iE_{y}\right)$$
(16.10)

and the functions (16.9) takes a form:

$$x \pm iy = A_{\pm}e^{i\omega t} = \frac{-\frac{e}{m}(E_x \pm iE_y)}{-\omega^2 + i\omega\gamma \mp \omega\omega_c}e^{i\omega t}.$$
 (16.11)

Above solutions are related to circular polarizations of the electromagnetic wave. The polarization  $E_x + iE_y$  is called right-hand circular polarization and marked as  $\sigma^+$  whereas  $E_x - iE_y$  is called left-hand circular polarization  $E_x \pm iE_y$  and marked as  $\sigma^-$ .

Taking derivative of above equation we obtain two velocities of electrons rotating in magnetic fields:

$$v_{\pm} = \left(x \pm iy\right)' = \frac{-i\frac{e}{m}(E_x \pm iE_y)}{-\omega^2 + i\omega\gamma \mp \omega\omega_c}e^{i\omega t}$$
(16.12)

and since:

$$\sigma = -nev \tag{16.13}$$

we obtain the complex conductivity in a form:

$$\sigma_{\pm}^* = -\frac{nev_{\pm}}{E_{\pm}} = \frac{ne^2}{m} \frac{i}{-\omega \mp \omega_c + i\gamma},$$
(16.14)

where n is the electrons concentration.

Since the complex conductivity is expressed by quantities measured in an experiment, it is the real conductivity  $\sigma$  and the real polarisibility  $\alpha$ :

$$\sigma^* = \sigma + i\omega\alpha \tag{16.15}$$

we obtain expressions the following expressions for conductivity:

$$\sigma_{\pm} = \frac{ne^2}{m} \frac{\gamma}{\left(\omega \pm \omega_c\right)^2 + \gamma^2}$$
(16.16)

and polarisibility:

$$\alpha_{\pm} = -\frac{ne^2}{\omega m} \frac{\omega \pm \omega_c}{\left(\omega \pm \omega_c\right)^2 + \gamma^2}.$$
(16.17)

Since the absorption coefficient  $\eta$  is proportional to conductivity  $\sigma$ , so that for the minus sign in equation (16.16) we have a resonant absorption. The Full Width at Half Maximum (FWHM) occurs when:

$$\Delta \omega = \omega - \omega_c = \gamma \,. \tag{16.18}$$

A sharp resonance occurs when:

$$\frac{1}{\tau} = \gamma = \Delta \omega \qquad \omega_c, \qquad (16.19)$$

where  $\tau$  is a relaxation time.

The equation (16.19) can be expressed also in a form:

$$\varsigma = \omega_c \tau \qquad 1, \tag{16.20}$$

where parameter  $\varsigma$  is equal to the mean angle path of an electron around the magnetic field (see also paragraph 7). It means that the sharp resonance occurs when an electron make many rotations around the magnetic field. In the Figure 16.1.

The mean angle path of an electron around the magnetic field  $\varsigma$  can be expressed in a form dependent on mobility  $\mu$  and magnetic field B:

$$\varsigma = \omega_C \tau = \frac{eB\tau}{mc} = \frac{e\tau}{m} \frac{B}{c} = \mu \frac{B}{c}$$
(16.20)

in a Gauss units.

In the SI units the above equation is expressed in a form:

$$\varsigma = \omega_C \tau = \frac{eB\tau}{m} = \frac{e\tau}{m} B = \mu B.$$
(16.21)

For most semiconductors the condition described by equation (16.20) is achieved in low temperatures (liquid helium T=4.2) and magnetic fields of a few Tesla. The angular frequency  $\omega_C$  is than in the range of  $\omega_C \sim 10^{10} - 10^{11} Hz$ , it is in microwave region. Such experiments can be performed very easily in most of laboratories.

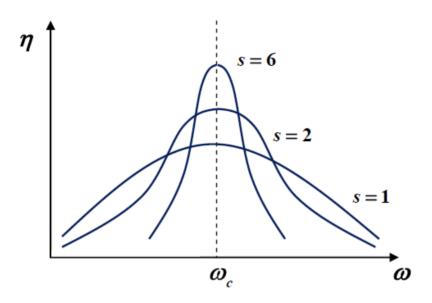


Fig. 16. 1. The evolution of absorption as a function of angular frequency in the resonance region for a few value of a parameter  $\varsigma$ .

#### 17. Inter bands transitions. Optical selection rules

In optical inter band transitions of an electron from a valence to a conduction band two conservation laws have to be fulfilled:

1<sup>0</sup> The energy conservation law

$$\hbar \omega_{photon} = E_f - E_i. \tag{17.1}$$

2<sup>0</sup> The momentum conservation law

$$\hbar \overline{k_i} + \hbar \overline{k_{photon}} = \hbar \overline{k_f}, \qquad (17.2)$$

where  $E_i$ ,  $\hbar \overline{k_i}$  and  $E_f$ ,  $\hbar \overline{k_f}$  are the energy and the momentum of an electron in an initial and final state respectively whereas  $\hbar \omega_{photon}$  and  $\hbar \overline{k_{photon}}$  are the energy and the momentum of incident photon. Energy gap of most of semiconductors is in the range of E<sub>g</sub>=1-2eV. Photons with the same energy have wave vector of the range of  $10^7 \text{m}^{-1}$  whereas electrons in the considered range have wave vector of the range of  $10^9 \cdot 10^{10} \text{m}^{-1}$  so the momentum conservation law takes a form:

$$\hbar \overline{k_i} = \hbar \overline{k_f} \,. \tag{17.3}$$

The optical transitions should obey also the selection rules dependent on symmetry of initial and final electron states. The full Hamiltonian of electrons in crystals under interaction of electromagnetic wave has a form:

$$\hat{H} = \hat{H}_{cr} + \hat{H}_{R} + \hat{H}_{int}, \qquad (17.4)$$

where  $\hat{H}_{cr}$ ,  $\hat{H}_{R}$ , and  $\hat{H}_{int}$  terms in Hamiltonian  $\hat{H}$  describe an electron in a crystal, radiation and interaction of electron with radiation respectively. Interaction of an electron with radiation in quantum mechanics is introduced via a general momentum and a vector potential  $\hat{A}$  of an electromagnetic field in a form:

$$\hat{H}_{int} = -\frac{e}{mc}\hat{p}\hat{A}.$$
(17.5)

When the interaction is small a perturbation theory can be applied. Than a transition probability is described by a square of the matrix element:

$$w \sim |< m|\hat{p}|n>|^2 = |p_{fi}|^2.$$
 (17.6)

In optical transition a dimensionless quantity called the oscillator strength is introduced. The oscillator strength express the strength of the transition and is given in a form:

$$f_{fi} = \frac{2 |p_{fi}|^2}{m(E_f - E_i)}.$$
(17.7)

### **18. Direct transitions**

In the frame of quasi-classical many harmonic oscillators the conductivity is expressed in a form:

$$\sigma = \sum_{fi} \frac{e^2}{4m} \frac{f_{fi} \gamma_{fi}}{(\omega - \omega_{fi})^2 + \frac{\gamma_{fi}^2}{4}}.$$
 (18.1)

# Direct allowed transitions

Direct allowed transitions are those for which matrix elements are non zero. In the calculation of absorption coefficient is it convenient to substitute a summation by an integration over the Brillouine zone:

$$\eta(\omega) = \frac{4\pi\sigma}{cn} = \frac{\pi e^2}{mcn} \int_{BZ} \frac{f(E)\delta(E)\rho(E)dE}{\left[\omega - \omega(E)\right]^2 + \frac{\gamma^2}{4}},$$
(18.2)

which with a good accuracy can be expressed as:

$$\eta(\omega) = \frac{2\pi e^2 \hbar}{mcn} \int_{BZ} f(E) \rho(E) \delta(E - \hbar \omega) dE. \qquad (18.3)$$

After a simple calculation the absorption coefficient for direct transitions can be expressed in a form:

$$\eta = \frac{2^{5/2} m_{\rm r}^{*3/2} e^2}{m \hbar^2 n c} (\hbar \omega - E_g)^{1/2}, \qquad (18.4)$$

where  $m_{\rm r}^*$  is so called reduced mass for an electron and a hole and equals to:

$$m_{\rm r}^* = \frac{m_h^* m_e^*}{m_h^* + m_e^*}.$$
(18.5)

# 19. Direct forbidden transitions

Direct forbidden transitions are those for which the matrix element for k = 0 vanishes:

$$\langle f | p^{i} | i \rangle_{k=0} = 0,$$
 (19.1)

when the initial and final states have the same symmetry.

In some cases we have however non vanishing matrix elements for  $k \neq 0$  which are usually proportional to  $k^2$ :

$$< f | p^{\uparrow} | i >_{k \neq 0} \sim k^{2}.$$
 (19.2)

So the absorption coefficient is dependent on energy in the power 3/2:

$$\eta(\hbar\omega) = Af(\hbar\omega)\rho(\hbar\omega) = A(\hbar\omega - E_g)(\hbar\omega - E_g)^{\frac{1}{2}} = A(\hbar\omega - E_g)^{3/2}.$$
 (19.3)

# 20. Indirect transitions

Indirect transition are those for which the matrix elements for direct transitions for any **k** are equal to zero. In this case transitions of electrons from valence to conduction bands take place with simultaneous additional absorption or emission of a quant of a lattice vibrations – phonons.

In this case two conservation laws are:

 $1^0$  The energy conservation law:

$$\hbar \omega_{photon} \pm \hbar \omega_{phonon} = E_f - E_i.$$
(20.1)

 $2^0$  The momentum conservation law:

$$\hbar \overline{k_i} + \hbar \overline{k_{photon}} \pm \hbar \overline{k_{phonon}} = \hbar \overline{k_f} .$$
(20.2)

The absorption coefficient for indirect transitions is described by a formula:

$$\eta(\hbar\omega) = D\left[\frac{\left(\hbar\omega_{photon} + \hbar\omega_{phonon} - E_g\right)^2}{e^{\frac{E_{phonon}}{kT}} - 1} + \frac{\left(\hbar\omega_{photon} - \hbar\omega_{phonon} - E_g\right)^2}{1 - e^{-\frac{E_{phonon}}{kT}}}\right], \quad (20.3)$$

where the first term describes process with absorption of phonon and the second its emission.

#### 21.Excitons. Effective mass approximation

In low temperatures the absorption as well as emission spectrum of solid states are strongly affected by interaction of photo-excited electrons from the conduction band with leftover holes in a Fermi sea in the valence band. This interaction and energies of complex electronhole systems can be calculated in a frame of so called on effective mass approximation. In the presence of additional potentials (except crystal potentials) and excitations of electrons the Bloch function is not longer a good solution of the Schrodinger equations. When those fields are weak and slowly vary with  $\overline{r}$  one can use the wave function in a following form:

$$\Psi(\overline{r}) = \phi_k(\overline{r}) u_{\overline{k}}(\overline{r}), \qquad (21.1)$$

where  $\phi_k(\overline{r})$  is so cold an envelope function. Without additional fields the envelope function is the solution of the effective mass equation:

$$-\frac{\hbar^2}{2}\nabla\bar{\overline{m}}^{*-1}\nabla\phi_{k_0} = E\phi_{k_0},$$
(21.2)

where  $\overline{\overline{m}}^*$  is an effective mass of electron or hole.

In the case of cubic crystals with a scalar effective mass  $m^*$  above equation can be written in a simplified form:

$$-\frac{\hbar^2}{2m^*}\Delta\phi_{k_0} = E\phi_{k_0}.$$
 (21.3)

In the presence of slowly varying fields equation the effective mass equation takes a form:

$$\left[-\frac{\hbar^2}{2m^*}\Delta + \hat{V}_{slow}(\overline{r})\right]\phi_{\overline{k}} = E\phi_{\overline{k}}.$$
(21.4)

When electron is excited from the valence to the conduction band the electron system is perturbated by the lack of one electron in the valence band. This is considerably different situation to that with additional electron in the conduction band a full valence band. Such an electron – hole pair couple via Coulomb interaction. In some cases this potential is slowly varying and we can use the effective mass approximation. The electron – hole Coulomb interaction can be than written in a form:

$$\hat{V}_{slow}(\overline{r}) = -\frac{1}{4\pi\varepsilon\varepsilon_0} \frac{e^2}{|\overline{r_e} - \overline{r_h}|},$$
(21.5)

where  $\mathcal{E}$  is an relative permittivity.

Effective mass equation takes a form:

$$\left[-\frac{\hbar^2}{2m^*}\Delta + -\frac{1}{4\pi\varepsilon\varepsilon_0}\frac{e^2}{\left|\overline{r_e} - \overline{r_h}\right|}\right]\phi_{\overline{k}}(\overline{r_e}, \overline{r_h}) = E\phi_{\overline{k}}(\overline{r_e}, \overline{r_h}).$$
(21.6)

The envelope function describes now two particles; an electron and a hole. It is convenient to introduce new variables – a relative electron – hole position and a position of a centre of mass:

$$\overline{r} = \overline{r_e} - \overline{r_h} \quad \overline{R} = \frac{m_e^* \overline{r_e} + m_h^* \overline{r_h}}{m_h^* + m_e^*}.$$
(21.7)

The reduce mass and the total mass of an electron – hole pair are:

$$m_{\rm r}^* = \frac{m_h^* m_e^*}{m_h^* + m_e^*} \quad M^* = m_h^* + m_e^*.$$
(21.8)

With this variables the envelope function can be expressed in a simple form as a product of two functions dependent only on these two new variables:

$$\phi_{\overline{k}}\left(\overline{r_{e}},\overline{r_{h}}\right) = \phi_{\overline{k}=0}\left(\overline{r}\right)\phi_{\overline{k}}\left(\overline{R}\right)\phi_{\overline{k}}\left(\overline{r_{e}},\overline{r_{h}}\right) = \phi_{\overline{k}=0}(\overline{r})\phi_{\overline{k}}(\overline{R}).$$
(21.9)

In the effective mass equation these variables may be separated into two independent equations:

$$-\frac{\hbar^2}{2M^*}\Delta\phi_{\bar{k}}\left(\bar{R}\right) = E_1\phi_{\bar{k}}\left(\bar{R}\right)$$
(21.10)

and

$$\left[-\frac{\hbar^2}{2m_{\rm r}^*}\Delta + -\frac{1}{4\pi\varepsilon\varepsilon_0}\frac{e^2}{r}\right]\phi_{\bar{k}=0}(\bar{r}) = E_2\phi_{\bar{k}=0}(\bar{r}).$$
(21.11)

The solutions of those two equations are well known in a quantum mechanics. The first one is a free electron like with effective mass  $M^*$  and the second one is a Hydrogen atom like with effective mass  $m_r^*$  and relative permittivity  $\varepsilon$ . The total energy can be expressed in a form:

$$E = E_1 + E_2 = \frac{\hbar^2 k^2}{2M^*} - Ry \frac{m_r^*}{\varepsilon^2} \frac{1}{n^2} \qquad n = 1, 2, 3..., \qquad (21.12)$$

where Ry = 13, 6eV is Rydberg energy for a Hydrogen atom. Since for typical semiconductors  $m_r^* = 0.1$  and  $\varepsilon = 10$  the so called effective Rydberg energy

$$Ry^* = Ry \frac{m_r^*}{\varepsilon^2}$$
(21.13)

is about three orders smaller and is of the range of a few milielectronvolts.

Such an electron hole object is called an exciton. Notice, that except quantized Coulomb interaction energy it posses also the unquantised energy of translator motion.

# 22. Magneto-optical effects –quantum mechanical picture. Landau quantization

The problem of the electron subjected to external magnetic field is fully solved in quantum mechanics in the Schrödinger picture, it is the Schrödinger equation has an exact solution. The quantization of the cyclotron orbits of charged particles in the magnetic field was for the first time solved by Lev Landau and so it is called the Landau quantization. The charged particles can only occupy orbits with discrete energy values, called Landau levels. The Landau levels are degenerate, with the number of electrons per level directly proportional to the strength of the applied magnetic field. Landau quantization is directly responsible for oscillations in electronic properties of materials as a function of the applied magnetic field.

In quantum mechanics the external magnetic field  $\overline{B}$  can be represented (as in a classical mechanic) by a vector potential  $\overline{A}$ :

$$\overline{B} = rot\overline{A} \tag{22.1}$$

introduced into the Hamiltonian via general momentum:

$$\hat{p} \rightarrow \left(\hat{p} + \frac{e}{c}\hat{A}\right).$$
 (22.2)

When we consider an electron in a crystal in one electron effective mass approximation the Hamiltonian takes a form:

$$\hat{H} = \frac{1}{2m^*} \left( \hat{p} + \frac{e}{c} \hat{A} \right)^2.$$
(22.3)

Let us consider an electron in crystal, it is three dimensional system with magnetic field B applied along z direction:

$$\overline{B} = (0, 0, B). \tag{22.4}$$

There is some freedom in the choice of vector potential for a given magnetic field. However, the Hamiltonian is gauge invariant, which means that adding the gradient of a scalar field to A changes the overall phase of the wave function by an amount corresponding to the scalar field. Physical properties are not influenced by the specific choice of gauge. We will take the so called Landau gauge with vector potential  $\overline{A}$  in a form:

$$\overline{A} = \left(-yB, 0, 0\right). \tag{22.5}$$

Putting above dependence to the Hamiltonian (22.3) and then into the stationary Schrödinger equation:

$$\hat{H}\psi = E\psi \tag{22.6}$$

we get:

$$\frac{1}{2m^*} \left[ \left( -i\hbar \frac{\partial}{\partial x} - \frac{e}{c} By \right)^2 - \hbar^2 \frac{\partial^2}{\partial y^2} - \hbar^2 \frac{\partial^2}{\partial z^2} \right] \psi = E \psi . \qquad (22.7)$$

The above equation differs from the equation for a free electron only by terms dependent on y so the solution can be expressed as a function:

$$\psi(x, y, z) = \varphi(y)e^{i(k_x x + k_z z)}.$$
(22.8)

Putting this function into the equation (22.7) and performing necessary calculation on x and z we obtain:

$$e^{i(k_{x}x+k_{z}z)}\left(\frac{\hbar^{2}k_{x}^{2}}{2m^{*}}+\frac{\hbar^{2}k_{z}^{2}}{2m^{*}}-\frac{\hbar^{2}}{2m^{*}}\frac{\partial^{2}}{\partial y^{2}}-\frac{\hbar k_{x}}{m^{*}}\frac{e}{c}By+\frac{e^{2}}{2m^{*}c^{2}}B^{2}y^{2}\right)\varphi(y)=$$

$$e^{i(k_{x}x+k_{z}z)}E\varphi(y).$$
(22.9)

Extracting the function  $e^{i(k_x x + k_z z)}$  from both sides of above equation we obtain the equation for the function  $\varphi(y)$  only.

Three terms in above equation can be written in a more compact form:

$$\left(\frac{\hbar^{2}k_{x}^{2}}{2m^{*}} + -\frac{\hbar k_{x}}{m^{*}c}\frac{e}{c}By + \frac{e^{2}}{2m^{*}c^{2}}B^{2}y^{2}\right) = \frac{1}{2}m^{*}\left(\frac{eB}{m^{*}c}\right)^{2}\left(y - \frac{\hbar k_{x}c}{eB}\right)^{2} = (22.10)$$
$$\frac{1}{2}m^{*}\omega_{c}^{2}\left(y - \frac{\hbar k_{x}c}{eB}\right)^{2},$$

where

$$\omega_c = \frac{eB}{m^* c} \tag{22.11}$$

is an cyclotron frequency.

Making a simple substitutions:

$$\zeta = y - \frac{\hbar k_x c}{eB},\tag{22.12}$$

$$E' = E - \frac{\hbar^2 k_z^2}{2m^*}$$
(22.13)

and since we have an obvious equality:

$$\frac{\partial^2}{\partial \zeta^2} = \frac{\partial^2}{\partial y^2},\tag{22.14}$$

the equation (22.9) takes a form:

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial\zeta^2} + \frac{1}{2}m\omega_c\zeta^2\right]\phi(y) = E'\phi(y). \qquad (22.15)$$

This equation resembles the equation of a quantum oscillator. The energy of such oscilator are quantized and in our case equal to:

$$E_{n} = \left(n + \frac{1}{2}\right) \hbar \omega_{c} + \frac{\hbar^{2} k_{z}^{2}}{2m^{*}}.$$
 (22.16)

This dependence is illustrated in the Fig. 22.1. The movement of an electron in the external magnetic field subjected along z axis  $\overline{B} = (0, 0, B)$  is free in direction z and quantized in a plane perpendicular to the magnetic field x, y. As the energy  $E_n$  is not dependent on the wave vector  $k_x$  as in the case of zero magnetic field we have a strong degeneration of energy states. The density of states in the ideal case of a perfect crystal (without any imperfection and electron – phonon interaction are presented in the Fig. 22.2. As in the case of quantum oscillator the optically allowed transition occur only without nearest states with:

$$\Delta n = \pm 1. \tag{22.17}$$

This transitions are called as in the classical mechanics the cyclotron resonance and appear only with one frequency  $\omega_c$  called cyclotron frequency. We can also evaluate a width of the energy states from the Heisenberg uncertainty principle:

$$\Delta E \cdot \tau \approx \hbar, \qquad (22.18)$$

where  $\tau$  is a life time of an electron on a given energy state.

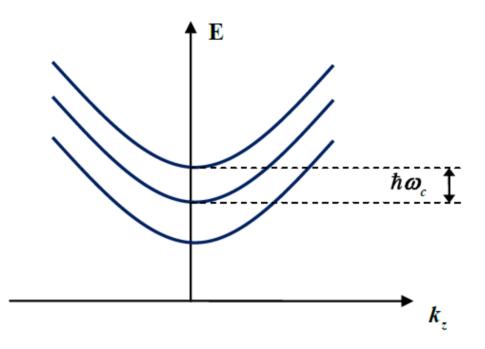


Fig. 22.2. The dependence of the electron energy in an external magnetic field for small wave vectors  $k_z$ 

The resonance is detected only when the energy width is smaller than the distance between energy levels:

$$\Delta E < \hbar \omega_c. \tag{22.19}$$

Putting dependence of  $\Delta E$  from equation (22.18) to equation (22.19) we get:

$$\frac{\hbar}{\tau} < \hbar \omega_c, \qquad (22.20)$$

which can be expressed in the more convenient form:

$$\zeta = \omega_c \tau > 1, \tag{22.21}$$

which resembles the classical mechanics solution (see paragraph 16). The requirements for the observation of cyclotron resonance is that the an electron should make number of circles around the magnetic field.

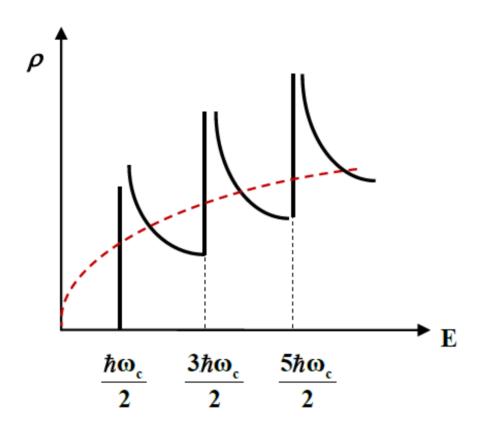


Fig. 22.1. The electron density of states in a magnetic field – solid lines. Dashed lines indicates electron density of states without magnetic field.

Except the condition (22.21) in order to observe cyclotron resonance in experiments additional condition have to fulfilled, it is the temperature have to be as low as the temperature broadening of the line have to be smaller that the distance between energy levels:

$$\hbar\omega_c > kT \,. \tag{22.22}$$

There are variety of effects related to Landau quantization in the magnetic field. In spectroscopy experiments we detect cyclotron resonance in a far infrared region as well as many effects observed in transitions of electrons from valence to conduction bands both in absorption and emission in visible, near infrared and near ultraviolet. Among them are cyclotron replicas of the main intensity lines going to both lower and higher energy with the increase of the magnetic field. In the transport experiments so called Shubnikov de Hass effect is observed as the oscillations of resistivity as a function of the magnetic fields. This effects reflects crossing of the Fermi energy by subsequent landau levels which energies increase with the magnetic field. Also the integer quantum Hall effect be long to this class of experiments. Also the magnetic susceptibility oscillates in magnetic fields. This effect is called the Hass van Alphen effect. In experiments in external magnetic field we should also take into account that an electron posses also the spin

$$s = 1/2$$
, (22.23)

which is fourth quantum number describing the internal degree of an electron state of freedom. The energy of an electron in a magnetic field connected with the spin is equal to:

$$E_{\mu} = g\mu_B \hat{\sigma} \overline{B} , \qquad (22.24)$$

where  $\hat{\sigma}$  is the spin operator and  $\mu_B$  is an magnetic moment of an electron so called the Bohr magneton equal to:

$$\mu_B = \frac{e\hbar}{2mc}.$$
(22.25)

Since the projection of the electron spin along the magnetic field is equal to:

$$s_z = \pm 1/2$$
 (22.26)

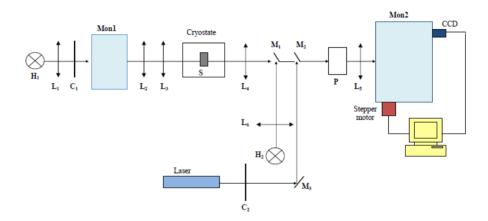
we have two energies related to spin connected with each Landau levels. The transition between Landau levels with the conservation of the spin projection are called the cyclotron resonance whereas the transition between the states with opposite spin but with the same Landau levels are called paramagnetic resonance.

#### Further reading

- 1. P. Yu, M. Cardona, "Fundamentals of Semiconductors", Springer, Berlin 1999
- H. Ibach, H. Luth, "Solid-State Physics, An introduction to Principles of Material Science" Springer-Verlag Berlin Heildelberg 1995
- 3. C. Kittel, "Introduction to Solid State", Wiley and Sons, New York 1996
- 4. W. A. Harrison, "Solid-State Physics", Wiley and Sons, New York 1995

# 23. The typical set up for an optical experiments. Determination of an absorption coefficient of bulk crystals

Typical set up for optical experiments is presented in Figure 1. In this configuration all main optical experiments can be performed, it is absorption, reflectivity, photoluminescence, photoluminescence excitation and combinations of these experiments.



The main parts of set up are a cryostat, a spectrophotometer and excitation sources.

The cryostats are used since most valuable information about physical properties of materials are obtained when they are in low temperatures and the studied effects are not influenced by interaction with vibrations of crystal lattice i.e. electron – phonon interactions. There are variety of cryostats used in experiments. In bath cryostats samples are immersed in a liquid Nitrogen or Helium in temperatures T=77K and T=4.2K respectively. The advantage of such cryostats is possibility of the use of high excitation power density however disadvantage is vaporisation of liquids and bulbs produce in such process what strongly increase noise of measured signal. The other type of cryostats are so called "cold finger" cryostats. In such cryostats sample is mounted in a vacuum on a holder cooled by liquid Nitrogen or Helium. Advantage of these cryostats is very easy operation however in this case a low density power excitation can be used.

The spectrometer consists of a monochromator which split the light in a necessary spectral regions, followed by detectors, step motors rotating a grating and a computer from which an experiment is directed. Monochromators with gratings are chosen according to the requirements of experiments, which is spectral region, resolution, efficiency etc. Nowadays CCD camera are commonly used due to low cost and ability to measure the whole analysed spectra. Unfortunately CCD camera operates only in spectral region in which Silicon has strong absorption it is from  $\lambda$ =1.1-0.2 µm. In spectral region down to  $\lambda$ =1.7 µm the In<sub>x</sub>Ga<sub>1</sub>. <sub>x</sub>As linear device can be used also to measure the whole spectra. Unfortunately this device is very expensive. Out of above regions other detectors have to be used. Very common in the were photomultipliers which usually have very strong signal but since they measure only one signal the spectra with their use were measured point by point which is very time consuming. In for infrared other detectors as thermopars and bolometer are used but their efficiency are very week in comparison to CCD cameras and photomultipliers.

The light sources should also be chosen according up to the studied spectral range. The most common sources are halogen lamps. They are very cheap and have very high efficiency in visible region (VIS) as well as in not far ultraviolet (UV) and infrared (NIR).

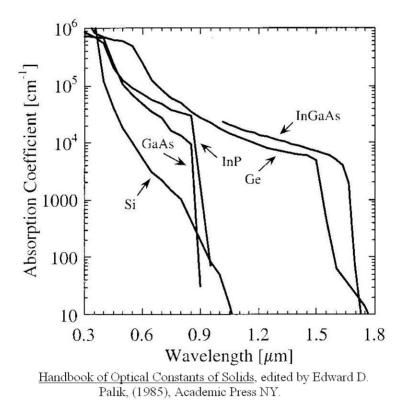
In infrared a black body source is used (with customer name a globar).

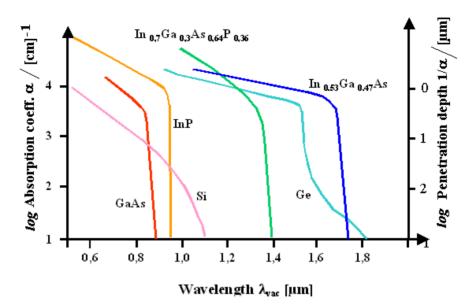
A Globar is a silicon carbide rod of 5 to 10 mm width and 20 to 50 mm length which is electrically heated up to temperatures ranging from 1,000 to 1,650 °C (1,832 to 3,002 °F). When combined with a downstream variable interference filter, it emits radiation from 4 to 15 micrometres wavelength. Globars are used as thermal light sources for infrared spectroscopy because their spectral behaviour corresponds approximately to that of a Planck black body radiator.

The most common material for lenses is glass since it is cheap and easy to manufacture. The typical glass transmit light from 0.4  $\mu$ m to 2  $\mu$ m. Quartz glass transmits light in a wider region from 0.2  $\mu$ m to 4  $\mu$ m. When operating beyond this region metal focussing mirrors are being used.

# Determination of an absorption coefficient of bulk crystals

In the case of semiconductors and dielectrics with direct energy gap an absorption coefficient in fundamental absorption edge region increases very quickly with increase of photon energy. In Figures bellow we see that for those materials as GaAs and InP absorption coefficient increase in a very narrow region up to  $10^{-5}$  cm<sup>-1</sup>. According to Lambert Beer law it means that in absorption experiments very thin samples should be used with a thickness of the range of micrometers. Such samples are very difficult to obtain and also very difficult to operate. During students laboratory a bulk samples with a thickness of about 100  $\mu$ m are being used.





In semiconductors with indirect energy gaps as Silicon the absorption coefficient above energy gap increases very slowly. Therefore transmission measurements of such samples above energy gap samples with thickness of even 1 mm could be used. Such samples are very easy to operate and are advised to use as a starting point for not experienced students.