MAGNETOTRANSPORT IN QUANTUM WIRES

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Abstract

Numerical calculation of magnetotransport in quantum wires is performed. Magnetoconductivities at $T = 100$K are evaluated by using the Kubo formula, where the electron-longitudinal optical phonon interaction is taken into account. The conductivities consist of two types contributions; one is related to the hopping motion between the localized cyclotron motion through the electron-phonon interaction, σ_{ep}, and the other is caused by the confinement potential, σ_{po}. The magnetic field and the wire width dependencies of these two types of contributions are studied.

1. INTRODUCTION

Recent developments in maicrofabrication technology have made it possible to produce ultranarrow wires of semiconductors. The width of the wires is comparable to the Fermi wavelength, and electrons are free only along the wires. Such quantum wires have revealed quite new features in transport properties, such as Aharonov-Bohn effect, quantized conductance and conductance fluctuations. In addition, the quantum wires provide a possibility to fabricate novel functional devices. Usually, it is required to operate such devices at room temperature, where the effects of scattering by optical phonons play important roles in conductivity. The purpose of the present paper is to study the magnetotransport in high magnetic field. Especially we review the method of calculation of the conductance.

It is well known that the magnetophonon resonances (MPR) are a powerful tool for studying electron-optical-phonon interactions in semiconductors [1–4]. An external magnetic field quantizes the electron energy into Landau levels leading to singularities in the density of states. When the separation of such quantized levels is tuned to a longitudinal optical (LO) phonon frequency, a resonant scattering occurs between the two Landau levels and the transverse conductance becomes maxima in three- or two-dimensional systems, where the magnetoresistance is measured as a function of the magnetic field. Vasilopoulos *et al.* have predicted that the same effect is expected to occur in quantum wires [5]. They calculated magnetoconductivity in quantum wires with parabolic confinement potential and found that the resonant condition is modified by the confinement potential. However their calculation is restricted to the case of wide quantum wires and neglects the effect of the confinement potential. We calculated the transverse conductivity using the Kubo formula in quantum wires with the structure similar to those of Vasilopoulos *et al.* Our calculation revealed that the confinement potential plays a significant role in the case of narrow quantum wires and the magnetic field dependence of the conductance exhibits maxima or minima depending on the confinement potential [6]. The confinement potential produced by split-gates fabricated on a single-heterostructure is parabolic at extremely low electron density. The Coulomb interaction results in a flattening of the bottom of the confinement potential, and thus the unharmonicity increases with increasing the electron density. The effect of the unharmonicity has been studied using square quantum wire model [7]. In this paper, we review the numerical study of the MPR in

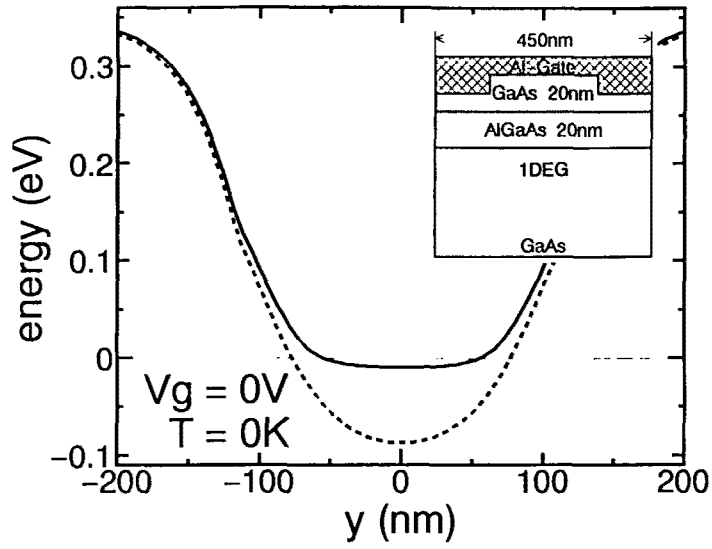

Figure 1: The self-consistent results of the potential in a structure shown in the inset, where the dashed curve represents potential profile along the y-direction in the case of empty electron density and the solid curve shows the potential profile in the presence of electrons ($n = 2 \times 10^6 \mathrm{cm}^{-1}$) at 0K.

quantum wires. The model and the electron states of quantum wires are given in Sec. 2. In Sec. 3 the method to calculate the conductivity is described. The numerical results are given in Sec. 4.

2. QUANTUM WIRES

We assume a model of a quantum wire in which ideal two-dimensional electron gas is confined by a potential in the y-direction, and electrons are free only along the wire. In this structure the heterointerface is normal to the z-axis. In Fig. 1 we present the self-consistent calculation of the potential in a structure shown in the inset, where the dashed curve represents potential profile along the y-direction in the case of empty electron density and the solid curve shows the potential profile in the presence of electrons ($n = 2 \times 10^6 \mathrm{cm}^{-2}$) at 0K. As seen in the figure, the potential for zero electron exhibits parabolic behavior, while the bottom of the potential becomes flat with finite electron density due to the Coulomb interaction. Present calculations were made in two different potential profiles, parabolic and square well potentials, which correspond to the two extreme cases, zero electron and high electron density, respectively. In the present calculations, however, the conductivities are evaluated by assuming Boltzmann distribution for electrons, for simplicity.

When a magnetic field $\mathbf{B}$ is applied in the z-direction, one-electron Hamiltonian for the two-dimensional system is written as

$$\mathcal{H} = \frac{1}{2m}(\mathbf{p} + e\mathbf{A})^2 + V(y), \tag{1}$$

where $V(y)$ is the confinement potential and $V(y) = \frac{1}{2}m\Omega^2 y^2$ for a parabolic potential, and

$$V(y) = \begin{cases} V_0, & |y| \geq \frac{1}{2}a \\ 0, & \text{otherwise} \end{cases}, \tag{2}$$

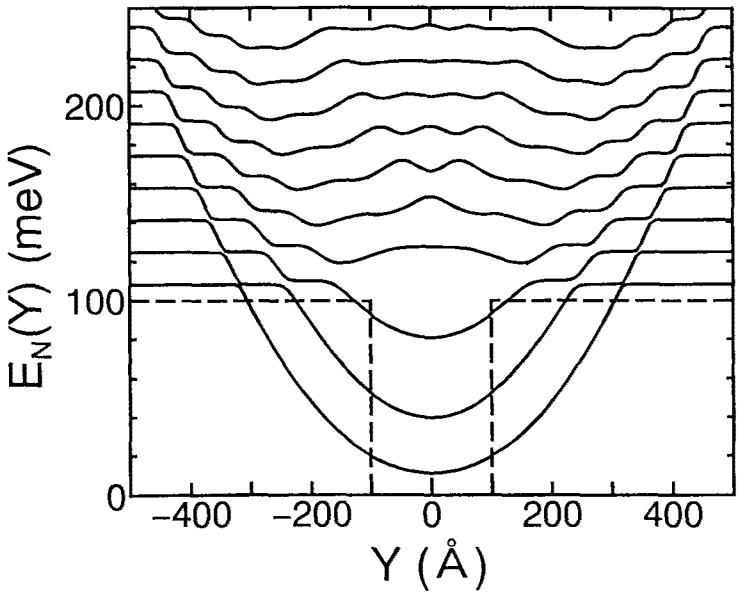

Figure 2: Electron energy $E_N(Y)$ as a function of center coordinate of cyclotron motion Y at $B = 10$T for $N = 0$ to 9 in a quantum wire of GaAs of $a = 200$Å and $V_0 = 100$meV. The dashed line shows the square confinement potential.

for a square well potential. $\mathbf{A} = (-By, 0)$, Ω is the strength of the confinement potential, a is the wire width and V_0 is the barrier height.

Calculations of electronic states in the parabolic potential are straightforward and the wave functions are well know simple harmonic-oscillator-line solutions. The results are give in our paper [6].

In the case of the square well potential, the calculations are made as the following. If we set $\ell \equiv 1/(eB)^{1/2} = 1$ and $\omega_c \equiv eB/m = 1$, the Schrödinger equation for eigenfunctions $e^{ikx}\varphi_N(y - Y; Y)$ ($Y \equiv \ell^2 k$) is given by

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}y^2 + V(y + Y)\right)\varphi_N(y; Y) = E_N(Y)\varphi_N(y; Y). \tag{3}$$

We discretize this equation in a uniform mesh, $y_i = -\frac{1}{2}L + ih$, $i = 0, 1, 2, \ldots, N$, ($L \sim 10$, $h = L/N$), and calculate eigenfunctions and eigenvalues by the Householder, bisection and inverse iteration method. In Fig. 2 we show the eigenvalues $E_N(Y)$ as a function of the y-component of the cyclotron center Y for a quantum wire of GaAs in which we take $a = 200$Å, $V_0 = 100$meV and $m = 0.07m_0$. We find in Fig. 2 that the lower energy states depend strongly on the location of the cyclotron center, while the higher energy states show weak oscillations.

3. CALCULATIONS OF MAGNETOCONDUCTANCE

At high magnetic fields, the transverse conductivity σ_{xx} is determined by the change in the center of cyclotron motion along the x-direction, $\dot{X}$. Since $\dot{X}$ is determined by the gradient of the potential along the y-direction, the term $\dot{X}$ for electrons in the quantum wire consists of two contributions, the one by the electron optical-phonon interaction potential $U_{ep}(\mathbf{r})$ and the other by the confinement

potential $V(y)$. $\dot{X}$ is given explicitly by the equation of motion and we have

$$\dot{X} = \frac{1}{eB}\frac{\partial U_{\rm ep}(\mathbf{r})}{\partial y} + \frac{1}{eB}\frac{\partial V(y)}{\partial y}$$
$$= \begin{cases} \dfrac{1}{eB}\dfrac{\partial U_{\rm ep}(\mathbf{r})}{\partial y} + m\Omega^2 y, & \text{for parabolic potential,} \\ \dfrac{1}{eB}\dfrac{\partial U_{\rm ep}(\mathbf{r})}{\partial y} + V_0\delta(y-\frac{1}{2}a) - V_0\delta(y+\frac{1}{2}a), & \text{for square potential.} \end{cases} \tag{4}$$

The first term on the right hand side of Eq. (4) gives the usual conductivity due to hopping motion of cyclotron center which is referred as $\sigma_{\rm ep}$, and the rest is related to the confinement potential giving the conductivity $\sigma_{\rm po}$. It should be noted that the conductivity $\sigma_{\rm po}$ will not appear in three- or two-dimensional systems.

Calculations of the magnetoconductivity for parabolic potential are reported in Ref. [6] in detail, and here we will present numerical calculations of the magnetoconductivity in quantum wires of square potential. The conductivity $\sigma_{\rm po}$ is calculated in the same manner as Ref. [6], and we have $\sigma_{\rm po} = ne^2\tau_{\rm po}/\tilde{m}$ with

$$\tau_{\rm po} = \frac{\beta\omega_{\rm c}\int dY \dfrac{1}{W_0(Y)}\{\ell\varphi_0^2(-\frac{1}{2}a - Y; Y) + \ell\varphi_0^2(\frac{1}{2}a - Y; Y)\}^2 {\rm e}^{-\beta E_0(Y)}}{\int dY\, {\rm e}^{-\beta E_0(Y)}}, \tag{5}$$

and

$$W_0(Y) = \alpha\omega_0 N_0 \sum_{N'}\int dq_x dq_y \frac{\omega_0}{k_0(q_x^2+q_y^2)^{1/2}} J^2_{N'Y}(q_x,q_y)\delta_\Gamma(E_0(Y)+\omega_0 - E_{N'}(Y+\ell^2 q_x)), \tag{6}$$

where n is the one-dimensional electron density, $\tilde{m} = (\omega_{\rm c}/V_0)^2 m$, α is the Fröhlich coupling constant of electron–optical-phonon interaction, ω_0 is the LO phonon frequency, N_0 is the occupation number of LO phonons, $k_0 = (2m\omega_0)^{1/2}$, $\delta_\Gamma(E) = \pi^{-1}\Gamma/(E^2+\Gamma^2)$ (Γ is the broadening energy), and

$$J^2_{N'Y}(q_x,q_y) = \left|\int \varphi_{N'}(y-\ell^2 q_x; Y+\ell^2 q_x){\rm e}^{iq_y y}\varphi_0(y;Y)dy\right|^2. \tag{7}$$

The matrix elements are calculated by the fast Fourier transform (FFT) method. We perform the FFT by using the uniform mesh such that the mesh size in k-space coincides with h in the units of $\ell = 1$, and we can readily perform the integration of Eqs. (6) and (5).

The hopping conductivity is also calculated in the same manner as Ref. [6], and we have $\sigma_{\rm ep} = ne^2\tau_{\rm ep}/m$, with

$$\tau_{\rm ep} = \int dY \tau(Y){\rm e}^{-\beta E_0(Y)} \Big/ \int dY {\rm e}^{-\beta E_0(Y)}, \tag{8}$$

and

$$\tau(Y) = \alpha N_0\beta\left(\frac{\omega_0}{\omega_{\rm c}}\right)^2 \sum_{N'}\int dq_x dq_y \frac{\omega_0 q_y^2}{k_0^3(q_x^2+q_y^2)^{1/2}} J^2_{N'Y}(q_x,q_y)\delta_\Gamma(E_0(Y)+\omega_0 - E_{N'}(Y+\ell^2 q_x)). \tag{9}$$

When we compare Eqs. (6) and (9), we find that these two equations are quite similar and thus the evaluation of the two terms given by Eqs. (5) and (8) are straightforward.

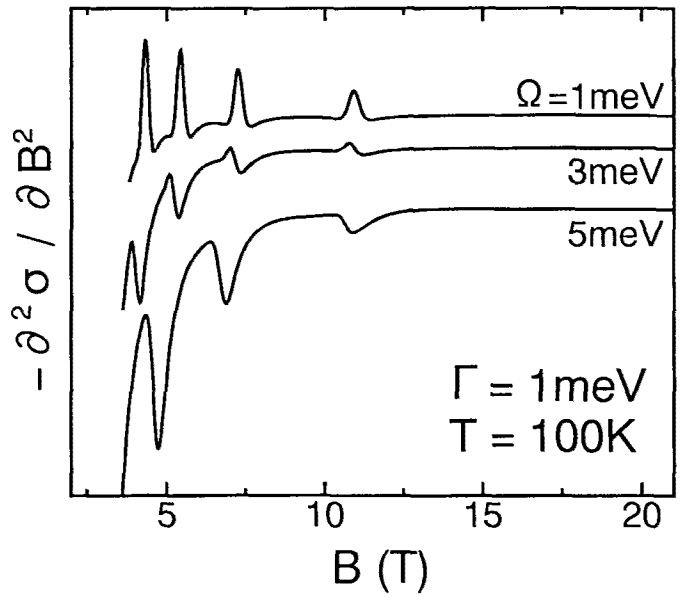

Figure 3: The calculated result of the second derivative of magnetoconductivity as a function of magnetic field in quantum wires of parabolic confinement potential Ω = 1, 3, and 5meV at T = 100K.

4. RESULTS

In Fig. 3 we present calculated result of magnetoconductivity as a function of magnetic field in quantum wires of parabolic confinement potential Ω = 1, 3, and 5meV at T = 100K, where the second derivative of the magnetoconductivity with respect to the magnetic field is plotted to show the oscillatory structures clearly. We used the following values for the material parameters for GaAs: α = 0.07 and ω_0 = 36.2meV. In the calculation, we assume that the broadening energy is 1meV. For weak confinement potential (Ω = 1meV), the magnetoconductivity exhibits maxima at resonances, and the feature is quite similar to the case of two-dimensional electron gas. The magnetoconductivity consists mostly of the hopping conductivity σ_{po}. On the other hand, for strong confinement potential (Ω = 5meV), the magnetoconductivity shows minima at resonates and the magnetoconductivity is dominated by the σ_{po} arising from the confinement potential.

We present calculated results of magnetoconductivity at T = 100K in square potential in Fig. 2, where we assumed quantum wires of GaAs of well width a = 200Å and barrier heights V_0 = 50, 70 and 100meV. We have to note that the calculations of the magnetoconductivity are carried out by taking into account electron scattering by LO phonons from the lowest Landau level to higher Landau levels. In addition the distribution function of electrons is assumed to be Maxwellian, for simplicity. We show the calculated conductivity σ_{po} due to confinement potential in Fig. 4(a) and the hopping conductivity σ_{ep} due to electron-phonon interaction in Fig. 4(b) as a function of applied magnetic field, where we plotted magnetoconductivity near the fundamental resonance region. The conductivity is normalized by $\sigma_0 = e/m\alpha\omega_0$. At resonance, σ_{ep} exhibits maxima and σ_{po} exhibits minima. These features are very similar to the result of high confinement potential in the parabolic case. The resonance is mainly caused by the resonant scattering between the lowest two Landau levels, because the electrons occupy the lowest state in Fig. 2 for low density case. The ratio of σ_{po} to σ_{ep} is found to increase with increasing the potential barrier V_0. This behavior is similar to that in the quantum wire having the parabolic confinement potential.

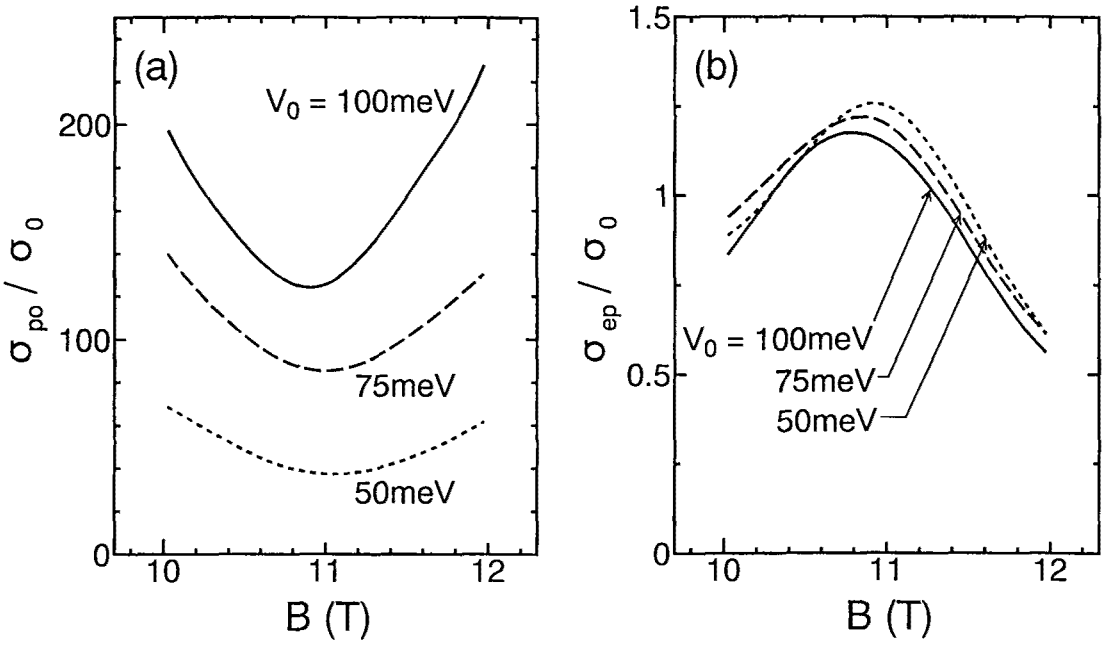

Figure 4: The calculated conductivity at $T = 100$K as a function of applied magnetic field B for a quantum wire of GaAs as treated in Fig. 2. (a) σ_{po} represents the conductivity caused by the current carried by electron motion affected by the confinement potential, and (b) σ_{ep} represents that related to the current carried by electron hopping motion between the localized cyclotron orbits through electron-phonon interaction.

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REFERENCES

[1] R.A. Stradling and R.A. Wood, J. Phys. C1 (1968) 1711.

[2] R.L. Peterson, The magnetophonon effect in *Semiconductors and Semimetals*, edited by R.K. Willardson and A.C. Beer, (Academic, New York, 1975), Vol. 10, p. 221.

[3] R.J. Nicholas, Prog. Quantum Electronics **10** (1985) 1.

[4] C. Hamaguchi and N. Mori, Physica B **164** (1990) 85.

[5] P. Vasilopoulos, P. Warmenbol, F.M. Peeters and J.T. Devreese, Phys. Rev. B**40** (1989) 1810.

[6] N. Mori, H. Momose and C. Hamaguchi, Phys. Rev. B**45** (1992) 4536.

[7] N. Mori, H. Momose and C. Hamaguchi, presented in IIAS Symposium on Sci. and Technol. of Mesoscopic Structures, Nara, Japan, 1991.