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TRANSPORT PROPERTIES OF A QUASI-TWO-DIMENSIONAL ELECTRON GAS IN A $Si/SiGe$ HETEROSTRUCTURE: TEMPERATURE AND MAGNETIC FIELD EFFECTS

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Abstract. *We investigate the mobility and resistivity of a quasi-two-dimensional electron gas (Q2DEG) in a Si/SiGe heterostructure (HS) at arbitrary temperatures for two cases: with and without in-plane magnetic field. We consider two scattering mechanisms: charged impurity and interface-roughness scattering. We study the dependence of the mobility on the temperature, magnetic field, carrier density, impurity concentration and position. At low temperatures our results reduce to those of Gold (Semicond. Sci. Technol. 26, 045017 (2011)). Our results and new measurements of transport properties can be used to obtain information about the scattering mechanisms in the Si/SiGe heterostructures.*

I. INTRODUCTION

Recently Gold has calculated the zero temperature mobility of the two-dimensional electron gas in Si/SiGe heterostructures for charged-impurity scattering, and interface-roughness scattering [1]. He has included the exchange-correlation and multiple-scattering effects (MSE) and obtained good agreement with experiment on a metal-insulator transition (MIT)[2, 3, 4, 5] . In this paper we generalize Gold's work to the finite temperature case. We show that even at low temperature ($T > 0.1T_F$) the temperature effect is considerable.

II. THEORY

We consider a Q2DEG in the xy-plane with parabolic dispersion. We describe extension effects of the Q2DEG perpendicular to the Si/SiGe interface by the triangular potential well using the Howard-Stern expression for the envelope wave function [1, 2]

$$\varsigma_0(z) = \left(\frac{b^3}{2}\right)^{1/2} z \exp\left(-\frac{1}{2}bz\right) \tag{1}$$

When the in-plane magnetic field B is applied to the system, the carrier densities for spin up/down are not equal [7, 8]. At $T = 0$ we have

$$\begin{aligned} n_\pm &= \frac{n}{2}\left(1 \pm \frac{B}{B_s}\right), && B < B_s \\ n_+ &= n, n_- = 0, && B \geq B_s \end{aligned} \tag{2}$$

Here $n = n_+ + n_-$ is the total density and B_s is the so-called saturation field given by $B_s = 2E_F/(g\mu_B)$, where g is the electron spin g-factor and μ_B is the Bohr magneton. For $T > 0$, $n_\pm$ is determined using the Fermi distribution function and given by

$$n_+ = \frac{n}{2} tln \left(\frac{1 - e^{2x/t} + \sqrt{(e^{2x/t} - 1)^2 + 4e^{(2+2x)/t}}}{2} \right)$$
$$n_- = n - n_+ \tag{3}$$

where $x = B/B_s$ and $t = T/T_F$ with T_F is the Fermi temperature. The energy averaged transport relaxation time for the $\pm$ components are given in the Boltzmann theory by [7]

$$\langle \tau_\pm(\epsilon) \rangle = \frac{\int_0^{+\infty} \tau(\epsilon)\epsilon[-\frac{\partial f^\pm(\epsilon)}{\partial \epsilon}]d\epsilon}{\int_0^{+\infty} \epsilon[-\frac{\partial f^\pm(\epsilon)}{\partial \epsilon}]d\epsilon} \tag{4}$$

$$\frac{1}{\tau(k)} = \frac{m^*}{2\pi\hbar^3 k^3} \int_0^{2k} \frac{\langle |U(q)|^2 \rangle}{[\epsilon(q)]^2} \frac{q^2 dq}{\sqrt{1 - (q/2k)^2}} \tag{5}$$

$$\epsilon(q) = 1 + \frac{2\pi e^2}{q\epsilon_L} F_C(q)[1 - G(q)]\Pi(q, T) \tag{6}$$

$$\Pi(q, T) = \Pi_+(q, T) + \Pi_-(q, T) \tag{7}$$

$$\Pi_\pm(q, T) = \frac{\beta}{4} \int_0^\infty d\mu' \frac{\Pi^0_\pm(q, \mu')}{cosh^2(\frac{\beta}{2}(\mu_\pm - \mu'))} \tag{8}$$

$$\Pi^0_\pm(q, E_{F\pm}) = \frac{g_\nu m^*}{\pi\hbar^2} \left[1 - \sqrt{1 - \left(\frac{2k_{F\pm}}{q} \right)^2} \theta(q - 2k_{F\pm}) \right] \tag{9}$$

$$F_C(q) = \frac{1}{8} \left[1 + \frac{q}{b} \right]^{-3} \left[8 + 9\frac{q}{b} + 3\left(\frac{q}{b} \right)^2 \right] \tag{10}$$

with $f^\pm(\varepsilon) = \frac{1}{1+\exp(\beta[\varepsilon - \mu_\pm(T)])}$, $\beta = (k_B T)^{-1}$, $\mu = \frac{1}{\beta} ln(exp[\beta E_{F\pm}] - 1)$, $E_{F\pm} = \frac{\hbar^2 k^2_{F\pm}}{2m^*}$ and $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$. Here, m^* is the effective mass in xy-plane and m_z is the effective mass perpendicular to the xy-plane, $G(q)$ is the local field correction (LFC) describing the exchange-correlation effects and $U(q)$ is the random potential which depends on the scattering mechanism [1]. For charged-impurities of density N_i located on the plane with $z = z_i$ we have

$$\langle |U_R(q)|^2 \rangle = N_i \left[\frac{2\pi e^2}{\epsilon_L q} \right]^2 F^2_R(q, z_i) \tag{11}$$

with $q_s = \frac{2g_\nu m^* e^2}{\epsilon_L \hbar^2}$, $F(q, z_i) = \frac{e^{-q|z_i|}}{(1+\frac{q}{b})^3}$ and $b = \left(\frac{33\pi n m_z e^2}{16\epsilon_L \hbar^2}\right)^{1/3}$. Here ϵ_L is the background static dielectric constant and g_ν is the valley degeneracy. For the interface-roughness scattering (IRS) the random potential is given by

$$\langle |U_S(q)|^2 \rangle = 4\pi^3 e^4 (\Delta \Lambda N)^2 \frac{e^{-q^2\Lambda^2/4}}{\epsilon_L} \tag{12}$$

where Δ represents the average height of the roughness perpendicular to the Q2DEG and Λ represents the correlation length parameter of the roughness in the plane of the Q2DEG. The mobility of the unpolarized and fully polarized Q2DEG is given by $\mu_0 = \frac{e\langle\tau\rangle}{m^*}$. The resistivity of the polarized Q2DEG is given by $\rho = \frac{1}{\sigma}$ where $\sigma = \sigma_+ + \sigma_-$ is the total conductivity and $\sigma_\pm$ is the conductivity of the $(\pm)$ spin subband given by

$$\sigma_\pm = \frac{n_\pm e^2 \langle \tau_\pm \rangle}{m^*} \tag{13}$$

We use the symbol μ for the mobility when MSE are taken into account at low electron densities. For $N > N_{MIT}$ the mobility can be written as $\mu = \mu_0(1 - A)$ with $A < 1$. The parameter A describes the importance of MSE and depends on the random potential, the screening function including the LFC and the compressibility of the electron gas and is given by [1, 9]

$$A = \frac{1}{4\pi N^2} \int_0^\infty dqq \frac{\langle |U(q)|^2 \rangle}{\epsilon(q)^2} \Pi^2(q, T) \tag{14}$$

For $N < N_{MIT}$, where $A > 1$, the mobility vanishes: $\mu = 0$.

III. NUMERICAL RESULTS

In this section, we present our numerical calculations for the mobility and resistivity of a Q2DEG in a Si/SiGe HS using the following parameters [1]: $\epsilon_L = 12.5$, $g_\nu = 2$, $m^* = 0.19m_0$, $m_z = 0.916m_0$, where m_0 is the vacuum mass of the electron. At zero temperature we have obtained the results given in Gold's work [1]. We study the dependence of the mobility and resistivity on the impurity position, temperature and magnetic field. Our results maybe of help in checking the validity of Gold's assumptions experimentally.

III.1. The impurity position effects:

The author of Ref. [1] has supposed two kinds of charged impurities: remote impurity of density N_{id} located at $z_i = 490$Å and interface impurity of density N_{i0} located at $z_i = 0$. The values of z_i are taken from the experiment [6] and the values of N_{id} and N_{i0} are chosen in order to obtain a reasonable agreement with the experiment. We have calculated the mobility versus density for remote impurity scattering (RIS) with different values of z_i and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and interface impurity scattering (IIS) with $z_i = 0$ and $N_{i0} = 5 \times 10^9 cm^{-2}$. The results shown in Fig. 1 indicate that the mobility increases and the critical electron density N_{MIT} decreases with increase in the distance of the impurity layer from the Si/SiGe interface.

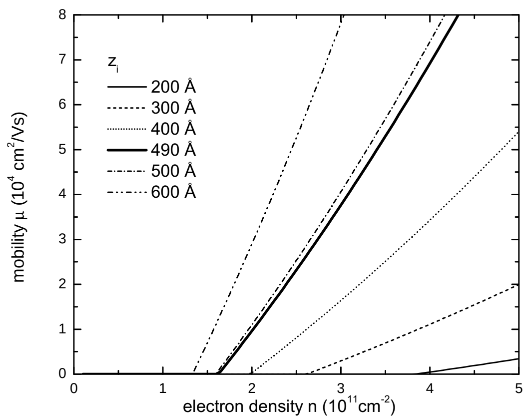

Fig. 1. Mobility versus density for RIS with different values of z_i and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and IIS with $z_i = 0$ and $N_{i0} = 5 \times 10^9 cm^{-2}$.

III.2. The temperature effects:

To see the temperature effects we calculate the mobility μ_0 versus density for remote impurities with $z_i = 490$Å and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and interface impurities with $z_i = 0$ and $N_{i0} = 5 \times 10^9 cm^{-2}$ at $t = 0, 0.1, 0.5$. The results shown in Fig. 2 indicate that for temperature $T \approx 0.5 T_F$ the mobility increases remarkably for high-density regions. Gold has shown [1] that the low temperature experimental data given in [6] can also be interpreted using RIS and IRS. We have generalized the Gold's work to the finite temperature case and the results are displayed in Fig. 3. It is seen that the temperature dependence of the mobility is similar to that shown in Fig. 2.

III.3. The magnetic field effects

The mobility μ_0 versus density for RIS with $z_i = 490$Å and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and IIS with $z_i = 0$ and $N_{i0} = 5 \times 10^9 cm^{-2}$ at $B = B_0$ and $B = B_s$ are plotted in Fig. 4. We observe that the mobility of the fully polarized Q2DEG is lower than that of the unpolarized Q2DEG. This effect is due to spin-splitting in the parallel magnetic field leading to reduced screening in a spin-polarized electron gas. We have also obtained similar results for RIS with $z_i = 490$Å and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and IRS with $\Lambda = 100$Å, $\Delta = 3.5$Å.

IV. CONCLUSIONS

The author of Ref. [1] has interpreted successfully the mobility data of the recent experiment [6] using IRS and charge-impurity scattering. In this paper we have investigated the impurity position, temperature and magnetic field effects on the mobility. At zero temperature our results reduced to those given in [1]. We have shown that the mobility increases and the critical electron density N_{MIT} decreases with increase in the distance of

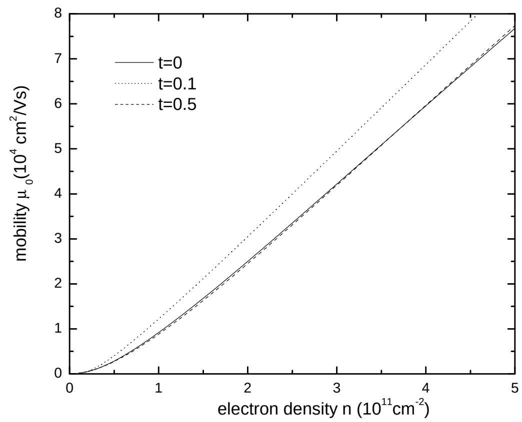

Fig. 2. Mobility μ_0 versus density for remote RIS with $z_i = 490\text{Å}$ and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and IIS with $z_i = 0$ and $N_{i0} = 5 \times 10^9 cm^{-2}$ at $t = 0, 0.1, 0.5$.

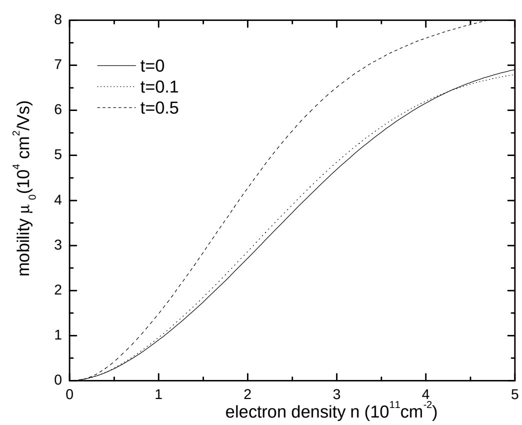

Fig. 3. Mobility $\mu_0$versus density for RIS with $z_i = 490\text{Å}$ and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and IRS with $\Lambda = 100\text{Å}$, $\Delta = 3.5\text{Å}$ at $t = 0, 0.1, 0.5$.

the impurity layer from the Si/SiGe interface and for temperature $T \approx 0.5T_F$ the mobility increases remarkably for the high density region. We also find that the mobility of the fully polarized Q2DEG is lower than that of the unpolarized Q2DEG. Finally, we note that our finite temperature results are valid only for electron densities much higher than the critical density N_{MIT} .

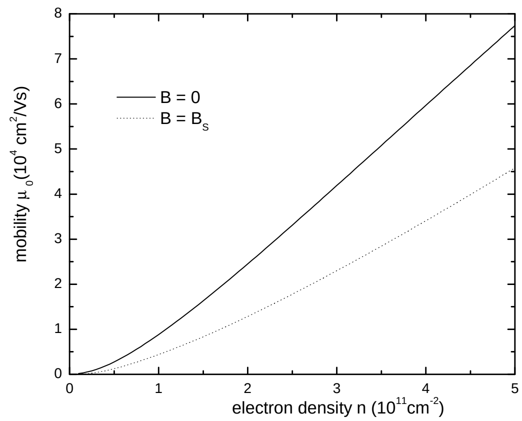

Fig. 4. Mobility μ_0 versus density for RIS with $z_i = 490\text{Å}$ and $N_{id} = 3.2 \times 10^{13} cm^{-2}$ and IIS with $z_i = 0$ and $N_{i0} = 5 \times 10^9 cm^{-2}$ at $B = B_0$ and $B = B_s$.

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