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On the Field Dependence of Magnetoresistance in Two-Dimensional Systems

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Weak localization theory of magnetoresistance in two-dimensional systems is re-investigated. A formulation is developed which is applicable up to magnetic field much larger than the exsisting theory. The result of the calculation is compared with the experiment on GaAs/AlGaAs heterojunction and the agreement between them is satisfactory.

§1. Introduction

Recently various anomalous properties of two-dimensional systems have been explained in terms of weak localization theory.[1] As for magnetoresistance the theory by Hikami, Larkin and Nagaoka[2] (HLN) can qualitatively explain experiments, but quantitatively deviation of experiments from HLN is not negligibly small and generally it becomes larger as the magnetic field increases.[3] In most cases the deviation was explained in terms of electron-electron interaction effects. According to the recent theories,[4,5] however, the interaction does not affect magnetoresistance very much except when the temperature is extremely low and the effect of Zeeman splitting shows up.[4,6] Therefore the discrepancy between experiments and theory has to be explained within one-particle theory. As will be shown below, HLN is correct when

$$\omega_c\tau \ll 1/\varepsilon_F\tau \ll 1, \tag{1}$$

where ω_c, ε_F and τ are cyclotron frequency, Fermi energy divided by $\hbar$ and momentum relaxation time of electrons, respectively. Since the parameter $1/\varepsilon_F\tau$ must be small enough in order that the weak localization theory is correct, HLN is applicable only to the regions of very weak magnetic field. If a theory of magnetoresistance which is valid for larger magnetic field is available, we will be able to extract more reliable information, for instance, that on energy relaxation time, spin-flip scattering time, etc. from the experiments.

Some years ago, the author proposed a theory[7] of magnetoresistance in three-dimensional systems which is valid when

$$\omega_c\tau,\ 1/\varepsilon_F\tau \ll 1, \tag{2}$$

and is applicable to much wider regions of magnetic field than HLN. In this paper the two-dimensional version of this theory will be discussed.

§2. Formulation

We consider a model of non-interacting electron gas with randomly distributed scattering center. The part of the conductivity associated with weak localization is given by[7,8]

$$\delta\sigma(H,\omega)=\frac{e^2}{\pi\hbar L^2}\left(-i\frac{\hbar}{m}\right)^2\int \mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_3\,\mathrm{d}\boldsymbol{r}_4\Gamma(\boldsymbol{r}_3,\boldsymbol{r}_4,\omega)$$
$$\times G^A(\boldsymbol{r}_4,\boldsymbol{r}_1,0)\frac{\partial}{\partial x_1}G^R(\boldsymbol{r}_1,\boldsymbol{r}_3,\omega)G^R(\boldsymbol{r}_4,\boldsymbol{r}_2,\omega)\frac{\partial}{\partial x_2}G^A(\boldsymbol{r}_2,\boldsymbol{r}_3,0), \tag{3}$$

where L is the linear dimension of the system, $G^R(\boldsymbol{r},\boldsymbol{r}',\varepsilon)$ and $G^A(\boldsymbol{r},\boldsymbol{r}',\varepsilon)$ are retarded and advanced one-electron Green's functions, and the diffusion propagator $\Gamma(\boldsymbol{r},\boldsymbol{r}',\omega)$ is to be obtained by solving the equation

$$\Gamma(\boldsymbol{r}_3,\boldsymbol{r}_4,\omega)=\left[\delta(\boldsymbol{r}_3-\boldsymbol{r}_4)+\int \mathrm{d}\boldsymbol{r}_5G^R(\boldsymbol{r}_3,\boldsymbol{r}_5,\omega)G^A(\boldsymbol{r}_3,\boldsymbol{r}_5,0)\Gamma(\boldsymbol{r}_5,\boldsymbol{r}_4,\omega)\right]\Big/2\pi\nu\hbar\tau, \tag{4}$$

ν being the density of states at the Fermi level. Under the condition $\omega_c \ll 1/\tau$, ε_F, the Green's function in magnetic field can be approximated as[7]

$$G^{R,A}(\boldsymbol{r}, \boldsymbol{r}', \varepsilon) = \exp\{i(x+x')(y'-y)/2l^2\} G_0^{R,A}(\boldsymbol{r}-\boldsymbol{r}', \varepsilon), \tag{5}$$

where $G_0^{R,A}(\boldsymbol{r}-\boldsymbol{r}', \varepsilon)$ are the Green's functions in the absence of magnetic field and $l=(c\hbar/eH)^{1/2}$ with H the magnetic field. It is important to note that in deriving (5) the condition (1) is not required. In order to solve (3), we expand the diffusion propagator and the product of the Green's function with the eigenstates of an electron in magnetic field of $\sqrt{2}H$;

$$\Gamma(\boldsymbol{r}, \boldsymbol{r}', \omega) = \sum_{N,X} \Gamma(N, \omega) \Psi_{NX}(\boldsymbol{r}) \Psi_{NX}^*(\boldsymbol{r}'), \tag{6}$$

$$G^R(\boldsymbol{r}, \boldsymbol{r}', \omega) G^A(\boldsymbol{r}, \boldsymbol{r}', 0) = \sum_{N,X} \Pi(N, \omega) \Psi_{NX}(\boldsymbol{r}) \Psi_{NX}^*(\boldsymbol{r}'), \tag{7}$$

where

$$\Psi_{NX}(\boldsymbol{r}) = \Phi_N(x-X) \exp(-2iyX/l^2)/\sqrt{L}, \tag{8}$$

$\Phi_N(x)$ being the Nth eigenstate of harmonic oscillator of frequency $\sqrt{2}\omega_c$ and we assume that $\Gamma(N, \omega)$ and $\Pi(N, \omega)$ are independent of X from the consideration of translational symmetry. Then making use of the relation[9]

$$\sum_X \Psi_{NX}(\boldsymbol{r}) \Psi_{NX}^*(\boldsymbol{r}') = \frac{1}{\pi l^2} \exp\{i(x+x')(y-y')/l^2\} \exp(-|\boldsymbol{r}-\boldsymbol{r}'|^2/2l^2) L_N(|\boldsymbol{r}-\boldsymbol{r}'|^2/l^2), \tag{9}$$

L_N being Laguerre polynomial, and noting the orthogonality of the functions $\exp(-x^2/2) L_N(x^2)$, we can solve (4) in the form

$$\Gamma(N, \omega) = [2\pi\nu\hbar\tau(1-P_N)]^{-1}, \tag{10}$$

with

$$P_N = (2\pi\nu\hbar\tau)^{-1} \int d\boldsymbol{r} L_N(r^2/l^2) \exp(-r^2/2l^2) G_0^R(\boldsymbol{r}, \omega) G_0^A(\boldsymbol{r}, 0). \tag{11}$$

From (2) it follows that $p_F \gg 1/\lambda$, $1/l$, p_F and λ being the Fermi wave number and the mean free path, and hence the integral in (11) is dominated by the contribution from the regions $p_F r \gg 1$. In these regions the Green's function can be approximated as

$$G_0^R(\boldsymbol{r}, \varepsilon) = G_0^{A*}(\boldsymbol{r}, \varepsilon) = -(im/2\hbar)(2/\pi r p_F)^{1/2} \exp i[r(p_F + \varepsilon/v_F + i/2\lambda) - \pi/4], \tag{12}$$

where v_F is the Fermi velocity. It has been argued by Anderson, Abrahams and Ramakrishnan[10] and by Fukuyama and Abrahams[11] that at zero frequency ω is to be replaced by $1/\tau_\varepsilon$, τ_ε being the energy relaxation time of electrons due to inelastic scattering. Then, putting (12) into (10) we find that

$$P_N = \frac{s}{1+z} \int_0^\infty dx L_N(x^2) \exp(-sx - x^2/2), \tag{13}$$

where

$$z = \tau/\tau_\varepsilon, \tag{14}$$

and

$$s = (1+z)/(2\omega_c \tau^2 \varepsilon_F)^{1/2}. \tag{15}$$

As is shown in the appendix P_0 can be evaluated with a simple numerical calculation and P_N for $N>0$ can be calculated with the use of the recursion formulas

$$P_1 = s^2/(1+z) - s^2 P_0, \tag{16}$$

$$P_{N+2} = [(N+1+s^2)(P_N - P_{N+1}) + NP_{N-1}]/(N+2). \quad (N \geqq 0) \tag{17}$$

Next we have to carry out the integration over $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ in (3). To do this it is convenient to use the following forms of G^R and G^A;[6]

$$G^R(\boldsymbol{r}, \boldsymbol{r}', \varepsilon)=G^{A*}(\boldsymbol{r}, \boldsymbol{r}', \varepsilon)=\sum_{N,X}\frac{\psi_{NX}(\boldsymbol{r})\psi^*_{NX}(\boldsymbol{r}')}{\varepsilon+\varepsilon_F-\varepsilon_N+i/2\tau}, \tag{18}$$

where $\psi_{NX}(\boldsymbol{r})$ is the eigenfunction of an electron in the magnetic field H and $\varepsilon_N=\omega_c(N+1/2)$. Here we neglect the energy dependence of τ because of the condition (2). Then we find that

$$\begin{aligned}\int d\boldsymbol{r}_1 G^A(\boldsymbol{r}_4, \boldsymbol{r}_1, 0)\frac{\partial}{\partial x_1}G^R(\boldsymbol{r}_1, \boldsymbol{r}_3, \omega)\\ =\sum_{N,X}\frac{1}{\sqrt{2}l}\frac{\psi_{NX}(\boldsymbol{r}_4)}{\varepsilon_F-\varepsilon_N-i/2\tau}\left[\frac{\sqrt{N+1}\psi^*_{N+1X}(\boldsymbol{r}_3)}{\varepsilon_F+\omega-\varepsilon_{N+1}+i/2\tau}-\frac{\sqrt{N}\psi^*_{N-1X}(\boldsymbol{r}_3)}{\varepsilon_F+\omega-\varepsilon_{N-1}+i/2\tau}\right].\end{aligned} \tag{19}$$

To carry out the summation over X we make use of the relation[9]

$$\sum_X \psi_{NX}(\boldsymbol{r}_4)\psi^*_{N-1X}(\boldsymbol{r}_3)=-\frac{r}{2\sqrt{2N}\pi l^3}L^{(1)}_{N-1}\left(\frac{r^2}{2l^2}\right)\exp\left[i\frac{(x_3+x_4)(y_3-y_4)}{2l^2}-\frac{r^2}{4l^2}+i\theta\right], \tag{20}$$

where $\boldsymbol{r}=\boldsymbol{r}_3-\boldsymbol{r}_4$ and θ is the angle between $\boldsymbol{r}$ and x axis. In the summation over N in (19) the contribution from the region $N\sim\varepsilon_F/\omega_c\gg 1$ is dominant. Therefore we can replace $N\pm 1$ with N and the Laguerre polynomial can be approximated with its asymptotic form;

$$L^{(1)}_N(y)=\pi^{-1/2}e^{y/2}y^{-3/4}N^{1/4}\cos\left[2(Ny)^{1/2}-3\pi/4\right]. \tag{21}$$

Then, replacing the summation with an integral we can evaluate the right hand side of (19), and putting it into (3) we obtain

$$\delta\sigma(H)=-\frac{e^2\tau^2 p_F}{\pi^2\hbar}\int d\boldsymbol{r}_3\, d\boldsymbol{r}_4 \Gamma(\boldsymbol{r}_3, \boldsymbol{r}_4, \omega)\cos^2\theta\exp\left[i(x_3+x_4)(y_3-y_4)/l^2-r/\lambda-r/\tau_\varepsilon v_F\right]. \tag{22}$$

Thus from (6), (9), (10) and (11) we finally obtain

$$\delta\sigma(H)=-\frac{2e^2}{\pi^2\hbar}A\sum_{N=0}^{N_0}\frac{P_N}{1-P_N}, \tag{23}$$

with $A=\omega_c\tau^2\varepsilon_F$. The cut off number N_0 is estimated as follows. For $N\gg 1$ we use the asymptotic form of L_N in (13);

$$\begin{aligned}P_N&=\int_0^\infty dy J_0(2\sqrt{2A(N+1/2)}y)\exp\{-(1+z)y\}\\ &=[8A(N+1/2)+(1+z)^2]^{-1/2}.\end{aligned} \tag{24}$$

To this integral the contribution from the region $y=r/\lambda\lesssim[A(N+1/2)]^{-1/2}$ is dominant while (12) is correct only for $rp_F\gg 1$. Therefore the summation in (23) should be cut off at

$$N_0=b(\varepsilon_F\tau)^2/A, \tag{25}$$

where b is a constant of order of unity. In the limit $H\to 0$ ($A\to 0$) we replace the summation over N in (23) with an integral and use (24). Then we obtain the expression for the magnetoresistance

$$\Delta\sigma(H)=\delta\sigma(H)-\delta\sigma(0)=-\frac{2e^2}{\pi^2\hbar}\left[A\sum_{N=0}^{N_0}\frac{1}{1-P_N}-\{F(A(N_0+1))-F(0)\}\right], \tag{26}$$

where we have subtracted 1 from the summand of (23), of which the contributions to $\delta\sigma(H)$ and $\delta\sigma(0)$ are identical, and

$$\begin{aligned}F(y)&=\int\frac{dy}{1-[8y+(1+z)^2]^{-1/2}}\\ &=[t^2/2+t+\ln(t-1)]/4,\end{aligned} \tag{27}$$

with $t=[8y+(1+z)^2]^{1/2}$. Using (24) we can easily see that $\Delta\sigma(H)$ tends to a finite value in the limit $N_0\to\infty$, and by numerical calculation it has been found that $\Delta\sigma(H)$ is practically independent of N_0 if $N_0>5\sim 10$ for realistic values of A and z.

§3. Effects of Spin-Orbit Interaction and Intervalley Scattering

Extension of the present theory to the case when spin-flip scattering of electrons due to spin-orbit interaction is considerably strong[2] is straightforward;

$$\Delta\sigma(H) = -\frac{2e^2}{\pi^2\hbar}\left[S(\beta_1) + \frac{1}{2}\{S(\beta_2) - S(1)\}\right], \tag{28}$$

where

$$S(\beta) = \sum_{N=0}^{N_0} \frac{A}{1-\beta P_N} - F_2(A(N_0+1), \beta) + F_2(0, \beta), \tag{29}$$

$$F_2(y, \beta) = [t^2/2 + \beta t + \beta^2 \ln(t-\beta)]/4, \tag{30}$$

t being defined as in (27), and

$$\beta_1 = 1 - 2\tau/\tau_{so}^x - 2\tau/\tau_{so}^z, \tag{31}$$

$$\beta_2 = 1 - 4\tau/\tau_{so}^x. \tag{32}$$

(As for the definition of τ_{so}^x and τ_{so}^z, the reader is referred to ref. 3). In the above we have neglected the effects of Zeeman splitting,[12] which is unimportant except when the magnetic field is parallel to the surface or g-factor is extremely large.

In the case of two-valley systems like (001) MOS, the effects of intervalley scattering have to be considered[13] and we obtain

$$\Delta\sigma(H) = -\frac{4e^2}{\pi^2\hbar}\left[S(\beta_3) + \frac{1}{2}\{S(1) - S(\beta_4)\}\right], \tag{33}$$

with $\beta_3 = 1 - \tau/\tau_i$ and $\beta_4 = 1 - 2\tau/\tau_i$, τ_i being the intervalley scattering time.

§4. Discussions

In Fig. 1 the result of the calculation of $\Delta\sigma(H)$ using (26) is compared with experiment[14] on a GaAs/AlGaAs heterojunction. For an appropriate value of τ_ε we can reproduce the experiment quite well in the whole region of the magnetic field while HLN gives $\Delta\sigma(H)$ considerably larger than the experiment for $H \gtrsim 30$ Gauss if the curve is fitted in the low field region. This tendency is seen in the most of the experiments. HLN can be obtained from the present theory by expanding P_N in A ($\sim 1/s^2$) up to the first order. To do this we have to expand $L_N(x^2)\exp(-x^2/2)$ in (13) to the first order in x^2. Up to the second order in A, P_N is given by

$$P_N = [1 - 2(2N+1)A/(1+z)^2 + 12\{2N(N+1)+1\}A^2/(1+z)^4]/(1+z), \tag{34}$$

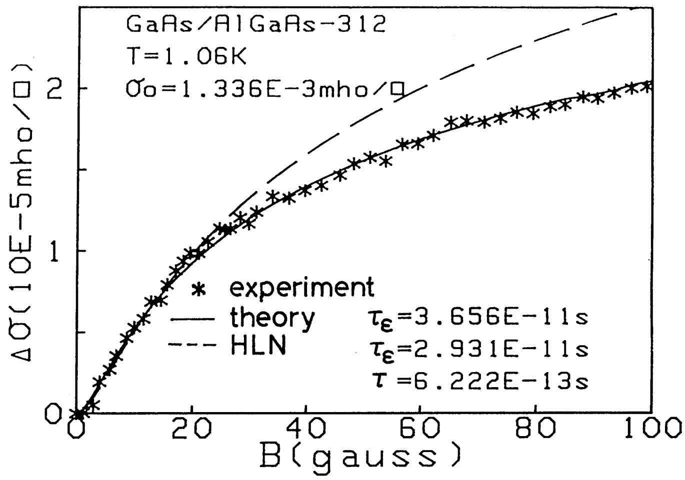

Fig. 1. The present theory and Hikami-Larkin-Nagaoka theory are compared with experiment on GaAs/AlGaAs heterojunction. For HLN τ_ε is chosen in such a way that the best fit is obtained in the low field region.

and we find that in HLN the deviation of P_N from 1 is overestimated and hence that the suppression of quantum interference effects is overestimated. Recently Ebisawa and Fukuyama published a theory[15] which is claimed to be valid under the condition (2). It gives, however, $\Delta\sigma(H)$ larger than HLN in the regions of large field and can not explain the above mentioned tendency of the experiments. In order to calculate the diffusion propagator in magnetic field they simply replaced the wave number q with $2l^{-1}\sqrt{N+1/2}$ in that in the absence of the field. This approximation is, however, correct only when $q\lambda \ll 1$ or $q \ll k_B T/\hbar v_F$,[16,17] and can not be applied to the case $l \lesssim \lambda$ at low temperatures. In ref. 17, for instance, the calculation is correct to infinite order in $\hbar v_F^2 \tau q^2/k_B T$ but only to the lowest order in $q\lambda$, and is applied only to the case $l \gg \lambda$.

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Appendix

We put

$$Q_N = (1+z)P_N/s = \int_0^\infty dx L_N(x^2) \exp(-sx - x^2/2). \tag{A·1}$$

Then, by integrating the right hand side by part and making use of the relations between the Laguerre polynomials and its derivatives, from (A·1) we obtain

$$Q_N = \frac{1}{s} + \frac{1}{s^2}\left[2\sum_{n=0}^{N-1} Q_n - 2NQ_N - (N+1)Q_{N+1} - NQ_{N-1}\right], \tag{A·2}$$

and hence

$$Q_{N+1} = \frac{1}{N+1}\left[2\sum_{n=0}^{N-1} Q_n - (2N+s^2)Q_N - NQ_{N-1} + s\right]. \quad (N \geqq 0) \tag{A·3}$$

It is straightforward to derive (16) and (17) from (A·3). For $N=0$, we can write (A·1) in the form

$$Q_0 = \sqrt{2}\, e^{s^2/2} \operatorname{Erfc}(s/\sqrt{2}). \tag{A·4}$$

The error function Erfc (x) can be calculated easily with the use of the expansion in x when $x<1$ and of the formula[18]

$$e^{x^2} \operatorname{Erfc}(x) = \frac{2x}{\pi}\int_0^\infty dt \frac{e^{-t^2}}{t^2+x^2}, \tag{A·5}$$

when $x>1$.

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