

# 8.231 Physics of Solids I — Fall 2017

## Recitation Note 1

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### 1 More on Drude Theory

#### 1.1 Hall Effect

##### 1.1.1 Historic Fact [1]

The story of the Hall effect begins with a mistake. The story of the Hall effect begins with a mistake made by James Clerk Maxwell. In the first edition of his book “*Treatise on Electricity and Magnetism*”, which appeared in 1873, Maxwell discussed the deflection of a current carrying wire by a magnetic field. Maxwell then says: *It must be carefully remembered that the mechanical force which urges a conductor ..., acts, not on the electric current, but on the conductor which carries it.* If the reader is puzzled that is OK, he should be.

In 1878 Edwin H. Hall, a student at Johns Hopkins University, was reading Maxwell for a class by Henry A. Rowland. Hall was puzzled by this passage and approached Rowland. Rowland told him that ... *he doubted the truth of Maxwell statement and had sometimes before made a hasty experiment ... though without success.* Hall made a fresh start, and tried to measure the magnetoresistance — a hard experiment. This experiment failed too and Maxwell appeared to be safe. Hall then decided to repeat the experiments made by Rowland, and following a suggestion of his advisor, replaced the original metal bar with a thin gold leaf and found that the magnetic field deflected the galvanometer needle. This earned Hall a position at Harvard.

##### 1.1.2 How to Measure Hall Effect

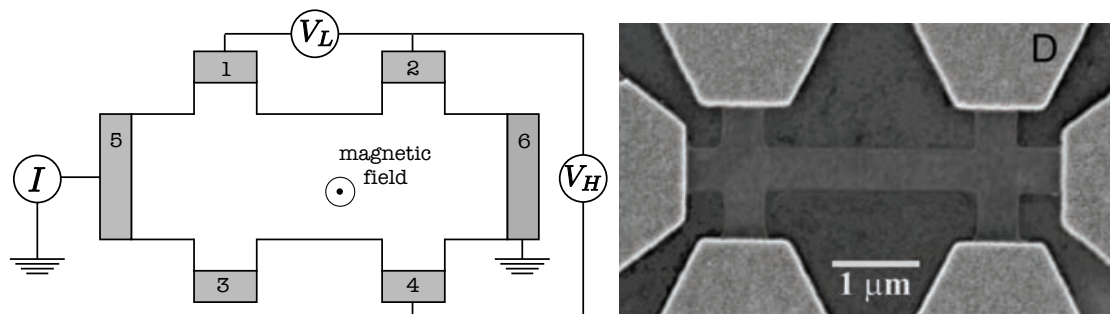


Figure 1: A Hall bar setup to measure Hall effect. Left: Schematic; Right: Scanning electron microscope image of the Hall bar setup to measure Hall effect in graphene [2].

$$J_x = I/W, \quad (1)$$

$$E_x = \frac{(V_1 - V_2) + (V_3 - V_4)}{2L}, \quad (2)$$

$$E_y = \frac{(V_1 - V_3) + (V_2 - V_4)}{2D}. \quad (3)$$

Here  $W$  is the area of the cross section of the Hall bar.  $L$  and  $D$  are the lengths of Hall bar at  $x$  and  $y$  directions, respectively.

### 1.1.3 Drude Theory Revisited

The equation of motion in Drude theory is

$$\frac{d\mathbf{p}}{dt} = -e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) - \frac{\mathbf{p}}{\tau}. \quad (4)$$

Here  $\mathbf{p}$  is interpreted as the averaged momentum of the electron. Let us consider the stationary solution  $d\mathbf{p}/dt = 0$ .

Without loss of generality, assume  $\mathbf{B} = B\hat{\mathbf{z}}$  and  $\mathbf{E} = E_x\hat{\mathbf{x}} + E_y\hat{\mathbf{y}}$ .

$$-e(E_x + v_y B_z) - \frac{mv_x}{\tau} = 0, \quad (5)$$

$$-e(E_y - v_x B_z) - \frac{mv_y}{\tau} = 0. \quad (6)$$

Since  $\mathbf{J} = -nev$ , we have

$$E_x = \frac{m}{ne^2\tau} J_x - \frac{B}{ne} J_y, \quad (7)$$

$$E_y = \frac{B}{ne} J_x + \frac{m}{ne^2\tau} J_y. \quad (8)$$

Define the resistivity tensor  $\rho$  as  $E_i = \sum_{ij} \rho_{ij} J_j$ , we have

$$\rho = \begin{pmatrix} \frac{m}{ne^2\tau} & -\frac{B}{ne} \\ \frac{B}{ne} & \frac{m}{ne^2\tau} \end{pmatrix} = \rho_0 \begin{pmatrix} 1 & -\omega_c\tau \\ \omega_c\tau & 1 \end{pmatrix}. \quad (9)$$

Here  $\rho_0 = 1/\sigma_0$ ,  $\sigma_0 = ne^2\tau/m$  is the DC conductivity in Drude theory.  $\omega_c = -eB/m$  is the cyclotron frequency.

The conductivity tensor  $\sigma$  is defined as  $J_i = \sum_{ij} \sigma_{ij} E_j$ . Thus  $\sigma = \rho^{-1}$ . It can be calculated as

$$\sigma = \frac{\sigma_0}{1 + (\omega_c\tau)^2} \begin{pmatrix} 1 & \omega_c\tau \\ -\omega_c\tau & 1 \end{pmatrix}. \quad (10)$$

Here we have defined the dimensionless quantity  $\omega_c\tau$  to characterize the how “large” is the magnetic field. It only makes physical sense to talk about “large” or “small” for dimensionless quantities.

For Hall effect, there are several quantities one can measure:

- Hall coefficient

$$R_H \equiv \frac{E_y}{BJ_x} = -\frac{1}{ne}. \quad (11)$$

It can tell us the density of the current carrier.

- Hall angle (under the assumption  $J_y = 0$ )

$$\tan \theta \equiv \frac{E_y}{E_x} = \frac{\rho_{yx}}{\rho_{xx}} = \omega_c \tau. \quad (12)$$

It can tell us the scattering time.

Figure 2 shows the measurement of  $\rho_{xx}$  and  $R_H$  for graphene. There is additional voltage at  $z$  direction called the “gate voltage”  $V_g$ . As we can see, the Hall coefficient even changes sign with  $V_g$ . There is also a peak for  $\rho_{xx}$  at the same time  $R_H$  changes sign. At least in some regimes of gate voltage, the behavior of graphene deviates drastically from Drude theory. We will be able to understand what happens in Figure 2 after first half of this course.

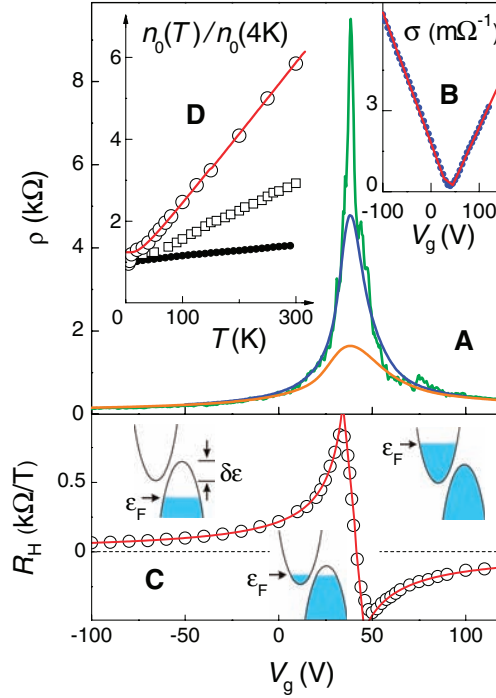


Figure 2: Measurement of Hall effect in graphene [2].

In the weak field limit  $\omega_c \tau \ll 1$ ,

$$\rho \rightarrow \rho_0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (13)$$

Hall angle  $\theta = 0$ . There is only transport along  $x$  direction. We reproduce the result of DC conductivity in Drude theory.

#### 1.1.4 Quantum Hall Effect

What about in the strong field limit  $\omega_c \tau \gg 1$ ? It seems

$$\rho \rightarrow \rho_0 \omega_c \tau \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (14)$$

Hall angle  $\theta = 90^\circ$ . There is only transport along  $y$  direction. Do you think Drude theory is still correct at this regime?

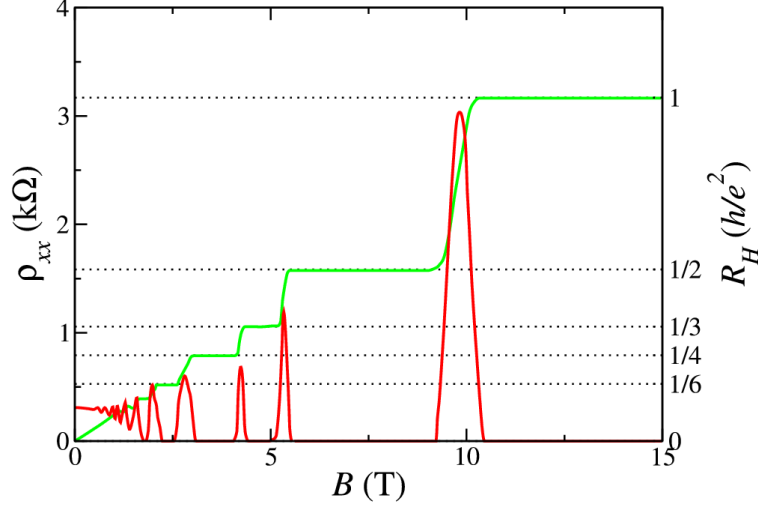


Figure 3: Typical magnetic field dependence of  $\rho_{xx}$  (red) and  $R_H$  (green) in the strong field limit  $\omega_c\tau \gg 1$ .

## 1.2 Thermal Conductivity [3]

Temperature gradient induces heat transfer. This can be summarized by the Fourier's law:

$$\mathbf{j} = -\kappa\nabla T, \quad (15)$$

where  $\mathbf{j}$  is the thermal current and  $\kappa$  is the thermal conductivity.

Suppose temperature only has spatial variation along  $x$  direction, i.e.  $T = T(x)$ . Denote  $\mathcal{E}(T)$  as the thermal energy per electron in equilibrium at temperature  $T$ . An electron whose last collision happens at  $x'$  will carry energy  $\mathcal{E}(T(x'))$ . The electrons arriving at  $x$ , on average will have their last collisions at  $x \pm v\tau$ . Therefore, the thermal current at position  $x$  is given by

$$j_x = \frac{nv}{6} [\mathcal{E}(T(x - v\tau)) - \mathcal{E}(T(x + v\tau))] \quad (16)$$

$$= \frac{nv^2\tau}{3} \frac{d\mathcal{E}}{dT} \left( -\frac{dT}{dx} \right). \quad (17)$$

The  $1/6$  factor is because there are six possible directions of the scattering:  $\pm x, \pm y, \pm z$ . For particles at  $x \pm v\tau$ , only particles scattered to  $\pm x$  contribute to the thermal current at  $x$ .

Also notice

$$n \frac{d\mathcal{E}}{dT} = \frac{N}{V} \frac{d\mathcal{E}}{dT} = \frac{1}{V} \frac{dE}{dT} = c_v, \quad (18)$$

which is the specific heat of the electron. In this way, we can identify

$$\kappa = \frac{1}{3} v^2 \tau c_v, \quad (19)$$

For classical ideal gas,  $c_v = 3nk_B/2$  and  $mv^2/2 = 3k_B T/2$  due to equipartition of energy. Therefore

$$\kappa = \frac{3}{2} k_B^2 T \frac{n\tau}{m} = \frac{3}{2} \left( \frac{k_B}{e} \right)^2 \sigma. \quad (20)$$

This is the Wiedemann-Franz law:

$$\frac{\kappa}{\sigma T} = \frac{3}{2} \left( \frac{k_B}{e} \right)^2 \approx 2.22 \times 10^{-8} \text{ W}\Omega/\text{K}^2. \quad (21)$$

$L \equiv \kappa/(\sigma T)$  is called the Lorenz number of the material. This law is universal, in the sense that all materials described by Drude theory will have the same Lorenz number, regardless of  $\tau$ .

For alkali metals, this number agrees well with experiments up to a factor of 2. However, this is due to pure luck. The classical ideal gas model overestimates the specific heat of electrons about 100 times larger and underestimates the averaged velocity 100 times smaller.

## 2 Review of Quantum Statistical Mechanics [4]

### 2.1 Grandcanonical Ensemble

Consider an isolated system with particle number  $N$  and energy  $E$ . We divide it into two parts as system and environment. The system has particle number  $N_1$  and energy  $E_1$ . The environment has particle number  $N_2$  and energy  $E_2$ .  $E = E_1 + E_2$  and  $N = N_1 + N_2$ . Assume the environment is much larger than the system so that  $E_1 \ll E_2$  and  $N_1 \ll N_2$ .

Denote  $\Omega_1(N_1, E_1)$  and  $\Omega_2(N_2, E_2)$  as the number of all possible microscopic states given particle number and energy for the system and for the environment respectively. The central *postulate* of statistical mechanics is the principle of equal a priori probabilities.

For an isolated system at thermal equilibrium, each microstate occurs with equal probability in the ensemble.

Therefore, for a microstate  $s$  in the system, its probability of occurrence is

$$\rho_s(N_1, E_1) = \frac{\Omega_2(N_2, E_2)}{\Omega_1(N_1, E_1)\Omega_2(N_2, E_2)}. \quad (22)$$

Let us expand the logarithmic of  $\Omega_2(N_2, E_2)$  as  $N_1$  and  $E_1$ :

$$\ln \Omega_2(N - N_1, E - E_1) \approx \ln \Omega_2(N, E) - \left( \frac{\partial \ln \Omega_2(N, E)}{\partial N} \right) N_1 - \left( \frac{\partial \ln \Omega_2(N, E)}{\partial E} \right) E_1. \quad (23)$$

Denote

$$\alpha = \frac{\partial \ln \Omega_2(N, E)}{\partial N}, \quad (24)$$

$$\beta = \frac{\partial \ln \Omega_2(N, E)}{\partial E}, \quad (25)$$

$$\Xi = \Omega_1(N_1, E_1). \quad (26)$$

Eq. (22) can be rewritten into

$$\rho_s(N_1, E_1) = \frac{1}{\Xi} e^{-\alpha N_1 - \beta E_1}. \quad (27)$$

Notice  $\alpha$  and  $\beta$  depend only on the environment. Any system that is in equilibrium with the environment will have the same  $\alpha$  and  $\beta$ . According to the thermodynamics, these two quantities are in fact

$$\alpha = -\frac{\mu}{k_B T}, \quad (28)$$

$$\beta = \frac{1}{k_B T}. \quad (29)$$

$k_B$  is the Boltzmann constant,  $\mu$  is the chemical potential and  $T$  is the temperature.

To summarize, the probability for a system to be in the microstate  $s$  with particle number  $N$  and energy  $E_s$  is

$$\rho_{Ns} = \frac{1}{\Xi} \exp\left(-\frac{E_s - \mu N}{k_B T}\right). \quad (30)$$

The normalization factor  $\Xi$  is the grand partition function<sup>1</sup>:

$$\Xi = \sum_{N=0}^{\infty} \sum_s \exp\left(-\frac{E_s - \mu N}{k_B T}\right). \quad (31)$$

Straightforward calculation gives the expectation value of the some thermodynamical quantities:

$$\bar{N} = \sum_N \sum_s N \rho_{Ns} = \frac{1}{\Xi} \sum_N \sum_s N e^{-\alpha N - \beta E_s} = -\frac{\partial}{\partial \alpha} \ln \Xi. \quad (32)$$

$$\bar{E} = \sum_N \sum_s E_s \rho_{Ns} = \frac{1}{\Xi} \sum_N \sum_s E_s e^{-\alpha N - \beta E_s} = -\frac{\partial}{\partial \beta} \ln \Xi. \quad (33)$$

## 2.2 Bose and Fermi Distribution

Suppose for a given particle, the possible energy eigenstates are specified by the index  $i$ . The  $i$ -th state has energy eigenvalue  $\epsilon_i$ . The particles are non-interacting so that all of them are distributed independently. The  $i$ -th state has been occupied by  $n_i$  particles. Since  $N$  and  $E$  are not fixed in the grand canonical ensemble,

$$\Xi = \sum_{\{n_i\}} e^{-\sum_i (\alpha + \beta \epsilon_i) n_i} = \prod_i \Xi_i, \quad (34)$$

where  $\Xi_i$  is the grand partition function for state  $i$ .

$$\Xi_i = \sum_{n_i} e^{-(\alpha + \beta \epsilon_i) n_i} = \begin{cases} \frac{1}{1 - e^{-\alpha - \beta \epsilon_i}} & \text{Boson, } \sum_{n_i=0}^{\infty}, \\ 1 + e^{-\alpha - \beta \epsilon_i} & \text{Fermion, } \sum_{n_i=0}^1. \end{cases} \quad (35)$$

Thus

$$\Xi = \prod_k [1 \pm e^{-\alpha - \beta \epsilon_k}]^{\pm g_k}, \quad (36)$$

$$\ln \Xi = \pm \sum_k g_k \ln (1 \pm e^{-\alpha - \beta \epsilon_k}). \quad (37)$$

Here we sum over the energy levels instead of energy eigenstates.  $g_k$  is the degeneracy of energy level  $\epsilon_k$ . + is for fermions and - is for bosons.

The expectation value of particle numbers of energy  $\epsilon_k$  is computed as

$$\bar{n}_k = -g_k \frac{\partial}{\partial \alpha} \ln \Xi_k = \frac{g_k}{e^{\alpha + \beta \epsilon_k} \pm 1}. \quad (38)$$

+ corresponds to Fermi-Dirac distribution. - corresponds to Bose-Einstein distribution.

In Figure 4 we plot Fermi-Dirac distribution at several temperatures. The chemical potential of Fermi gas is called ‘‘Fermi energy’’, and is denoted as  $E_F$ .

<sup>1</sup>In our previous derivation, the total particle number is finite. Since  $N \gg N_1$ , it is same to push the summation to infinity.

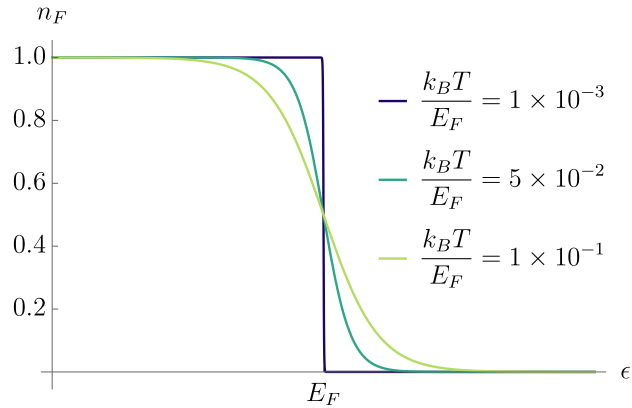


Figure 4: Fermi-Dirac distribution at various temperatures. The chemical potential is set to be  $E_F$ .

## References

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- [4] R. K. Pathria and Paul D. Beale. Chapter 4 - 6. In *Statistical Mechanics (3rd Edition)*. Elsevier Ltd., 2011.