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THE CONDUCTIVITY OF THE SPIN-POLARIZED TWO-DIMENSIONAL ELECTRON GAS: EXCHANGE/CORRELATION AND STRONG DISORDER EFFECTS

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The conductivity of a spin-polarized two-dimensional electron gas is calculated and compared with the conductivity of the unpolarized electron gas. Disorder effects are considered within the self-consistent current relaxation theory, which gives rise to a crossover point from metallic to insulating behavior. Many-body effects due to exchange and correlation are taken into account and are described by a local-field correction. Our calculations are in good agreement with recent experimental results on the magnetoresistance of Silicon inversion layers.

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In recent experiments the transport properties of the two-dimensional electron gas (2DEG) as realized in Si inversion layers and GaAs heterostructures have been studied by applying a parallel magnetic field [1 – 13]. The term "parallel magnetic field" means that the magnetic field is in the plane of the electron gas. The renewed interest into the metal-insulator transition (MIT) [14 – 19] in a 2DEG initiated much interest on transport measurements. In the metallic phase a strong positive magnetoresistance was found. The experimental fact that the magnetoresistance saturates above the magnetic field B_c, corresponding to a totally polarized electron system, was interpreted as manifestation for the importance of the spin-polarization [8, 9].

In a recent paper [20] we compared the transport properties of an unpolarized and of a polarized 2DEG and found a positive magnetoresistance. Our calculation was made for weak disorder and the screening behavior was treated within the random-phase approximation. The random-phase approximation is valid if the Winger – Seitz parameter $r_s = (\pi N a^{*2})^{-1/2}$ is small, which is not the case in the experiments. $a^* = 22.9\,\text{Å}$ is the effective Bohr radius, defined with the effective mass m^* and the background dielectric constant ϵ_L, and N is the electron density. Moreover, at low electron density the disorder effects in Si inversion layers are large because a MIT takes place around $N = N_c \approx 1 \cdot 10^{11}\,\text{см}^{-2}$ ($r_s = 7.8$) . For relatively high density $N > 2N_c$ our theory was in fair agreements with experimental results [8, 9].

Very recent experiments [10, 13] concerning the magnetoresistance showed that our theory [20] failed to describe experiments for $N < 2N_c$. Therefore, in the present paper we take into account exchange-correlation effects, which are important for large r_s, and we consider multiple-scattering effects, which lead to a MIT at low carrier density.

We assume that the 2DEG electron gas has zero width in the direction perpendicular to the interface and we consider only charged impurity scattering. Screening effects are taken into account within the random-phase approximation and including exchange/correlation effects (many-body effects) described by the local-field correction (LFC) [21]. Such a

theory is also valid in the dilute limit where r_s is large. Multiple scattering effects are treated within the self-consistent current relaxation theory [22 – 26]. We apply in this paper the transport theory for an interacting electron gas in two-dimensions [22, 26] and screening effects, including exchange and correlation, are taken into account by using an analytical expression for the LFC [27].

The electron density defines the Fermi wave number k_F of the 2DEG via $N = g_s g_v k_F^2/2\pi$. Here g_v and g_s is the valley and the spin degeneracy factors, respectively. For Si inversion layers and Si quantum wells we use $g_v = 2$. For zero field the spin degeneracy is $g_s = 2$, while for large magnetic field the degeneracy factor is given by $g_s = 1$. We assume that the disorder is due to charged impurities of density N_i located in the plane of the electron gas and the random potential for wave number q is given by $\langle |U(q)|^2 \rangle = N_i (2\pi e^2/\epsilon_L q)^2$ [28]. The magnetic field applied parallel to the 2DEG plane leads to a Zeeman energy $\Delta E = \pm g^* \mu_B B/2$. g^* is the effective Landé g-factor. The system be total spin-polarized if ΔE is larger that the Fermi energy ϵ_F. This condition defines a critical magnetic field B_c for complete spin-polarization, which is given by $B_c = 2\epsilon_F/g^*\mu_B$. In the following we discuss the conductivity for the unpolarized electron gas ($B = 0$) and for the fully polarized electron gas ($B \geq B_c$).

The LFC $G(q)$ for wave number q takes into account corrections to the random-phase approximation due to exchange and correlations. The LFC is important for small distances and for small electron densities [29]. We use a theory [27] where the LFC is written in a Hubbard form with three coefficients $C_i(r_s)$, which are calculated self-consistently by using the Singwi – Tosi – Land – Sjölander approach [21]: $G(q) = 1.402 r_s^{2/3} q/[2.644 q_0^2 C_1(r_s)^2 + q^2 C_2(r_s)^2 - q q_0 C_3(r_3)]^{1/2}$ with $q_0 = 2/r_s^{2/3} a^*$. The LFC reduces the screening properties of an electron gas compared to the random-phase approximation – the Coulomb interaction potential $V(q) = 2\pi e^2/q$ in the screening function is replaced by $[1 - G(q)]V(q)$.

In the self-consistent current relaxation theory [23] the dynamical conductivity is expressed in terms of the current relaxation kernel. The current relaxation kernel represents a generalized inverse scattering time. The current modes decay into density modes and the current relaxation kernel is expressed by the golden rule expression with the squared coupling matrix element $qU(q)$ (the gradient of the random potential) and the density of final states (the density correlation function). The density correlation function depends on the current relaxation kernel and this gives rise to a self-consistent theory for the conductivity of the 2DEG. For details we refer the reader to Ref.[22]. We note that mobility measurements of the 2DEG in strongly disordered remote doped $GaAs/Al_xGa_{1-x}As$ heterostructures have successfully been described by our theory [25, 26].

In our approach quantum interference effects for non-interacting electrons [30], which lead to weak-localization effects, are ignored. We argued before that the "relevance of interference effects for the strongly disordered *interacting* 2DEG is not understood" [22]. We claim that the recent measurements [17] of the temperature dependent conductivity of Si inversion layers near the MIT reinforces our argument.

In the transport theory [22] for the strongly disordered 2DEG with Coulomb interaction effects, the conductivity σ at zero temperature is given by [24, 26]

$$\sigma = \sigma_0 (1 - A), \tag{1a}$$

where $\sigma_0 = Ne^2\tau_0/m^*$, τ_0 is the scattering time at zero temperature calculated in Born approximation [28], $1/\tau_0$ is proportional to the impurity density N_i and expressed by [22]

$$\frac{1}{\tau_0} = \frac{1}{4\pi m^* N} \int_0^\infty dqq^3 \frac{\langle |U(q)|^2 \rangle \Phi_0''(q, \omega = 0)}{[1 + V(q)[1 - G(q)]X_0(q)]^2}. \tag{1b}$$

$\Phi_0(q, \omega)$ is the density-density correlation function of the free 2DEG for wave number q and frequency ω, $X_0(q)$ is the Lindhard function in two dimensions [28]. The parameter A describes multiple scattering effects and is given by [22]

$$A = \frac{1}{4\pi N^2} \int_0^\infty dqq \frac{\langle |U(q)|^2 \rangle X_0(q)^2}{[1 + V(q)[1 - G(q)]X_0(q)]^2}. \tag{1c}$$

For small impurity concentration and (or) high electron density the parameter A is small and can be neglected. In this limit the theory is described by the lowest order result σ_0. The conductivity becomes zero for $A = 1$, which means that for fixed impurity density a critical electron concentration N_c exists and the conductivity is zero for $N \leq N_c$. The condition $A = 1$ describes the MIT. For $N_c \approx 10^{11}\,\mathrm{cm}^{-2}$ we find $A = (N_c/N)^{1.7}$ and we conclude that A becomes small for $N \gg N_c$.

We have calculated A numerically by taking into account exchange and correlation via the LFC. For $10^{10}\,\mathrm{cm}^{-2} < N_c < 10^{12}\,\mathrm{cm}^{-2}$ we find for the non-polarized 2DEG

$$N_c/N_i \approx 10.5\,[10^{11}\,\mathrm{cm}^{-2}/N_c]^{0.75} \tag{2a}$$

and for the fully polarized 2DEG

$$N_c/N_i \approx 12.5\,[10^{11}\,\mathrm{cm}^{-2}/N_c]^{0.75}. \tag{2b}$$

From Eq.(2) we conclude that for $N_c \approx 10^{11}\,\mathrm{cm}^{-2}$, as found in experiments [19], one impurity localizes about 11 electrons. This shows that the localized electrons are not bound to impurities, as in the hydrogen atom – localized states are different from bound states and the physics of an impurity band is not appropriate in this case. If we neglect correlation effects and only take into account exchange effects we find for the unpolarized 2DEG $N_c/N_i \approx 2.3[10^{11}\,\mathrm{cm}^{-2}/N_c]^{0.33}$. We conclude that correlation effects are important in order to get realistic numbers for N_c.

In Fig.1 we show N_i versus N_c for the unpolarized system and the fully polarized system. We see that for given N_i the critical electron density N_c for the polarized system

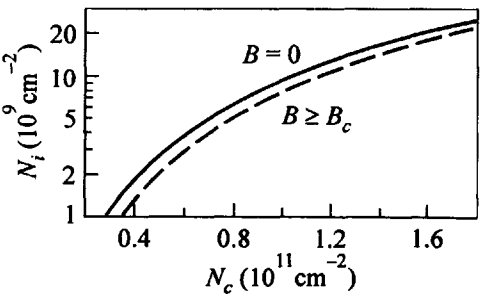

Fig.1. Critical electron density N_c for a given impurity density N_i of a 2DEG in Si with no spin polarization (solid line) and with full spin polarization (dashed line)

is larger than for the unpolarized electron gas, in agreement with experiments, and we find numerically $N_c(B \geq B_c) \approx 1.1 N_c(B = 0)$. This relation means that a magnetic field can suppress the metallic behavior. From experiment it was deduced that $N_c(B \geq B_c) \approx$ $\approx 1.4 N_c(B = 0)$ [1]. We believe that finite extension effects (orbital effects), which lead to a larger effective mass the 2DEG when a parallel magnetic field is applied [28], will increase $N_c(B \geq B_c)$.

From experiment the impurity density is not know. We determine N_i by the conductivity at high electron density $N \gg N_c$ using $\sigma \approx \sigma_0$. With N_i determined the critical density N_c is defined by $A = 1$. In Fig.2. we show the conductivity versus density for $N_i = 4 \cdot 10^9\,\mathrm{cm}^{-2}$ in comparison with recent experimental results from Ref.[10].

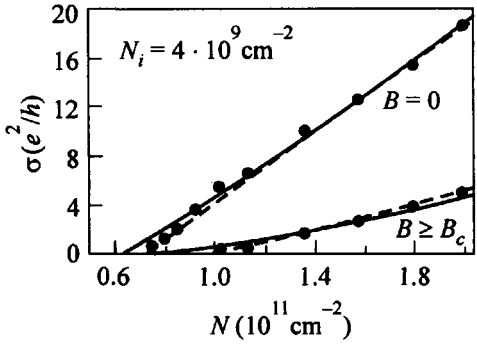

Fig.2. Conductivity σ in units of e^2/h as function of the electron density N for an impurity density $N_i = 4 \cdot 10^9\,\mathrm{cm}^{-2}$ as solid lines. The unpolarized electron gas ($B = 0$) shows a higher conductivity than the polarized electron gas ($B \geq B_c$). The solid circles are experimental results [10] for Si inversion layers for $B = 0$ and $B \geq B_c$. The dashed lines represent our fits to the experimental data, see the text

At high electron density ($N > 1.5 \cdot 10^{11}\,\mathrm{cm}^{-2}$) there is good agreement and even at lower density good qualitative agreement is obtained. The conductivity scale for the unpolarized system is about a factor 4 larger than for the polarized system due to σ_0 [20]. The discrepancies between theory and experiment seen in Fig.2 for $N < 1.5 N_c$ are due to the fact that our theory is not able to predict the critical electron density for the MIT in *perfect* agreement with the experiment. The experimental data [10] can be fitted by $\sigma(B = 0) = 10.5(e^2/h)(N - N_c)/N_c$ with $N_c = 7.2 \cdot 10^{10}\,\mathrm{cm}^{-2}$ and by $\sigma(B \geq B_c) = 4.8(e^2/h)[N - N_c]/N_c$ with $N_c = 9.8 \cdot 10^{10}\,\mathrm{cm}^{-2}$, see Fig.2. We conclude that $N_c(B \geq B_c)/N_c(B = 0) = 1.36$, in reasonable agreement with earlier experimental results [1].

From our numerical results for A and σ_0 and $N < 1.5 N_c$ (see Fig.2) we get for the unpolarized electron gas ($B = 0$)

$$\sigma = \frac{e^2}{h} 0.53 \frac{N_c}{N_i} \left[\frac{N_c}{10^{11}\,\mathrm{cm}^{-2}}\right]^{0.44} \left(\frac{N - N_c}{N_c}\right) \tag{3a}$$

and for the polarized electron gas ($B \geq B_c$) we find

$$\sigma = \frac{e^2}{h} 0.10 \frac{N_c}{N_i} \left[\frac{N_c}{10^{11}\,\mathrm{cm}^{-2}}\right]^{0.79} \left(\frac{N - N_c}{N_c}\right). \tag{3b}$$

These results are in qualitative agreement with the conductivity near the MIT as observed in the hole system of $GaAs/Al_xGa_{1-x}As$ [18].

In Fig.3 we show the resistivity ration $\rho(B \geq B_c)/\rho(B = 0)$ versus electron density. The lowest order result within the random-phase approximation is shown by the dotted line. Exchange/correlation effects are taken into account for the dashed-dotted

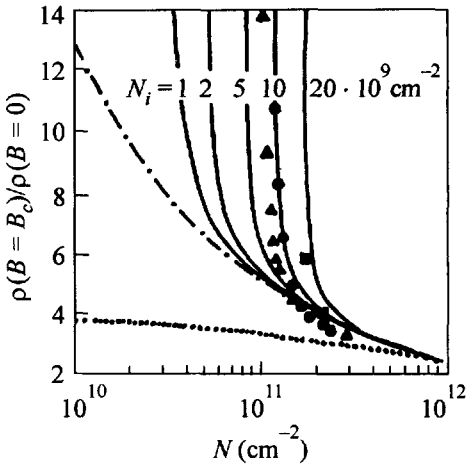

Fig.3. Resistivity ratio $\rho(B \geq B_c)/\rho(B = 0)$ as function of the electron density N for parameters corresponding to Si inversion layers. The dotted line represents the calculation within the random-phase approximation. The dashed-dotted line includes many-body effects (exchange and correlation) via the LFC. The solid lines include multiple scattering effects (the MIT) and results for different impurity densities N_i are show. The solid points represent experimental results for three different Si inversion layers: solid squares from Okamoto et al. [8], solid triangles from Pudalov et al. [10], and solid circles from Shashkin et al. [13]

line, where multiple scattering effects are neglected and in this approximation the ratio $\rho(B \geq B_c)/\rho(B = 0)$ does not depend on the impurity density. Multiple scattering effects, which lead to a MIT, are taken into account for the solid lines. Experimental results [8, 10, 13] are in good agreement with the theory if we compare with the solid line for $N_i \approx 1 \cdot 10^{10}\,\mathrm{cm}^{-2}$. The strong enhancement $\rho(B \geq B_c)/\rho(B = 0) \to \infty$ seen in Fig.3 is due to the MIT at N_c in the fully polarized 2DEG. It would be interesting to study Si inversion layers with an impurity density $N_i \approx 1 \cdot 10^9\,\mathrm{cm}^{-2}$. For such structures the exchange-correlation enhancement of $\rho(B \geq B_c)/\rho(B = 0)$ could be better observed than in the samples of Ref.[10] and Ref.[13], see Fig.3. We believe that the 2DEG in $Si/Si_{1-x}Ge_x$, where disorder effects are reduced by remote doping, is an ideal system in order to test separately interaction and disorder effects.

It was argued that finite width effects are important in $GaAs/Al_xGa_{1-x}As$ heterostructures [12] and lead to orbital effects, which are neglected in our model. Orbital effects have recently been discussed for a non-interacting 2DEG [31].

In conclusion we have shown that our theory of the transport properties of an unpolarized and a polarized 2DEG, where strong disorder and interaction effects are taken into account, is in astonishing agreement with very recent experimental data on Si inversion layers.

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