

# Screening Effect and Impurity Scattering in Monolayer Graphene

Tsuneya ANDO

Department of Physics, Tokyo Institute of Technology  
2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551

The static polarization function is calculated in two-dimensional graphite and used for the calculation of the conductivity limited by charged-impurity scattering. The conductivity increases in proportion to the electron concentration and the mobility remains independent of the Fermi energy, in qualitative agreement with experiments. The screening increases in proportion to temperature at sufficiently high temperatures in contrast to the behavior in conventional two-dimensional systems, leading to the mobility increase proportional to the square of temperature.

Keywords: two-dimensional graphite, screening effect, charged impurity, mobility

## §1. Introduction

Quite recently, an atomically thin graphene, or a single layer graphite, was fabricated,<sup>1-3)</sup> and the magnetotransport was measured and the integer quantum Hall effect was observed.<sup>4,5)</sup> In an effective-mass approximation, an electron in a graphite monolayer is described by Weyl's equation for a massless neutrino. Transport properties in such an exotic electronic structure are quite intriguing, and the conductivity with/without a magnetic field including the Hall effect,<sup>6-10)</sup> quantum corrections to the conductivity,<sup>11,12)</sup> and the dynamical transport<sup>9,13)</sup> were investigated theoretically. The results show that the two-dimensional graphite exhibits various characteristic behaviors different from conventional two-dimensional systems.<sup>14)</sup> The purpose of this paper is to study screening effect and roles of charged-impurity scattering.

The two-dimensional graphite is often called a zero-gap semiconductor because the density of states vanishes at zero energy in proportion to the linear power of the energy. The Boltzmann conductivity if calculated properly remains independent of the energy for scatterers with strength independent of the electron concentration.<sup>6)</sup> This is a result of the fact that the scattering probability proportional to the density of states cancels the increase of the density of states. Because of the vanishing density of states at zero energy, however, the conductivity exhibits a singular behavior in its vicinity. A calculation in a self-consistent Born approximation shows that the conductivity exhibits a sharp drop to a universal value  $\sim e^2/\pi^2\hbar$ .<sup>6)</sup> This behavior was observed recently,<sup>4,5)</sup> although the actual value of the conductivity minimum is larger than predicted.

In addition to this slight difference in the conductivity dip, the experiments show that the conductivity does not exhibit a saturation and increases almost in proportion to the electron concentration.<sup>4,5)</sup> In this paper we consider charged impurities as a possible candidate for dominant scatterers in the system and calculate the corresponding conductivity. Because the screening effect is known to be of vital importance for charged impurities, we have to study the static polarization function. It is revealed that the screening property in the two-dimensional graphite exhibits behavior significantly

different from that in conventional two-dimensional metals.

## §2. Screening Effect

### 2.1 Effective-mass description

In a graphite sheet the conduction and valence bands consisting of  $\pi$  orbitals cross at K and K' points of the Brillouin zone, where the Fermi level is located.<sup>15,16)</sup> Electronic states of the  $\pi$ -bands near a K point are described by the  $\mathbf{k}\cdot\mathbf{p}$  equation:<sup>17-20)</sup>

$$\mathcal{H}_0\mathbf{F}(\mathbf{r}) = \varepsilon\mathbf{F}(\mathbf{r}), \quad (2.1)$$

with

$$\mathcal{H}_0 = \gamma \begin{pmatrix} 0 & \hat{k}_x - i\hat{k}_y \\ \hat{k}_x + i\hat{k}_y & 0 \end{pmatrix} = \gamma(\sigma_x\hat{k}_x + \sigma_y\hat{k}_y), \quad (2.2)$$

where  $\gamma$  is a band parameter,  $\sigma_x$  and  $\sigma_y$  are the Pauli spin matrices, and  $\hat{\mathbf{k}} = (\hat{k}_x, \hat{k}_y) = -i\vec{\nabla}$  is a wave-vector operator.

The wave function is written as

$$\mathbf{F}_{s\mathbf{k}}(\mathbf{r}) = \frac{1}{L}\mathbf{F}_{s\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}), \quad (2.3)$$

with

$$\mathbf{F}_{s\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta_{\mathbf{k}}} \\ s \end{pmatrix}, \quad (2.4)$$

where  $L^2$  is the area of the system,  $s = +1$  and  $-1$  denote the conduction and valence bands, respectively, and

$$k_x = k \cos \theta_{\mathbf{k}}, \quad k_y = k \sin \theta_{\mathbf{k}}, \quad k = \sqrt{k_x^2 + k_y^2}. \quad (2.5)$$

The corresponding energy is given by

$$\varepsilon_{s\mathbf{k}} = s\varepsilon_{\mathbf{k}}, \quad (2.6)$$

with

$$\varepsilon_{\mathbf{k}} = \gamma|\mathbf{k}|. \quad (2.7)$$

The Schrödinger equation for the K' point is given by replacing  $\sigma_y$  by  $-\sigma_y$  in the above and therefore the corresponding wave functions are obtained easily in a similar manner. The density of states is given by

$$D(\varepsilon) = g_v g_s \frac{|\varepsilon|}{2\pi\gamma^2}, \quad (2.8)$$

with the valley degeneracy  $g_v = 2$  due to the K and

K' points and the spin degeneracy  $g_s = 2$ . The energy dispersion and the density of states are illustrated in Fig. 1.

## 2.2 Coulomb Interaction

The matrix element for the interaction shown in Fig. 2 is given by

$$V_{(s_1, \mathbf{k}_1 + \mathbf{q}, s_1 \mathbf{k}_1)(s_2 \mathbf{k}_2, s_2' \mathbf{k}_2 + \mathbf{q})} = \frac{2\pi e^2}{\kappa_0 q} (\mathbf{F}_{s_1', \mathbf{k}_1 + \mathbf{q}}^\dagger \cdot \mathbf{F}_{s_1, \mathbf{k}_1}) (\mathbf{F}_{s_2, \mathbf{k}_2}^\dagger \cdot \mathbf{F}_{s_2', \mathbf{k}_2 + \mathbf{q}}), \quad (2.9)$$

with

$$(\mathbf{F}_{s\mathbf{k}}^\dagger \cdot \mathbf{F}_{s'\mathbf{k}'}') = \frac{1}{2} [\exp(i\theta_{\mathbf{k}} - i\theta_{\mathbf{k}'}') + ss'], \quad (2.10)$$

where  $\kappa_0$  is the static dielectric constant. If we neglect effects of polarization inside the two-dimensional graphite completely, the screening constant is given by the average of that of the substrate  $\text{SiO}_2$ ,  $\kappa_{\text{ox}} = 3.9$ , and that of the vacuum due to the image effect,<sup>(14)</sup> i.e.,  $\kappa_0 = (\kappa_{\text{ox}} + 1)/2 \approx 2.5$ . Actually, we have to consider contributions of electrons in  $\sigma$  bands and  $\pi$  bands away from the Fermi level. This contribution is known to be  $\kappa_0 \approx 2.4$  in bulk graphite,<sup>(21)</sup> but is not known for the present system and may not be written as in eq. (2.9). In spite of this, we shall use eq. (2.9) assuming that  $\kappa_0$  can be larger than that estimated above.

## 2.3 Polarization Function

The static dielectric function is written as

$$\varepsilon(\mathbf{q}) = 1 + \frac{2\pi e^2}{\kappa_0 q} \Pi(\mathbf{q}), \quad (2.11)$$

where the polarization function is given by

$$\Pi(\mathbf{q}) = -\frac{g_v g_s}{L^2} \sum_{s, s', \mathbf{k}} (f_{s\mathbf{k}} - f_{s'\mathbf{k}+\mathbf{q}}) \frac{|(\mathbf{F}_{s\mathbf{k}}^\dagger \cdot \mathbf{F}_{s'\mathbf{k}+\mathbf{q}})|^2}{\varepsilon_{s\mathbf{k}} - \varepsilon_{s'\mathbf{k}+\mathbf{q}}}, \quad (2.12)$$

where  $f_{s\mathbf{k}}$  is the Fermi distribution function,

$$f_{s\mathbf{k}} = f(\varepsilon_{s\mathbf{k}}) \equiv \left[ \exp\left(\frac{\varepsilon_{s\mathbf{k}} - \zeta}{k_B T}\right) + 1 \right]^{-1}, \quad (2.13)$$

with  $\zeta$  being the chemical potential,  $T$  the temperature, and  $k_B$  the Boltzmann constant. Because the system is isotropic, the polarization function is determined by  $q \equiv |\mathbf{q}|$ , as can easily be proved by the above expression.

First, we define

$$\Pi^0(q) \equiv -\frac{g_v g_s}{L^2} \sum_{s, s', \mathbf{k}} (f_{s\mathbf{k}}^0 - f_{s'\mathbf{k}+\mathbf{q}}^0) \frac{|(\mathbf{F}_{s\mathbf{k}}^\dagger \cdot \mathbf{F}_{s'\mathbf{k}+\mathbf{q}})|^2}{\varepsilon_{s\mathbf{k}} - \varepsilon_{s'\mathbf{k}+\mathbf{q}}}, \quad (2.14)$$

where

$$f_{s\mathbf{k}}^0 = \begin{cases} 1 & (s = -1); \\ 0 & (s = +1). \end{cases} \quad (2.15)$$

This  $\Pi^0(q)$  describes effects of polarization of electrons in the valence band due to virtual interband transitions

into the conduction band. It is calculated as

$$\Pi^0(q) = 2g_v g_s \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{1}{2} \frac{1 - \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}})}{\gamma|\mathbf{k}| + \gamma|\mathbf{k}+\mathbf{q}|} = \frac{g_v g_s q}{16\gamma}. \quad (2.16)$$

This result has been obtained previously.<sup>22,23)</sup>

Because this polarization function is proportional to  $q$ , its effect can be incorporated into the renormalization of the effective dielectric constant  $\kappa_0$  to  $\kappa$ , with

$$\frac{\kappa}{\kappa_0} = 1 + g_v g_s \frac{\pi^2}{4} U_0, \quad (2.17)$$

where the dimensionless interaction parameter  $U_0$  is defined by

$$U_0 = \frac{e^2}{2\pi\kappa_0\gamma}. \quad (2.18)$$

For the band parameter  $\gamma = 6.46 \text{ eV} \cdot \text{\AA}$ , corresponding to  $\gamma = (\sqrt{3}/2)\gamma_0 a$  with  $\gamma_0 = -3.03 \text{ eV}$  and  $a = 2.46 \text{ \AA}$ , where  $\gamma_0$  is the transfer integral between  $\pi$  orbitals of nearest-neighbor carbon atoms and  $a/\sqrt{3}$  is their distance, we have  $U_0 = 0.3545/\kappa_0$ . For  $\kappa_0 \approx 2.5$ , we have  $U_0 \approx 0.14$ , giving  $\kappa/\kappa_0 \approx 2.4$  or  $\kappa \approx 6.0$ . Correspondingly, the renormalized interaction parameter defined by

$$U = \frac{e^2}{2\pi\kappa\gamma}, \quad (2.19)$$

becomes  $U \approx 0.06$ . Effects of interband polarization can be fully included by using these  $\kappa$  and  $U$  instead of  $\kappa_0$  and  $U_0$ .

In the following we shall confine ourselves to the case that the Fermi level lies in the conduction band. Define

$$\tilde{f}_{s\mathbf{k}} = f_{s\mathbf{k}} - f_{s\mathbf{k}}^0. \quad (2.20)$$

Then, we have

$$\Pi(\mathbf{q}) = -\frac{g_v g_s}{L^2} \sum_{s, s', \mathbf{k}} (\tilde{f}_{s\mathbf{k}} - \tilde{f}_{s'\mathbf{k}+\mathbf{q}}) \frac{|(\mathbf{F}_{s\mathbf{k}}^\dagger \cdot \mathbf{F}_{s'\mathbf{k}+\mathbf{q}})|^2}{\varepsilon_{s\mathbf{k}} - \varepsilon_{s'\mathbf{k}+\mathbf{q}}}. \quad (2.21)$$

This can be rewritten as

$$\Pi(\mathbf{q}) = -2 \frac{g_v g_s}{L^2} \sum_{s, s', \mathbf{k}} \tilde{f}_{s\mathbf{k}} \frac{|(\mathbf{F}_{s\mathbf{k}}^\dagger \cdot \mathbf{F}_{s'\mathbf{k}+\mathbf{q}})|^2}{\varepsilon_{s\mathbf{k}} - \varepsilon_{s'\mathbf{k}+\mathbf{q}}}. \quad (2.22)$$

Substituting eq. (2.10) and performing the summation over  $s' = \pm 1$ , we have

$$\Pi(\mathbf{q}) = -2 \frac{g_v g_s}{L^2} \sum_{\mathbf{k}} f^+(\varepsilon_{\mathbf{k}}) \frac{\gamma|\mathbf{k}| + \gamma|\mathbf{k}+\mathbf{q}| \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}})}{\gamma^2|\mathbf{k}|^2 - \gamma^2|\mathbf{k}+\mathbf{q}|^2}, \quad (2.23)$$

with

$$f^+(\varepsilon_{\mathbf{k}}) \equiv \sum_{s=\pm 1} s \tilde{f}_{s\mathbf{k}} = f(\varepsilon_{\mathbf{k}}) + f(\varepsilon_{\mathbf{k}} + 2\zeta). \quad (2.24)$$

The integration over the direction of  $\mathbf{q}$  can be performed easily and we have

$$\Pi(q) = \frac{g_v g_s}{2\pi\gamma} \left[ \int_0^\infty f^+(\varepsilon_{\mathbf{k}}) d\mathbf{k} - \int_0^{q/2} f^+(\varepsilon_{\mathbf{k}}) \sqrt{1 - \left(\frac{2\mathbf{k}}{q}\right)^2} d\mathbf{k} \right]. \quad (2.25)$$

At the absolute zero of temperature, we have

$$f^+(\varepsilon) = \begin{cases} 1 & (\varepsilon < \varepsilon_F); \\ 0 & (\varepsilon > \varepsilon_F). \end{cases} \quad (2.26)$$

For  $q < 2k_F$ , therefore, we have

$$\Pi(q) = \frac{g_v g_s k_F}{2\pi\gamma} \left(1 - \frac{\pi}{4} \frac{q}{2k_F}\right), \quad (2.27)$$

and for  $q > 2k_F$ , on the other hand, we have

$$\Pi(q) = \frac{g_v g_s k_F}{2\pi\gamma} \left[1 - \frac{1}{2} \sqrt{1 - \left(\frac{2k_F}{q}\right)^2} - \frac{1}{2} \frac{q}{2k_F} \sin^{-1} \frac{2k_F}{q}\right], \quad (2.28)$$

with the Fermi wavenumber  $k_F = \varepsilon_F/\gamma$ . At  $q = 2k_F$ , it becomes

$$\Pi(2k_F) = \frac{g_v g_s k_F}{2\pi\gamma} \left(1 - \frac{\pi}{4}\right), \quad (2.29)$$

and the first derivative is also continuous. This behavior is quite different from that in conventional two-dimensional metals where the polarization function is constant for  $q < 2k_F$  and decreases for  $q > 2k_F$  with a divergent first derivative at  $q = 2k_F$ .<sup>14)</sup>

The reason lies in the vanishing Coulomb matrix element for the backward scattering  $\mathbf{k} \rightarrow -\mathbf{k}$  as shown by eq. (2.10). The polarization function is dominated by virtual transitions between states with similar energy because of small energy denominator. Such energy conserving processes are present only for  $q < 2k_F$  and disappear suddenly at  $q = 2k_F$ . This singular behavior is known to be the origin of the large Kohn anomaly in two-dimensional systems.<sup>14)</sup> In two-dimensional graphite, the contributions of energy conserving processes become weaker with the increase of  $q$  even for  $q < 2k_F$  because of the decrease of the matrix element for large angle scattering, leading to the decrease of  $\Pi(q)$  for  $q < 2k_F$ . At  $q = 2k_F$ , the matrix element of energy conserving processes vanishes identically due to the absence of backscattering and therefore no strong singular behavior can appear at  $q = 2k_F$ .

In the long-wavelength limit, the dielectric function is written as

$$\varepsilon(q) = 1 + \frac{q_s}{q}, \quad (2.30)$$

where  $q_s$  is called the screening constant given by

$$q_s = \frac{2\pi e^2}{\kappa} \Pi(0). \quad (2.31)$$

It is easily shown that

$$\Pi(0) = \int_{-\infty}^{\infty} \left(-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right) D(\varepsilon) d\varepsilon, \quad (2.32)$$

which is known as the compressibility sum-rule.

The above results show that the static polarization function vanishes identically for  $\varepsilon = 0$  at the absolute zero of temperature, meaning that the screening is totally absent to the linear order except for the renormalization of the dielectric constant mentioned above. This corresponds to the inadequate linear screening noted previously in graphite intercalation compounds.<sup>24)</sup> When

the Fermi level is away from  $\varepsilon = 0$  or at nonzero temperatures, however, the linear polarization function does not vanish and the linear screening is expected to become appropriate.

Let us consider the case that the Fermi level  $\varepsilon_F$  lies in the conduction band at zero temperature. The chemical potential  $\zeta$  is determined by the condition

$$n_s = \frac{1}{2\pi\gamma^2} \int_0^{\infty} f^-(\varepsilon) \varepsilon d\varepsilon = \frac{1}{2} \frac{\varepsilon_F^2}{2\pi\gamma^2}. \quad (2.33)$$

with

$$f^-(\varepsilon) = f(\varepsilon) - f(\varepsilon + 2\zeta), \quad (2.34)$$

where  $n_s$  is the electron concentration. This gives

$$\zeta = \varepsilon_F - \frac{\pi^2}{6} \frac{(k_B T)^2}{\varepsilon_F} + \dots, \quad (2.35)$$

at low temperatures ( $k_B T \ll \varepsilon_F$ ), and

$$\zeta \approx \frac{1}{4 \ln 2} \frac{\varepsilon_F^2}{k_B T}. \quad (2.36)$$

at high temperatures ( $k_B T \gg \varepsilon_F$ ).

Correspondingly, the screening constant, i.e., the long-wavelength polarization function, becomes

$$\Pi(0) = \frac{g_v g_s \varepsilon_F}{2\pi\gamma^2} \left[1 - \frac{\pi^2}{6} \left(\frac{k_B T}{\varepsilon_F}\right)^2 + \dots\right], \quad (2.37)$$

at low temperatures and

$$\Pi(0) \approx 2 \ln 2 \frac{g_v g_s}{2\pi\gamma^2} k_B T. \quad (2.38)$$

at high temperatures. In conventional systems, the screening constant at high temperatures (Debye-Hückel) is proportional to the inverse of temperature. In the present system, the situation is completely different and the screening increases in proportion to the temperature. This is a direct consequence of the linear energy dependence of the density of states and the presence of the Dirac sea below  $\varepsilon = 0$ .

Figure 3 shows the temperature dependence of the screening constant, i.e., long-wavelength limit of the polarization function, together with the chemical potential. The screening constant takes a small minimum around  $k_B T/\varepsilon_F \sim 0.5$  and increases linearly at high temperatures. Figure 4 shows the polarization function as a function of the wave vector at different temperatures.

### §3. Impurity Scattering

#### 3.1 Boltzmann Transport Equation

The Boltzmann transport equation for the distribution function  $f_{s\mathbf{k}}^E$  is given by

$$\begin{aligned} & \frac{d\mathbf{k}}{dt} \cdot \frac{\partial f_{s\mathbf{k}}^E}{\partial \mathbf{k}} \\ &= - \sum_{s'} \int \frac{d\mathbf{k}'}{(2\pi)^2} [f_{s\mathbf{k}}^E (1 - f_{s'\mathbf{k}'}^E) - f_{s'\mathbf{k}'}^E (1 - f_{s\mathbf{k}}^E)] W(s'\mathbf{k}', s\mathbf{k}), \end{aligned} \quad (3.1)$$

with

$$W(s'\mathbf{k}', s\mathbf{k}) = \frac{2\pi}{\hbar} \langle |V_{s'\mathbf{k}', s\mathbf{k}}|^2 \rangle \delta(\varepsilon_{s\mathbf{k}} - \varepsilon_{s'\mathbf{k}'}), \quad (3.2)$$

where  $V_{s'\mathbf{k}', s\mathbf{k}}$  is the matrix element of scattering poten-

tial and  $\langle \dots \rangle$  denotes the average over configurations of scatterers. We shall confine ourselves to the case of elastic scattering and therefore neglect interband processes ( $s' \neq s$ ). To the lowest order in the applied electric field  $\mathbf{E}$ , we have

$$f_{s\mathbf{k}}^{\mathbf{E}} = f(\varepsilon_{s\mathbf{k}}) + g_{s\mathbf{k}}, \quad (3.3)$$

where  $f(\varepsilon)$  is the Fermi distribution function and  $g_{s\mathbf{k}}$  is the deviation proportional to  $\mathbf{E}$ . Then, we have

$$\frac{d\mathbf{k}}{dt} \cdot \frac{\partial f_{s\mathbf{k}}^{\mathbf{E}}}{\partial \mathbf{k}} = -e\mathbf{E} \cdot \mathbf{v}_{s\mathbf{k}} \frac{\partial f}{\partial \varepsilon_{s\mathbf{k}}} - \frac{e}{c\hbar} (\mathbf{v}_{s\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial g_{s\mathbf{k}}}{\partial \mathbf{k}}, \quad (3.4)$$

where  $\mathbf{B}$  is the magnetic field perpendicular to the system and  $\mathbf{v}_{s\mathbf{k}}$  is the velocity given by

$$\mathbf{v}_{s\mathbf{k}} = \frac{\partial \varepsilon_{s\mathbf{k}}}{\hbar \partial \mathbf{k}} = \frac{\gamma}{\hbar} \frac{s\mathbf{k}}{|\mathbf{k}|}. \quad (3.5)$$

The vector product is defined as  $\mathbf{v} \times \mathbf{B} = -\mathbf{v} \times \mathbf{B} = B(v_y, -v_x)$  for vector  $\mathbf{v} = (v_x, v_y)$ .

The transport equation is rewritten as

$$\begin{aligned} e\mathbf{E} \cdot \mathbf{v}_{s\mathbf{k}} \left( -\frac{\partial f}{\partial \varepsilon_{s\mathbf{k}}} \right) &= \frac{e}{c\hbar} (\mathbf{v}_{s\mathbf{k}} \times \mathbf{B}) \cdot \frac{\partial g_{s\mathbf{k}}}{\partial \mathbf{k}} \\ &- \int \frac{d\mathbf{k}'}{(2\pi)^2} (g_{s\mathbf{k}} - g_{s\mathbf{k}'}) \frac{2\pi}{\hbar} \langle |V_{s\mathbf{k}',s\mathbf{k}}|^2 \rangle \delta(\varepsilon_{s\mathbf{k}} - \varepsilon_{s\mathbf{k}'}). \end{aligned} \quad (3.6)$$

Introduce the relaxation time given by

$$\frac{\hbar}{\tau(\varepsilon_{s\mathbf{k}})} = 2\pi \int \frac{d\mathbf{k}'}{(2\pi)^2} \langle |V_{s\mathbf{k}',s\mathbf{k}}|^2 \rangle [1 - \cos(\theta_{\mathbf{k}} - \theta_{\mathbf{k}'})] \delta(\varepsilon_{s\mathbf{k}} - \varepsilon_{s\mathbf{k}'}), \quad (3.7)$$

and the cyclotron frequency

$$\omega_c(\varepsilon_{s\mathbf{k}}) = \frac{eBv^2}{c\varepsilon_{s\mathbf{k}}}, \quad (3.8)$$

with

$$v \equiv |\mathbf{v}_{s\mathbf{k}}| = \frac{\gamma}{\hbar}. \quad (3.9)$$

Then, the solution becomes

$$g_{s\mathbf{k}} = -e\tau \left( -\frac{\partial f}{\partial \varepsilon_{s\mathbf{k}}} \right) \frac{1}{1 + \omega_c^2 \tau^2} \mathbf{v}_{s\mathbf{k}} \cdot \left( \mathbf{E} + \omega_c \tau \frac{\mathbf{B}}{B} \times \mathbf{E} \right), \quad (3.10)$$

with  $\omega_c = \omega_c(\varepsilon_{s\mathbf{k}})$  and  $\tau = \tau(\varepsilon_{s\mathbf{k}})$ . It should be noted that the cyclotron frequency diverges in proportion to the inverse of the energy at zero energy and changes the signature corresponding to change in the carrier type from an electron to a hole.

Define

$$\bar{D} = \frac{g_v g_s}{2\pi\gamma^2} \int \left( -\frac{\partial f}{\partial \varepsilon} \right) |\varepsilon| d\varepsilon, \quad (3.11)$$

and the average of function  $p(\varepsilon)$  by

$$\langle p(\varepsilon) \rangle \equiv \frac{1}{\bar{D}} \int \left( -\frac{\partial f}{\partial \varepsilon} \right) \frac{g_v g_s}{2\pi\gamma^2} |\varepsilon| p(\varepsilon) d\varepsilon. \quad (3.12)$$

Then, we have the diagonal conductivity

$$\sigma_{xx} = \sigma_{yy} = \frac{e^2 \gamma^2}{2\hbar^2} \bar{D} \left\langle \frac{\tau}{1 + \omega_c^2 \tau^2} \right\rangle, \quad (3.13)$$

and the Hall conductivity

$$\sigma_{xy} = -\sigma_{yx} = -\frac{e^2 \gamma^2}{2\hbar^2} \bar{D} \left\langle \frac{\omega_c \tau^2}{1 + \omega_c^2 \tau^2} \right\rangle. \quad (3.14)$$

These are essentially the same as the expressions in conventional semiconductors or metals except that  $\omega_c$  depends strongly on the energy while the velocity remains independent.

The Hall coefficient is given by

$$R_H = -\frac{\sigma_{yx}}{B(\sigma_{xx}^2 + \sigma_{xy}^2)}, \quad (3.15)$$

and the Hall mobility is given by

$$\mu = c|R_H|\sigma_0. \quad (3.16)$$

At zero temperature in weak magnetic fields, we have

$$R_H = -\frac{s}{n_s e c}, \quad (3.17)$$

with the electron concentration given by eq. (2.33). The Hall mobility becomes

$$\mu_0 = \frac{ev^2}{\varepsilon_F} \tau(\varepsilon_F), \quad (3.18)$$

and then the conductivity is given by

$$\sigma_0 = n_s e \mu, \quad (3.19)$$

as in conventional two-dimensional systems.

As mentioned above, the cyclotron frequency  $\omega_c(\varepsilon)$  diverges at  $\varepsilon = 0$  and as will become clear in the following the relaxation time  $\tau(\varepsilon)$  diverges also. As a result, the integral over the energy giving the Hall conductivity in eq. (3.14) and the field-dependent part of the diagonal conductivity in eq. (3.13) diverges at  $\varepsilon = 0$  at nonzero temperatures if we neglect  $\omega_c^2 \tau^2$  in the denominator. Thus, the Hall coefficient and mobility and the magnetoresistivity can exhibit a singular behavior in the limit of vanishing magnetic field. As will be shown below, however, this singularity is weak for charged-impurity scattering and easily washed out if effects of a nonzero density of states at  $\varepsilon = 0$  are considered.<sup>6)</sup>

### 3.2 Charged Impurity Scattering

The Fourier transform of the potential of a charged impurity is given by

$$V_i^0(\mathbf{q}) = \frac{2\pi e^2}{\kappa q}. \quad (3.20)$$

Then the matrix element becomes

$$(s'\mathbf{k} + \mathbf{q} | V_i^0 | s\mathbf{k}) = \frac{2\pi e^2}{\kappa q} (\mathbf{F}_{s'\mathbf{k}+\mathbf{q}}^\dagger \cdot \mathbf{F}_{s\mathbf{k}}). \quad (3.21)$$

In the presence of the screening effect, this is modified as

$$(s'\mathbf{k} + \mathbf{q} | V_i | s\mathbf{k}) = \frac{2\pi e^2}{\kappa q \varepsilon(\mathbf{q})} (\mathbf{F}_{s'\mathbf{k}+\mathbf{q}}^\dagger \cdot \mathbf{F}_{s\mathbf{k}}). \quad (3.22)$$

With the use of eq. (2.10), the transport relaxation time

for energy  $\varepsilon$  ( $\varepsilon > 0$ ) is given by

$$\frac{\hbar}{\tau(\varepsilon)} = 2\pi n_i D(\varepsilon) \int_0^\pi \frac{d\theta}{\pi} \frac{1}{2} (1 - \cos^2 \theta) \left( \frac{2\pi e^2}{\kappa q \varepsilon(q)} \right)^2. \quad (3.23)$$

where  $n_i$  is the concentration of impurities and  $q = 2(\varepsilon/\gamma) \sin(\theta/2)$  in the integrand. This equation shows that the probability of backward scattering  $\theta = \pi$  vanishes identically, which corresponds to the absence of backscattering in metallic carbon nanotubes.<sup>20,25)</sup>

The relaxation time can be rewritten as

$$\tau(\varepsilon) = \frac{n_s}{\pi g_v g_s n_i} \frac{\hbar}{|\varepsilon|} H(\varepsilon), \quad (3.24)$$

with the dimensionless quantity  $H(\varepsilon)$  defined by

$$H(\varepsilon)^{-1} = \int_0^\pi \frac{d\theta}{\pi} \frac{1}{2} (1 - \cos^2 \theta) \left( \frac{1}{2\pi U} \frac{\gamma q}{\varepsilon_F} + g_v g_s \tilde{\Pi}(q) \right)^{-2}, \quad (3.25)$$

where  $\tilde{\Pi}(q)$  is the dimensionless quantity defined by

$$\Pi(q) \equiv \frac{g_v g_s \varepsilon_F}{2\pi \gamma^2} \tilde{\Pi}(q). \quad (3.26)$$

At zero temperature,  $H_0 \equiv H(\varepsilon_F)$  is independent of the electron concentration and determined by  $U$  alone. The mobility becomes

$$\mu_0 = \frac{e}{4\pi^2 \hbar n_i} H_0, \quad (3.27)$$

which is independent of  $n_s$ . The conductivity becomes

$$\sigma_0 = \frac{e^2}{4\pi^2 \hbar} \frac{n_s}{n_i} H_0, \quad (3.28)$$

which is proportional to  $n_s$ . Figure 5 shows  $H_0$  as a function of  $U$ . It is clear that  $H_0$  increases in proportion to  $U^{-2}$  for small  $U$  and approaches a constant for sufficiently large  $U$ . For  $U \approx 0.06$ , we have  $H_0 \approx 120$ .

The temperature dependence of the conductivity for a fixed electron concentration is shown in Fig. 6. At low temperatures  $k_B T/\varepsilon_F < 0.5$ , the conductivity decreases slightly with temperature because of the decrease of the screening effect as shown in Figs. 3 and 4. At sufficiently high temperatures the conductivity increases roughly in proportion to  $T^2$  because of the increase of the screening effect and also of the average kinetic energy. The conductivity takes a shallow minimum around  $k_B T/\varepsilon_F \sim 0.5$ .

Figure 7 shows the diagonal and Hall conductivity as a function of the effective magnetic field  $\omega_{c0}\tau_0$  at various temperatures, where  $\omega_{c0} = \omega_c(\varepsilon_F)$  and  $\tau_0 = \tau(\varepsilon_F)$  at zero temperature. We have assumed  $U = 0.05$  (slightly smaller than 0.06 for  $\kappa_0 = 2.5$ ). Results for different values of  $U$  are qualitatively the same. The diagonal conductivity exhibits the usual behavior  $\propto (1 + \omega_{c0}^2 \tau_0^2)^{-1}$  at sufficiently low temperatures, but its feature deviates considerably at high temperatures. In fact, the conductivity decreases with the field rapidly particularly in the vicinity of zero field because the contribution in the vicinity of zero energy drops rapidly due to the divergent cyclotron frequency. In high magnetic fields, on the other hand, contributions of states with higher energies

with small  $\omega_c$  become important and the conductivity-decrease becomes slower. The Hall conductivity starts to decrease when holes start to be populated in the valence band ( $k_B T/\varepsilon_F \sim 1$ ) due to the cancellation of contributions of electrons and holes (two-carrier regime).

Figure 8 shows the inverse of the Hall coefficient. It exhibits a large field dependence in the low-field regime at low temperatures due to the contribution of states near  $\varepsilon = 0$ . At higher temperatures the Hall coefficient is reduced considerably due to the cancellation of electron and hole contributions. Figure 9 shows the Hall mobility. It exhibits a singular increase near zero field again due to the contribution of states  $\varepsilon = 0$ , but the singularity is weak and can be smeared out easily by nonzero density of states at  $\varepsilon = 0$ . At higher temperatures it is reduced considerably due to the cancellation of electron and hole contributions.

#### §4. Discussion

In the previous calculation of the conductivity,<sup>6)</sup> short-range scatterers with amplitude independent of the electron concentration were assumed. In this case the scattering probability  $\hbar/\tau(\varepsilon_F)$  is proportional to the final-state density of states with a coefficient independent of  $\varepsilon_F$ . Because the density of states is proportional to  $\varepsilon_F$ , the relaxation time is inversely proportional to  $\varepsilon_F$ . As a result the mobility is inversely proportional to  $n_s \propto \varepsilon_F^2$ , leading to the conductivity independent of the Fermi energy and the electron concentration. For charged-impurity scattering, the matrix element itself is proportional to the inverse of the Fermi energy both in the presence and absence of screening. Consequently, the low-temperature mobility becomes independent of the electron concentration and the conductivity increases in proportion to the electron or hole concentration  $n_s$ .

Recent experiments seem to indicate that the mobility at low  $n_s$  decreases rapidly with increasing  $n_s$  and nearly converges at a value independent of  $n_s$  for sufficiently large  $n_s$ .<sup>5)</sup> The rapid reduction at low  $n_s$  is consistent with the singular behavior predicted previously.<sup>6)</sup> The observed value at high  $n_s$  close to  $\mu \sim 10^4 \text{ cm}^2/\text{Vs}$ <sup>5)</sup> corresponds to the impurity concentration of  $n_i \sim 4 \times 10^{11} \text{ cm}^{-2}$ . Such amount of impurities are highly likely to be present on a substrate surface. It is interesting that this concentration is comparable to the concentration of charged impurities present in the vicinity of the Si and SiO<sub>2</sub> interface in typical MOSFET's.<sup>14)</sup>

The singularity appearing in the magnetoconductivity in weak magnetic fields at nonzero temperatures should be removed by nonvanishing density of states in actual systems with disorder.<sup>13)</sup> This nonzero density of states causes a singular drop of the conductivity from the Boltzmann value to a universal value  $e^2/\pi\hbar$  in the vicinity of zero energy.<sup>6)</sup> The observed minimum conductivity at zero energy<sup>4,5)</sup> is 3~4 times as large as the predicted conductivity for model short-range scatterers.<sup>6)</sup> It is difficult to discuss this conductivity in the vicinity of zero energy assuming realistic charged-impurity scattering, because a self-consistent determination of the screening and the density of states is necessary. Further, the linear

screening may not be valid near  $\varepsilon \approx 0$ .<sup>24)</sup> This problem is left for a future study.

## §5. Summary and Conclusion

The static dielectric function has been calculated in a monolayer graphite system and shown to be considerably different from that in conventional two-dimensional systems mainly due to the absence of backward scattering. The result has been used for the calculation of transport coefficients based on a Boltzmann transport equation. The mobility limited by charged impurities is shown to be independent of the electron concentration, leading to the conductivity proportional to the electron concentration. This dependence is consistent with recent experimental results.

## Acknowledgments

The author thanks useful discussion with Mikito Koshino and Hidekatsu Suzuura. This work was supported in part by a 21st Century COE Program at Tokyo Tech “Nanometer-Scale Quantum Physics” and by Grant-in-Aid for Scientific Research from Ministry of Education, Culture, Sports, Science and Technology Japan. Numerical calculations were performed in part using the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

## References

- 1) K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva and A. A. Firsov: *Science* **306** (2004) 666.
- 2) C. Berger, Z. Song, T. Li, X. Li, A. Y. Ogbazghi, R. Feng, Z. Dai, A. N. Marchenkov, E. H. Conrad, P. N. First and W. A. de Heer: *J. Phys. Chem. B* **108** (2004) 19912.
- 3) Y. Zhang, J. P. Small, W. V. Pontius and P. Kim: *Appl. Phys. Lett.* **86** (2005) 073104.
- 4) K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos and A. A. Firsov: *Nature* **438** (2005) 197.
- 5) Y. Zhang, Y. -W. Tan, H. L. Stormer and P. Kim: *Nature* **438** (2005) 201.
- 6) N. H. Shon and T. Ando: *J. Phys. Soc. Jpn.* **67** (1998) 2421.
- 7) Y. Zheng and T. Ando: *Phys. Rev. B* **65** (2002) 245420.
- 8) V. P. Gusynin and S. G. Sharapov: *Phys. Rev. Lett.* **95** (2005) 146801.
- 9) N. M. R. Peres, F. Guinea and A. H. Castro Neto: *Phys. Rev. B* **73** (2006) 125411.
- 10) H. Kumazaki and D. S. Hirashima: to be published.
- 11) H. Suzuura and T. Ando: *Phys. Rev. Lett.* **89** (2002) 266603.
- 12) E. McCann, K. Kechedzhi, V. I. Falko, H. Suzuura, T. Ando and B. L. Altshuler, cond-mat/0604015.
- 13) T. Ando, Y. Zheng and H. Suzuura: *J. Phys. Soc. Jpn.* **71** (2002) 1318.
- 14) T. Ando, A. B. Fowler and F. Stern: *Rev. Mod. Phys.* **54** (1982) 437.
- 15) P. R. Wallace: *Phys. Rev.* **71** (1947) 622.
- 16) G. S. Painter and D. E. Ellis: *Phys. Rev. B* **1** (1970) 4747.
- 17) J. W. McClure: *Phys. Rev.* **108** (1957) 612.
- 18) J. C. Slonczewski and P. R. Weiss: *Phys. Rev.* **109** (1958) 272.
- 19) H. Ajiki and T. Ando: *J. Phys. Soc. Jpn.* **62** (1993) 1255.
- 20) T. Ando: *J. Phys. Soc. Jpn.* **74** (2005) 777.
- 21) E. A. Taft and H. R. Philipp: *Phys. Rev.* **138** (1965) A197.
- 22) J. Gonzalez, F. Guinea and M. A. H. Vozmediano: *Nucl. Phys. B* **424** (1994) 595.
- 23) J. Gonzalez, F. Guinea and M. A. H. Vozmediano: *Phys. Rev. B* **59** (1999) 2474.
- 24) D. P. DiVincenzo and E. J. Mele: *Phys. Rev. B* **29** (1984) 1685.
- 25) T. Ando and T. Nakanishi: *J. Phys. Soc. Jpn.* **67** (1998) 1704.

## Figure Captions

**Fig. 1** A schematic illustration of the dispersion relation and the density of states of the two-dimensional graphite.

**Fig. 2** The matrix element of the Coulomb interaction (a) and the diagram of the polarization function (b).

**Fig. 3** Calculated temperature dependence of the long-wavelength dielectric function  $\Pi(0)$  and chemical potential  $\zeta$ . The dotted lines denote the approximate results at zero and high temperatures.

**Fig. 4** The polarization function as a function of the wave vector at different temperatures. It does not exhibit an apparent singularity at  $q/k_F = 2$  even at zero temperature.

**Fig. 5** The dimensionless conductivity  $H(\varepsilon_F)$  as a function of the effective Coulomb interaction  $U$  at zero temperature. It is proportional to  $U^{-2}$  for small  $U$  and approaches a constant due to the screening for large  $U$ .

**Fig. 6** The conductivity limited by charged-impurity scattering as a function of the temperature.

**Fig. 7** The diagonal and Hall conductivity limited by charged-impurity scattering as a function of the effective magnetic field at various temperatures.  $\sigma(T)$  is the conductivity in the absence of a magnetic field.  $\omega_{c0} = \omega_c(\varepsilon_F)$ .  $\tau_0 = \tau(\varepsilon_F)$ .  $U = 0.05$ .

**Fig. 8** The inverse of the Hall coefficient limited by charged-impurity scattering as a function of a magnetic field at different temperatures.  $U = 0.05$ .

**Fig. 9** The Hall mobility limited by charged-impurity scattering as a function of a magnetic field at different temperatures.  $\mu_0$  is defined in eq. (3.27).  $U = 0.05$ .

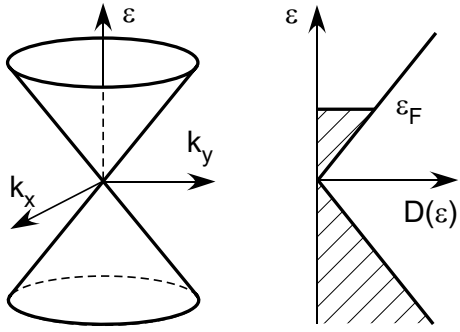


Fig. 1

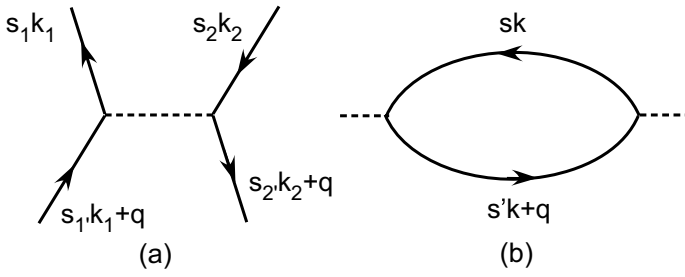


Fig. 2

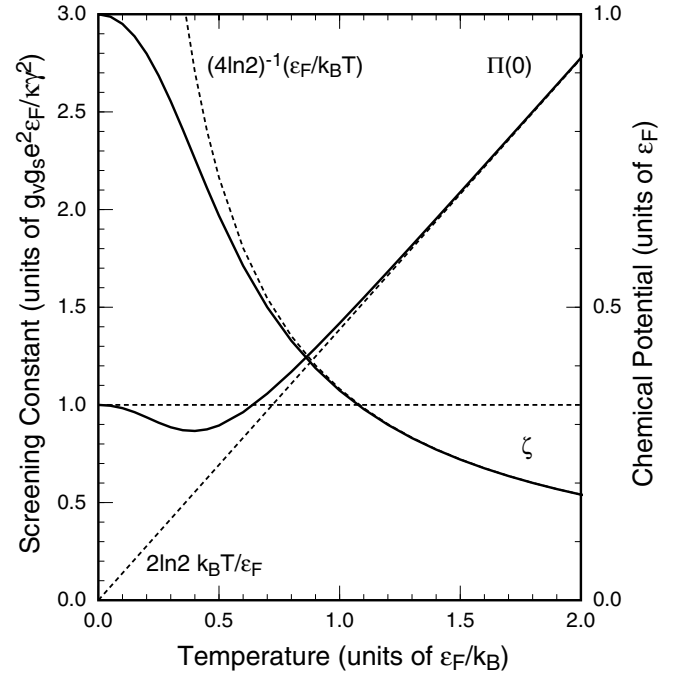


Fig. 3

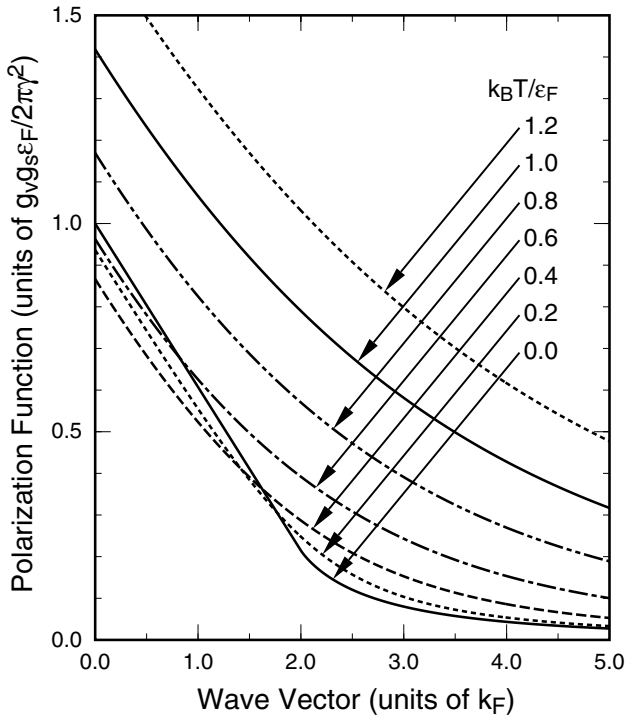


Fig. 4

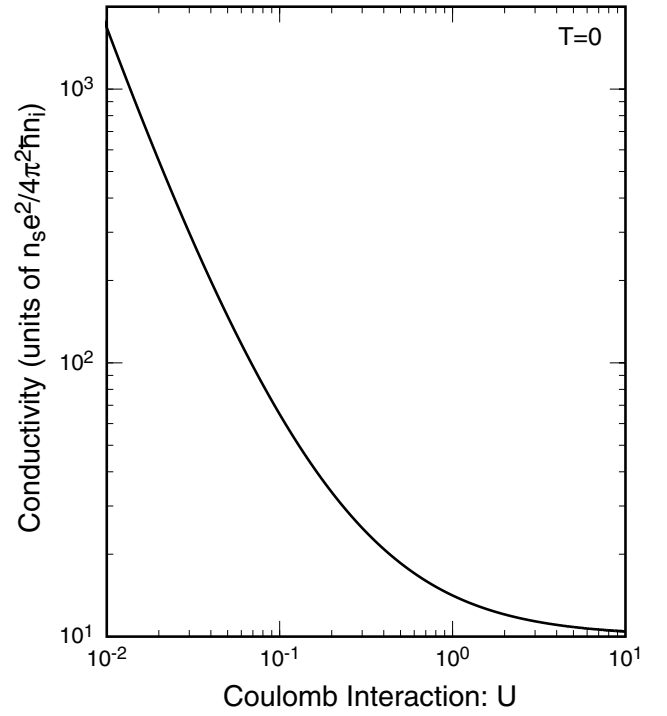


Fig. 5

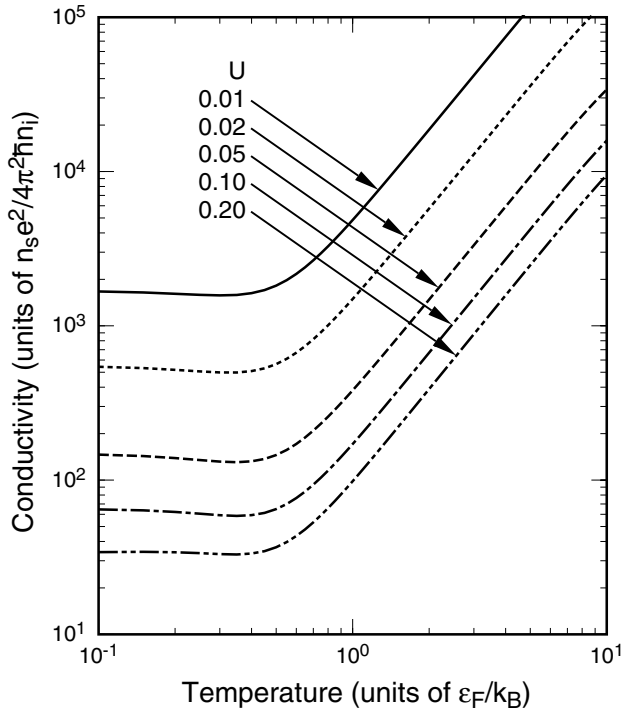


Fig. 6

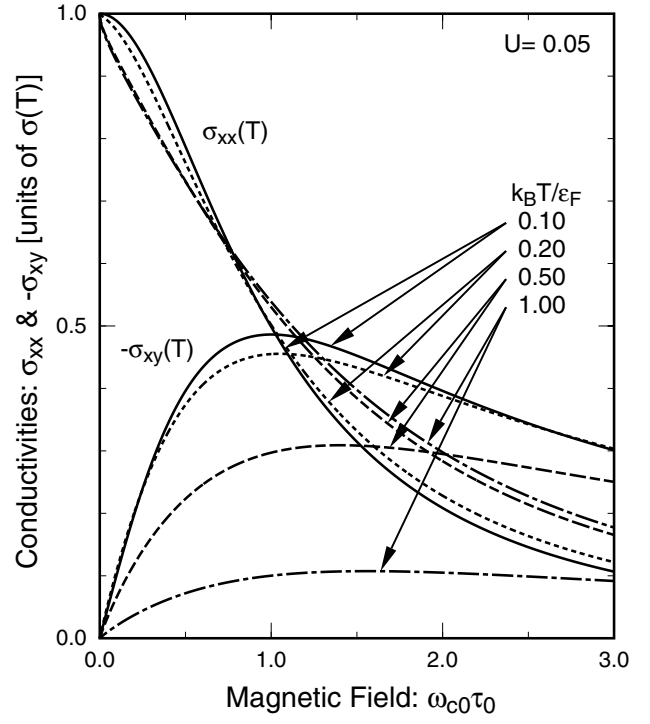


Fig. 7

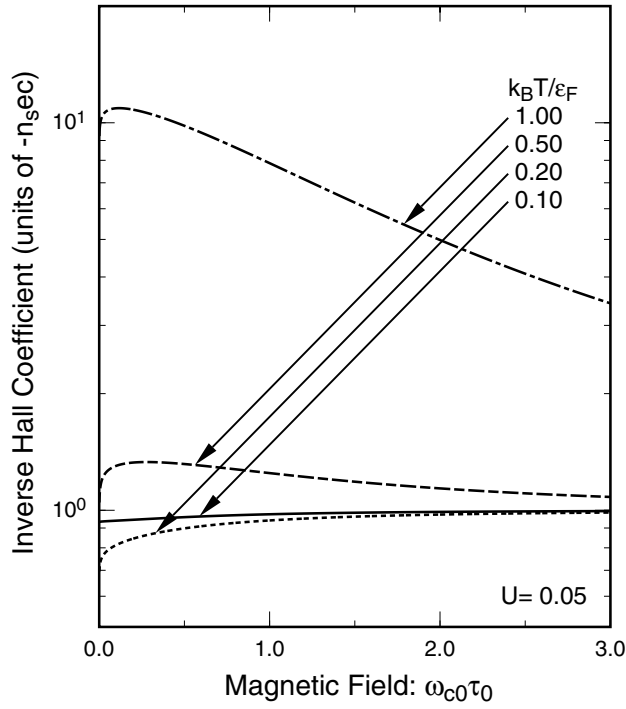


Fig. 8

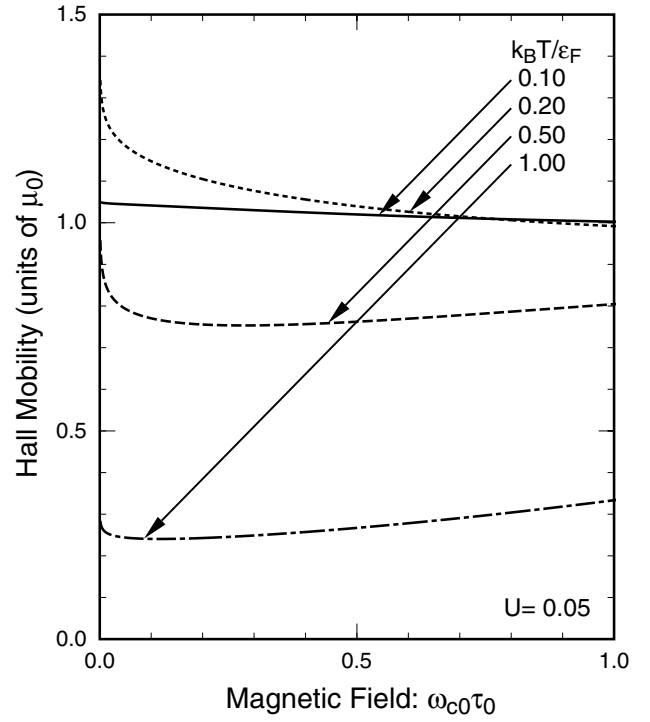


Fig. 9