Chapter 2

Theory

This chapter presents a classical equation of motion of an electron in electric and magnetic fields. Boltzmann equation is presented briefly. The provided theory aims at forming a model of multi-carrier transport in a magnetic field.

2.1 Classical equation approach

Considering a homogeneous material with an isotropic effective mass and the energy-independent relaxation time approximation, the motion of the electron with charge -e in a uniform external electric field $\mathbf{E} = (E_x, E_y, 0)$ and a magnetic field $\mathbf{B} = (0, 0, B_z)$ is described simply by the classical equation of motion

$$m^* \frac{d\mathbf{v}}{dt} + \frac{m^*}{\tau} \mathbf{v} = (-e) \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right), \tag{2.1}$$

where \mathbf{v} is a velocity, m^* is an effective mass of the carrier, and τ is a constant relaxation time. A standard geometry of Hall and magnetoresistivity measurement is shown in Fig. 2.1. In Eq. (2.1), an electrical charge -e will be replaced by a positive value e for hole carriers. Under a steady-state condition, the acceleration term is vanished and the velocity of the carrier becomes

$$v_x = \frac{(-e)\,\tau}{m^*} E_x + \frac{(-e)\,\tau B_z}{m^*} v_y \tag{2.2}$$

and

$$v_y = \frac{(-e)\,\tau}{m^*} E_y + \frac{(-e)\,\tau B_z}{m^*} v_x. \tag{2.3}$$

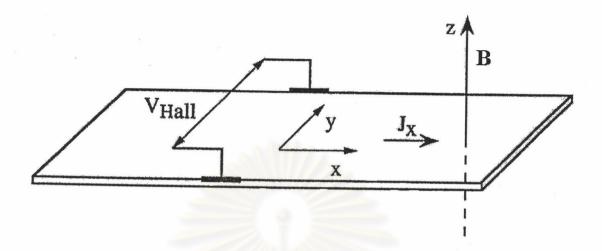


Figure 2.1: Standard geometry for Hall effect and magnetoresistivity measurements. V_{Hall} is the Hall voltage and J_x is the current density in the flow direction (after Grosso et al. (2000)).

Solving these coupling equations, one can present the solution in terms of a current density $\mathbf{J} = ne\mathbf{v}$ and the electric field \mathbf{E} as

$$\begin{bmatrix} j_x \\ j_y \end{bmatrix} = \begin{bmatrix} \sigma_{xx}(B) & -\sigma_{xy}(B) \\ \sigma_{xy}(B) & \sigma_{xx}(B) \end{bmatrix} \begin{bmatrix} E_x \\ E_y \end{bmatrix}, \tag{2.4}$$

where

$$\sigma_{xx} = \frac{ne\mu}{1 + (\mu B)^2},\tag{2.5}$$

$$\sigma_{xy} = \frac{ne\mu^2 B}{1 + (\mu B)^2},\tag{2.6}$$

and

$$\mu = \frac{e\tau}{m^*}.\tag{2.7}$$

The second-rank magnetoconductivity tensor $\sigma(B)$ is defined where σ_{xx} and σ_{xy} are the longitudinal and transverse magnetoconductivity tensor components respectively. n is a carrier concentration and μ is an electrical mobility. It shows that, under the influence of a magnetic field, the motion of carrier is deflected and the current density is no longer parallel to the applied electric field, E_x . The transverse electric field E_y is called Hall field. The magnetoresistivity ρ_{xx} and the Hall

coefficient R_H are defined and obtained form the measurement,

$$\rho_{xx} = \frac{E_x}{j_x} \tag{2.8}$$

and

$$R_H = \frac{1}{B} \frac{E_y}{j_x}. (2.9)$$

By inversion of $\sigma(B)$, the magnetoresistivity tensor $\rho(B)$ is provided as

$$\rho(B) = \begin{bmatrix} \rho_{xx}(B) & BR_H(B) \\ -BR_H(B) & \rho_{xx}(B) \end{bmatrix}, \qquad (2.10)$$

and its components relate to magnetoconductivity components with

$$\sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2 + (BR_H)^2} \tag{2.11}$$

and

$$\sigma_{xy} = \frac{BR_H}{\rho_{xx}^2 + (BR_H)^2}. (2.12)$$

On the other hand, we obtain

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2} \tag{2.13}$$

and

$$R_H = \frac{\rho_{xy}}{B} = \frac{\sigma_{xy}}{B\left(\sigma_{xx}^2 + \sigma_{xy}^2\right)}.$$
 (2.14)

In this approximation, an isotropic effective mass and constant relaxation time are assumed. ρ_{xx} and R_H can be expressed as

$$\rho_{xx} = \frac{1}{ne\mu} \tag{2.15}$$

and

$$R_H = \frac{1}{n\left(-e\right)}. (2.16)$$

It can be said that the magnetoresistivity and Hall coefficient are independent of the magnetic field. By Eqs. (2.15) and (2.16), the type of carrier, mobility and carrier

concentration are obtained from the measurement of ρ_{xx} and R_H . This is a simple way to characterize the material having single carrier species.

This model can be applied to both cases of holes and electrons. Considering a sample having hole group of concentration n_1 and mobility μ_1 , and electron group of concentration n_2 and mobility μ_2 , respectively. By assuming that there are no interaction between them, the diagonal components are merely the summation of the conductivity component from each species, but the off-diagonal components are the difference between the conductivity components of hole and electron species. The resultant magnetoconductivity tensor is obtained as

$$\sigma = \begin{bmatrix} \frac{n_1 e \mu_1}{1 + (\mu_1 B)^2} + \frac{n_2 e \mu_2}{1 + (\mu_2 B)^2} & \frac{n_1 e \mu_1^2 B}{1 + (\mu_1 B)^2} - \left(\frac{n_2 e \mu_2^2 B}{1 + (\mu_2 B)^2}\right) \\ -\left(\frac{n_1 e \mu_1^2 B}{1 + (\mu_1 B)^2}\right) + \frac{n_2 e \mu_2^2 B}{1 + (\mu_1 B)^2} & \frac{n_1 e \mu_1}{1 + (\mu_1 B)^2} + \frac{n_2 e \mu_2}{1 + (\mu_2 B)^2} \end{bmatrix}. \quad (2.17)$$

For the mobility spectrum analysis, these equations are generalized to

$$\sigma_{xx} = \sum_{i} \frac{(s_i^p + s_i^n)}{1 + \mu_i^2 B^2} \tag{2.18}$$

and

$$\sigma_{xy} = \sum_{i} \frac{(s_i^p - s_i^n) \,\mu_i B}{1 + \mu_i^2 B^2},\tag{2.19}$$

where $s_i^p = n_i^p e \mu_i$ and $s_i^n = n_i^n e \mu_i$ are the partial conductivity of hole species and electron species to be solved. For more realistic case, the energy dependence of the relaxation time and other complicated structure of energy band are considered. Then the rigorous formalism such as Boltzmann equation is required to describe accurately the transport properties in a complex sample.

2.2 Quasi-classical Boltzmann equation

The Boltzmann equation is used to describe the transport of an electrical carrier under the influence of an external electric field, a magnetic field, and a

temperature gradient. In the case of an electron gas, the equation can be written as [Beer (1963)]

$$-\frac{e}{\hbar} \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \cdot \nabla_k f + \mathbf{v} \cdot \nabla_r f = \left(\frac{\partial f}{\partial t} \right)_{coll}, \tag{2.20}$$

where **E** is the electric field, **B** is the magnetic field, and **v** is the carrier velocity. The distribution function f = f(k, r, t) is the carrier distribution in phase space which is modified when the external field is applied. For simplicity, the temperature gradient in a material is neglected. One can use a relaxation time approximation when the thermal energy is large compared to the energy of carriers, which is

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\left(\frac{f - f_0}{\tau}\right),$$
(2.21)

where f_0 is the equilibrium distribution.

McClure (1956) solved Boltzmann equation (Eq. (2.20)) with the relaxation time approximation (Eq. (2.21)) for a general energy band structure at an arbitrary magnetic field. By assuming that the relaxation time is constant around a cyclotron orbit, McClure expressed the magnetoconductivity tensor components as a Fourier series expansion B(m) in harmonic m of the cyclotron frequency ω . For a single band, the expression is [see Kiatgamolchai (2000)]

$$\sigma_{xx/xy} = \frac{e^2}{(2\pi)^3} \int d^3k \frac{\partial f_0}{\partial E} \tau S_{xx/xy}, \qquad (2.22)$$

where

$$S_{xx} = \sum_{m=1}^{\infty} \frac{|B(m-1)|^2 + |B(-(m+1))|^2}{1 + (m\omega\tau)^2}$$
 (2.23)

and

$$S_{xy} = \sum_{m=1}^{\infty} \frac{m\omega\tau \left[|B(m-1)|^2 - |B(-(m+1))|^2 \right]}{1 + (m\omega\tau)^2}.$$
 (2.24)

It is easy to generalize these expressions to multiple bands by summing each single band term. These expressions are more fruitful than other Boltzmann solutions because they are valid for a wide range of magnetic field strength. In particular, they allow a finite number of conduction bands, nonparabolic bands, and energy-dependent scattering mechanisms with field-dependent mass and relaxation time [Beck and Anderson (1987)].

Beck and Anderson (1987) transformed Eq. (2.22) from the wave vector space into the mobility space, which gave

$$\sigma_{xx}(B) = \int_{-\infty}^{\infty} \frac{s(\mu)}{1 + (\mu B)^2} d\mu \qquad (2.25)$$

and

$$\sigma_{xy}(B) = \int_{-\infty}^{\infty} \frac{s(\mu) \mu B}{1 + (\mu B)^2} d\mu \qquad (2.26)$$

where

$$s(\mu) = \begin{cases} n^p e \mu, & \mu > 0 \\ n^n e |\mu|, & \mu < 0 \end{cases}$$
 (2.27)

 $s(\mu)$ is the conductivity density as a quasi-continuous function of mobility, also called "mobility spectrum". In this formalism, holes have positive mobilities and electrons have negative mobilities.

Eqs. (2.25) and (2.26) are valid only in classical limit where quantum effect is neglected. At a large magnetic field, $\hbar\omega \geq kT$ where \hbar is plank's constant and k is Boltzmann's constant, Landau levels are formed and the energy band is split. The presence of discrete density of states leads to quantum effect; for example, the Shubnikov-de Haas oscillations where the magnetoresistance oscillates with magnetic field and Hall resistivity becomes stepwise.

2.3 Parameters from mobility spectrum

The Hall factor is the ratio of Hall mobility (μ_H) , measured at a low magnetic field, to drift mobility (μ_D) , measured in the absence of the magnetic field, or the ratio of carrier concentration n to Hall concentration n_H ;

$$r_H = \frac{\mu_H}{\mu_D} = \frac{n}{n_H},$$
 (2.28)

or [Swanson (1955)]

$$r_H = \frac{R_H (B \to 0)}{R_H (B \to \infty)} = \frac{\rho_{xy} (B \to 0)}{\rho_{xy} (B \to \infty)}.$$
 (2.29)

By using Eqs. (2.14), (2.18) and (2.19),

$$\lim_{B \to 0} \rho_{xy} = \frac{\sum_{i} s_i \mu_i}{\left(\sum_{i} s_i\right)^2} \tag{2.30}$$

and

$$\lim_{B \to \infty} \rho_{xy} = \frac{1}{\sum_{i} \frac{s_i}{\mu_i}},\tag{2.31}$$

which leads to

$$r_{H} = \frac{\left(\sum_{i} \frac{s_{i}}{\mu_{i}}\right) \left(\sum_{i} s_{i} \mu_{i}\right)}{\left(\sum_{i} s_{i}\right)^{2}}.$$

$$(2.32)$$

Hall mobility and concentration of each carrier species can be calculated by considering the mobility range that covers the peak of interest in a mobility spectrum. Hall mobility is defined as

$$\mu_H = \frac{R_H (B \to 0)}{\rho_{xx} (B = 0)}.$$
 (2.33)

By using Eqs. (2.13), (2.14), (2.18) and (2.19), it can be shown that

$$\mu_H = \frac{\sum_i s_i \mu_i}{\sum_i s_i}.$$
(2.34)

Carrier concentration is also the summation over the selected mobility range,

$$n_H = \sum_i \frac{s_i}{e\mu_i}. (2.35)$$

The drift mobility is defined as

$$\mu_D = \frac{R_H \left(B \to \infty \right)}{\rho_{xx} \left(B = 0 \right)}.$$
 (2.36)

Using Eqs. (2.28) and (2.32), it is easy to obtain

$$\mu_D = \frac{\sum_i s_i}{\sum_i \frac{s_i}{\mu_i}}.$$
(2.37)

