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Linear temperature dependence of mobility in quantum wells and the effects of exchange and correlation

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Abstract

We study the temperature dependence of the mobility for elastic scattering in quantum wells. Due to anomalous screening in two-dimensional systems the mobility decreases linearly with temperature. The parameter for this linear temperature dependence is a function of well width and of carrier density. It is expressed in terms of the density dependence of the form factor for finite width effects and by the local-field correction for many-body effects (exchange and correlation). We argue that alloy-disorder scattering should lead to the linear temperature dependence of the mobility.

1. Introduction

At low temperature the mobility in Si metal–oxide–semiconductor structures decreases linearly with increasing temperature [1–6]. This behaviour has also been found in Si/SiGe heterostructures for holes [7] and electrons [8]. The physical origin of this linear temperature dependence is an anomalous screening effect in two-dimensional systems as found in numerical calculations in [9]. An analytical expression for the temperature dependent mobility due to charged impurity scattering and interface-roughness scattering and a linear temperature dependence was derived in [10]. A peak mobility due to the interplay between weak localization effects and the anomalous screening effect was predicted in [11] and found in experiments for holes in Si/SiGe heterostructures [7]. So far this anomalous screening effect has only been found experimentally in Si structures.

In order to show that this phenomenon is related to two-dimensional systems in general it would be interesting to observe this behaviour in structures not containing Si. We argued before that this anomalous screening effect is difficult to measure in remote doped AlGaAs/GaAs heterostructures due to reduced backscattering in the case of remote impurities [12].

In this paper we propose to measure the anomalous screening in GaInAs structures where alloy-disorder scattering is the dominant scattering mechanism. Such a measurement would be

particularly interesting because, from the theoretical point of view, there exists a controversy concerning the importance of screening for alloy-disorder scattering. Alloy-disorder scattering, where screening was neglected, has been discussed in [13]. In [14] for heterostructures and in [15] for quantum wells (QWs) it was argued that screening has to be taken into account in order to study mobility. A confirmation of the linear temperature dependence for alloy-disorder scattering would support the latter statement. Experimentally, mobility measurements [16,17] of $Ga_{0.47}In_{0.53}As$ QW structures indicate that the alloy-disorder scattering is the dominant scattering mechanism in the large density regime [15].

The screening properties of a degenerate electron gas are usually calculated within the random-phase approximation (RPA). We show in this paper that the improvement of the RPA by taking into account many-body effects (exchange and correlation) via the local-field correction (LFC) [18] is important on a qualitative level if the carrier density becomes small (the Wigner–Seitz parameter r_s becomes large). In [10] only exchange effects have been taken into account for the LFC and the validity range of our theory was $r_s < 1$. In this paper we also take into account correlation effects and extent the validity range of our theory to the regime of the strongly correlated electron gas.

Very recently, the study of the temperature dependence of the conductivity in two-dimensional systems has attracted much attention [19–22]. Transport measurement of p-type GaAs in [19] indicated a linear temperature dependence. The coefficient of the linear temperature dependence was independent of the carrier density, as predicted by our theory [10] for very small carrier density ($r_s \to \infty$). The spin-polarized two-dimensional electron gas in SiGe generated by applying a parallel magnetic field, showed a mobility that was nearly linear dependent on the temperature [20]. From measurements of the metallic phase of holes in SiGe and a linear temperature dependence of the conductivity it was concluded that the system must be considered as a Fermi liquid up to a Wigner–Seitz parameter of $r_s < 8$ [21]. The large value for r_s in the samples used in [21] indicates that many-body effects are important. In Si-MOS structures the temperature dependent screening was also considered to be important in order to explain the experimental results of high-mobility samples away from the metal–insulator transition [22]. Some anomalies of the temperature dependence in Si-MOS systems and the connection with the metal–insulator transition have been reviewed in [23]. The recent experimental results with samples having a large Wigner–Seitz parameter [19–22] demand a more careful study of many-body effects. This study is performed in this paper for QWs.

The strictly linear temperature dependence of the conductivity [10] has been confirmed recently for transport theory approaches [24,25]. In addition we find it interesting that recently theoretical results appeared in the literature concerning the 'leading temperature correction to Fermi-liquid theory in two dimensions' and a linear T-terms was claimed to be the leading term [26].

The paper is organized as follows. The model and the theory are described in section 2. In section 3 we present our results for the temperature dependence of the mobility. The discussion is in section 4 and the conclusion in section 5.

2. Model and theory

We consider a two-dimensional electron gas in a QW of width L. We assume infinite barriers and thus, penetration effects into the barriers are neglected. The two-dimensional electron density N defines the Fermi wavenumber k_F via $N = g_v k_F^2/2\pi$. The effective Bohr radius $a^* = \varepsilon_L/m^* e^2$ is given in terms of the effective mass m^* and the dielectric constant ε_L of the host material. The Wigner–Seitz parameter r_s is determined by the electron density as $r_s^2 = 1/\pi N a^{*2}$. For $Ga_{0.47}In_{0.53}As$ with $m^* = 0.041 m_e$ and $\varepsilon_L \sim 13.3$ we find $a^* = 172$ Å.

m_e is the electron mass in the vacuum. The effective Rydberg is $Ry^* = 3.15$ meV. The Coulomb interaction potential is given by [27] $V(q) = 2\pi e^2 F(q, L)/\varepsilon_L q \cdot F(q, L)$ is the form factor due to the finite width effects [28]

$$F(q, L) = \frac{1}{4\pi^2 + q^2L^2}\left[3qL + \frac{8\pi^2}{qL} - \frac{32\pi^4}{q^2L^2}\frac{1 - \exp(-qL)}{4\pi^2 + q^2L^2}\right]. \tag{1}$$

The random potential for alloy-disorder scattering was given in analytical form in [15] and we refer to that paper. The parameter α characterizes the behaviour of the random potential $\langle|U(q|^2\rangle$ for the small wavenumber: $\langle|U(q \to 0|^2\rangle \propto q^{2\alpha}$. It is important that the alloy-disorder scattering potential is a short-range potential and the Fourier transform is independent of the wavenumber $q(\alpha = 0)$.

In [10] we derived the analytical result for the temperature dependent conductivity $\sigma(T)$ for elastic scattering for $k_B T \ll \varepsilon_F$ as

$$\sigma(T) = \sigma(0)\left[1 - C(r_s, \alpha)\frac{k_B T}{\varepsilon_F} - D(r_s, \alpha)\left(\frac{k_B T}{\varepsilon_F}\right)^{3/2} + O(T^2)\right] \tag{2}$$

with

$$C(r_s, \alpha) = 2C(r_s)C(\alpha) \tag{3a}$$

and

$$D(r_s, \alpha) = 2.45C(r_s)^2C(\alpha) \tag{3b}$$

$\sigma(0)$ is the conductivity at zero temperature. The temperature dependence described by $C(r_s, \alpha)$ and $D(r_s, \alpha)$ depends on the density via the function $C(r_s)$ and on the scattering mechanism via $C(\alpha)$. These two functions are given later.

The origin of this anomalous temperature dependence is the anomalous temperature dependence of the static susceptibility $\boldsymbol{X}_0(q, T)$ which determines the screening function. The anomalous temperature dependence of the static susceptibility, with $\boldsymbol{X}_0(q \leqslant 2k_F, T = 0) = \rho_F$ and $\boldsymbol{X}_0(q > 2k_F, T = 0) = \rho_F(1 - 4k_F/q^2)^{1/2}$ [27], is the consequence of the non-continuity of the first q-derivative at $q = 2k_F$. ρ_F is the density of states. This behaviour of $\boldsymbol{X}_0(q, T = 0)$ at $q = 2k_F$ is related to Friedel oscillations and gives rise to the linear T-dependence of the static conductivity [10].

The coefficient $C(r_s)$ is given by

$$C(r_s) = \frac{F(2k_F, L)[1 - G(2k_F, L)]}{F(2k_F, L)[1 - G(2k_F, L)] + k_F a^*/g_v} \tag{4}$$

with $k_F a^* = [2/g_v]^{1/2} r_s$. Alloy-disorder scattering is characterized by $\alpha = 0$ with

$$C(\alpha = 0) = 8\ln[2]/3 = 1.848. \tag{5}$$

The prefactor $\sigma(0)$ in (2) for alloy-disorder scattering was calculated by various authors using the approximation of non-interacting electrons [13] and of interacting electrons [14, 15, 29, 30]. Analytical results have been given for $\sigma(0)$ and these results can be used to compare with the experimental data.

$G(q, L)$ in (4) is the LFC. In [31] the LFC for two-dimensional systems (heterostructures and QWs) has been calculated within a sum-rule approach of the Singwi–Tosi–Land–Sjölander (STLS) theory [32, 33]. The LFC in [31] is given as an analytical expression, which is parametrized by two parameters $C_{12}(r_s, L)$ and $C_{22}(r_s, L)$. These two parameters are calculated within the STLS approach. The sum-rule version [31] of the STLS-approach is particularly interesting because it is numerically simple and can be applied to study width effects in QWs and heterostructures. We use this approach to calculate the LFC.

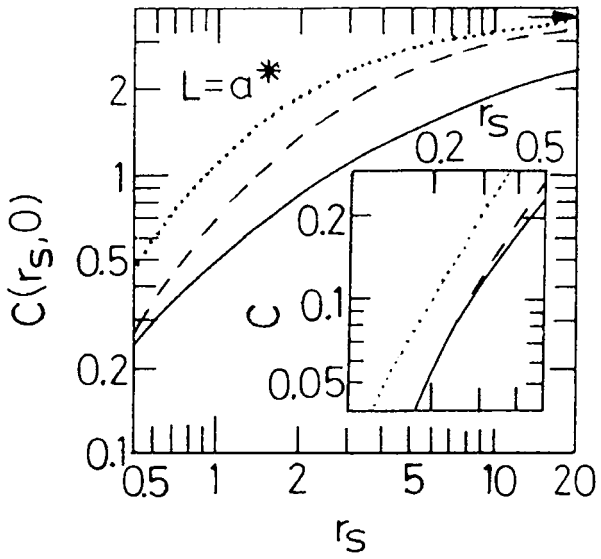

Figure 1. Coefficient $C(r_s, \alpha = 0)$ versus the RPA parameter r_s according to $(3a)$ for a QW of width $L = a^*$ as the solid curve with a^* as the effective Bohr radius. The dashed and dotted curve represents the Hubbard approximation and the RPA, respectively. In the inset we show $C(r_s, \alpha = 0)$ for large densities $0.1 < r_s < 0.5$. The valley degeneracy is $g_v = 1$.

We would like to point out that our earlier study [10] was made within the Hubbard (H) approximation $G_H(q) = q/[2g_v(q^2 + k_F^2)^{1/2}]$ [33] for the LFC where only the exchange is taken into account. The width effects for the exchange are also neglected in the Hubbard approximation. One finds $G_H(2k_F) = 1/5^{1/2}g_v = 0.45/g_v$. In the sum-rule approach [31] both exchange and correlation effects are taken into account.

We note that for $k_F \to 0\,(r_s \to \infty)$ the coefficient $C(r_s)$ becomes independent of r_s: $C(r_s \to \infty) = 1$. This result is independent of the LFC and we conclude that the LFC becomes unimportant for large $r_s\,(r_s > 100)$. For $k_F \to \infty\,(r_s \to 0)$ the coefficient $C(r_s)$ becomes $C(r_s \to 0) = [1 - 0.45/g_v)]/(k_F a^*/g_v)$ and the many-body effects (exchange) are important even for $r_s \to 0$ and cannot be neglected. This is an important topic because in the numerical calculations of the temperature dependence made by Stern [9] many-body effects in the screening function were neglected and the RPA was used.

We note that the coefficients $C(r_s, \alpha = 0)$ and $D(r_s, \alpha = 0)$ are independent of the model parameters for the alloy-disorder scattering and only depend on the parameters of the electron gas (density and width).

3. Results

The numerical results for $C(r_s, \alpha = 0)$ versus r_s are shown in figure 1 for $L = a^*$. The solid curve is the result with the LFC in the sum-rule approximation. The dashed curve is the result in Hubbard approximation and the dotted curve is the result with $G(q, L) = 0$ (RPA). Note that we used a logarithmic scale. The finite LFC reduces $C(r_s, \alpha = 0)$ in the given r_s-range by approximately a factor 2. For $r_s < 0.5$ (inset) the correlation effects can be neglected and the LFC is determined by the exchange effect. The arrow in figure 1 indicates the low-density limit $C(r_s \to \infty, \alpha = 0) = 2C(\alpha = 0) = 3.70$. For $r_s < 20$ we conclude that many-body effects are very important and must be included in the calculation of the temperature dependence of transport properties.

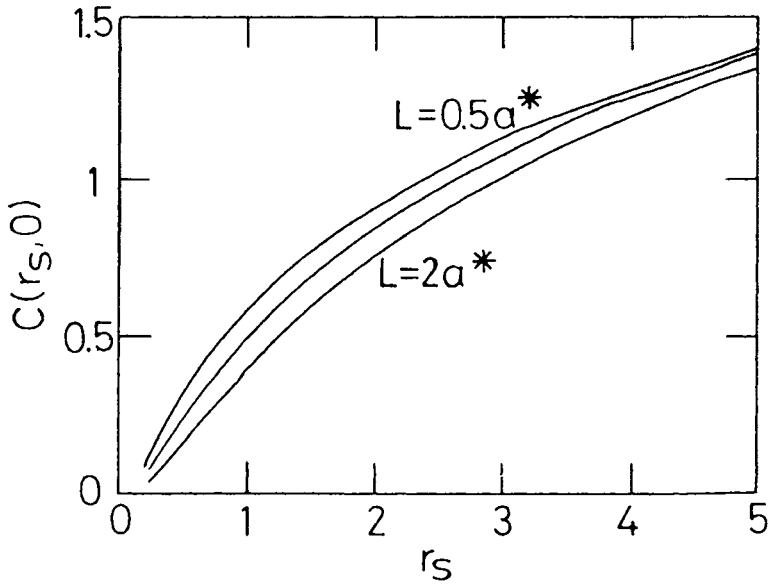

Figure 2. Coefficient $C(r_s, \alpha = 0)$ versus the RPA parameter r_s according to (3a) for QWs of width $L = a^*/2$, $L = a^*$ and $L = 2a^*$ with a^* as the effective Bohr radius. The valley degeneracy is $g_v = 1$.

In figure 2 we have shown $C(r_s, \alpha = 0)$ versus r_s for different well widths. We conclude that the well width does not give very large effects for $r_s > 3$. However, for small r_s values the well width is a very important variable and this effect has to be taken into account. Width effects are described by the parameter $2k_F L$, see (1). For small density (k_F small) this parameter is small and the width does not play an important role. However, in the high-density limit this parameter becomes large and the width effects become dominant.

The numerical results for $D(r_s, \alpha = 0)$ versus r_s are shown in figure 3 for $L = a^*$. The solid curve is the result within the full LFC in the sum-rule approximation. The dashed curve is the result given by the Hubbard approximation and the dotted curve is the result with $G(q, L) = 0$ (RPA). Note that we used a logarithmic scale. The finite LFC strongly reduce $D(r_s, \alpha = 0)$ by approximately a factor of 2. The arrow in figure 3 indicates $D(r_s \to \infty, \alpha = 0) = 2.45C(\alpha = 0) = 4.53$. Numerical results for $D(r_s, \alpha)$ have not been given in [10] and our result given in figure 3 could help experimenters correctly estimate the corrections to the linear T-term in the conductivity.

In figure 4 we show $D(r_s, \alpha = 0)$ versus r_s for the different well widths $L = a^*/2$, $L = a^*$ and $L = 2a^*$. We conclude that a finite well width does not give a very large effect for $r_s > 3$. For smaller r_s values the well width is an important variable as already found for $C(r_s, \alpha = 0)$, see figure 2. Comparing figure 2 with figure 4 we conclude that $C(r_s, \alpha = 0) \sim 3D(r_s, \alpha = 0)$.

In order to discriminate the $k_B T/\varepsilon_F$-term in (2) from the $(k_B T/\varepsilon_F)^{3/2}$-term the condition $(k_B T/\varepsilon_F)^{1/2} \ll C(r_s, \alpha)/D(r_s, \alpha)$ must be fulfilled: with $C(r_s, \alpha = 0)/D(r_s, \alpha = 0) = 3$ we find $k_B T/\varepsilon_F \ll 9$. Therefore, we argue that structures with a large Fermi energy are necessary to study the $(k_B T/\varepsilon_F)^{3/2}$ term. The T^2 term in (2) contains in principle three contributions: (i) the Sommerfeld term, (ii) the $[C(r_s, \alpha)T]^2$-contribution and (iii) an additional T^2-term due to the expansion of the screening function. Without knowing the exact coefficient of the T^2 term in (2) we suggest using the safer condition $k_B T \ll \varepsilon_F$ in order to determine the coefficient $C(r_s, \alpha)$ from the experimental results. In any case, the estimate $k_B T/\varepsilon_F \ll 9$, by using figures 2 and 4, indicates that it might be difficult to measure the $(k_B T/\varepsilon_F)^{3/2}$-term of (2).

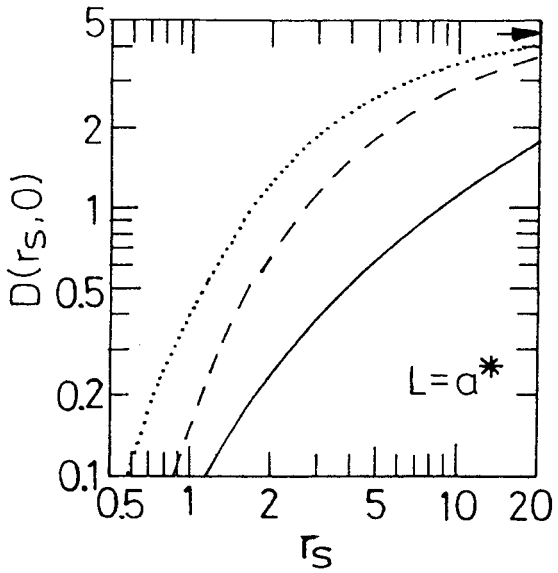

Figure 3. Coefficient $D(r_s, \alpha = 0)$ versus the RPA parameter r_s according to (3*b*) for a QW of width $L = a^*$ as the solid curve with a^* as the effective Bohr radius. The dashed and dotted curve represents the Hubbard approximation and the RPA, respectively. The valley degeneracy is $g_v = 1$.

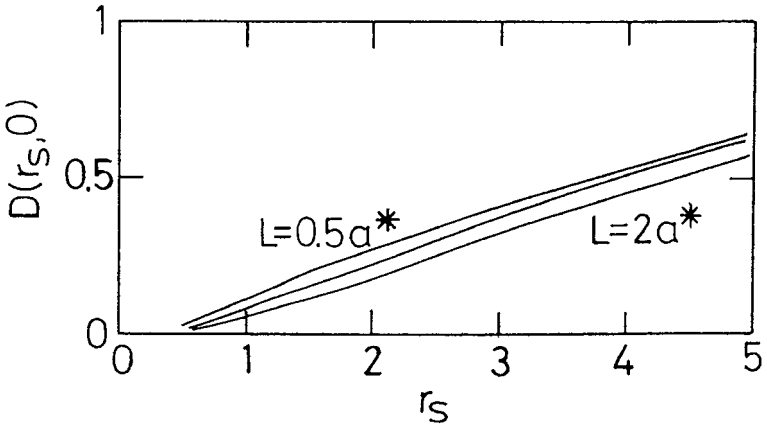

Figure 4. Coefficient $D(r_s, \alpha = 0)$ versus the RPA parameter r_s according to (3*b*) for QWs of width $L = a^*/2$, $L = a^*$ and $L = 2a^*$ with a^* as the effective Bohr radius. The valley degeneracy is $g_v = 1$.

4. Discussion

4.1. Theory

We used a model where the penetration effects into the barrier are neglected. Penetration effects become important for small well widths and the results for alloy-disorder scattering are given in [29,30]. A one-subband model with parabolic dispersion is used, and non-parabolicity effects are neglected.

Our model for the alloy-disorder scattering applies if the two-dimensional electron gas is present in the region of the alloy as in $Ga_{0.47}In_{0.53}As/InP$ and $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$.

In Si/SiGe, where the electron gas is in the Si, alloy-disorder scattering can only be relevant via penetration effects.

Our theory should also apply to the two-dimensional electron gas as realized in AlGaN/GaN QWs. Recent mobility measurements indicate that the samples now become well defined [34].

Our calculation of the mobility is made within the Born approximation including screening beyond the RPA and the disorder effects must be small. This means that the measurements must be made in the density regime where the multiple-scattering effects are small. At a critical carrier density N_c a metal–insulator transition is expected [23] and in order for the Born approximation to apply one must be away from the metal–insulator transition. A reasonable estimate of the critical density for the metal–insulator transition is given by $N_c^{1/2}a^* = 0.3$, assuming non-remote charged impurity scattering, see also [15].

We have presented our results for $C(r_s, \alpha = 0)$ and $D(r_s, \alpha = 0)$ as a function of the Wigner–Seitz parameter r_s. The Wigner–Seitz parameter was chosen because our results are not only valid for Si, but are also relevant for GaAs QWs or other QWs (GaN) if the mobility is determined by a short-range scattering potential [12].

4.2. Other scattering mechanisms

We mention that the linear temperature dependence due to the anomalous screening behaviour exists for ionized-impurity scattering ($\alpha = -1$) and for interface-roughness scattering ($\alpha = 0$ for short-range scattering) [10]. Indeed, for short-range interface-roughness scattering the coefficient for the anomalous temperature dependence is the same as for alloy-disorder scattering. However, the prefactor $\sigma(0)$ in (2) is different for the two scattering mechanisms. For impurity scattering, where the impurities are located in the QW (short-range random potential), the function $C(r_s, \alpha = 0)$ and $D(r_s, \alpha = 0)$ in (2) have to be replaced by $C(r_s, \alpha = -1) = 0.75C(r_s, \alpha = 0)$ and $D(r_s, \alpha = -1) = 0.75D(r_s, \alpha = 0)$. We conclude that the results given in figure 2 and 4 are also relevant for impurity scattering. For remote doping (long-range random potential) $C(r_s, \alpha = -1)$ becomes very small due to the reduction in backscattering as discussed in [12].

The measurements of the temperature dependent conductivity should be accompanied by Shubnikov–de Haas measurements in order to specify the scattering mechanism. The measurement of the transport scattering time τ_t (conductivity) and the single-particle relaxation time τ_s (Shubnikov–de Haas) can give information on the dominant scattering mechanism. For alloy-disorder scattering we expect $\tau_t/\tau_s \sim 0.7$–1, depending on the carrier density [15].

4.3. Experimental

The mobility measurements of $Ga_{0.47}In_{0.53}As$ QWs [16] covered the range 3×10^{10} cm^{-2} $< N < 1 \times 10^{12}$ cm^{-2} ($0.33 < r_s < 1.9$). The electron density range of the mobility measurements in [17] was 8×10^{10} cm^{-2} $< N < 2 \times 10^{11}$ cm^{-2} ($0.74 < r_s < 1.2$). The many-body effects induced bandgap renormalization in $Ga_{0.47}In_{0.53}As$ QWs was measured for 3×10^{11} cm^{-2} $< N < 2\times10^{12}$ cm^{-2} [35]. These estimates clearly show that $Ga_xIn_{1-x}As$ QWs are suitable to observe the anomalous screening of alloy-disorder scattering in two-dimensional systems. However, from figure 1 it becomes clear that the r_s values in the experiments [17] are small and the coefficient $C(r_s, \alpha = 0)$ will also be small. Therefore we suggest to search for this linear temperature dependence in samples with a lower carrier density than used in [17] but with $N \gg N_c$.

The random potential (alloy-disorder scattering) in $Ga_xIn_{1-x}As$ is proportional to $x(1-x)$: $\sigma(0) \propto 1/[x(1-x)]$. In strained QWs with $x \neq 0.47$ the alloy-disorder scattering can be strongly reduced for $x \to 0$ and $x \to 1$. While other scattering mechanisms (background impurities) might become important for weak alloy-disorder scattering we argue that systematic studies of the x-dependence of the mobility can be performed, as shown already in experiment [36]. We mention that $C(r_s, \alpha = 0)$ and $D(r_s, \alpha = 0)$ are independent of x.

Alloy-disorder scattering was studied in theory for holes in Si/Si_xGe_{1-x} QWs [37]. Experimental results for electrons in Si/Si_xGe_{1-x} heterostructures have been reviewed in [8] and also showed the linear temperature dependence, as reported earlier [7] for holes. For high-mobility samples the low-temperature mobility was interpreted as interface-roughness scattering [8, 38].

The linear temperature dependence of the mobility found for holes in GaAs [19] could be an important contribution to show that this effect is not material dependent. However, the density independence of the coefficient $C(r_s)$ found in experiment needs confirmation.

4.4. Comments

The temperature dependence of the mobility for alloy-disorder scattering in QWs was calculated within a one-subband approximation. For QWs a simple estimate of the subband energies for the subbands $n = 1, 2, \ldots$ gives $\varepsilon_n = Ry^*(\pi n a^*/L)^2$. We conclude that the condition $\varepsilon_2 - \varepsilon_1 = 3\varepsilon_1 > \varepsilon_F$ must be fulfilled in order to have only the lowest subband occupied. Due to the expansion in k_BT/ε_F in (2) the temperature must be low: $k_BT \ll \varepsilon_F$. Therefore, we argue that structures with a large Fermi energy (small mass and, therefore, small density of states) are in general better systems to study this anomalous temperature dependence. Note, however, that with increasing density (decreasing r_s) the coefficients $C(r_s, 0)$ and $D(r_s, 0)$ decrease.

Other sources of a unconventional temperature dependence of the conductivity are weak localization effects and interaction anomalies as discussed in [23]. They give rise to a logarithmic decrease of the conductivity with decreasing temperature. Together with the linear increase as discussed in this paper a maximum of the conductivity was predicted [11] and found in experiment [7].

Inelastic scattering effects due to acoustic phonons can also give rise to a linear contribution for the resistance, for a review see [27]. We mention that the Bloch–Grüneisen (BG) law predicts a T^5 dependence of the resistance at low temperatures $T < T_{BG}$ (T_{BG} is the Bloch–Grüneisen temperature) and a linear T dependence of the resistance for high temperatures $T > T_{BG}$, see [39] for AlGaAs/GaAs structures and [40] for AlGaN/GaN structures. Clearly, the temperature range, where the linear temperature dependence due to the elastic scattering can be discriminated from the linear temperature dependence due to inelastic scattering is given by $k_BT \ll \varepsilon_F$ and $T < T_{BG}$.

5. Conclusion

The temperature dependence of the mobility for elastic scattering in QWs was calculated. Many-body effects (exchange and correlation) are shown to be quantitatively important in the high and intermediate density regime and reduce the temperature dependence of the mobility. The coefficients $C(r_s, \alpha = 0)$ and $D(r_s, \alpha = 0)$ are independent of model parameters of the scattering process but depend on the electron density via r_s. We argued that the alloy-disorder is screened and the conductivity should show this linear temperature dependence. The functions $C(r_s, \alpha = 0)$ and $D(r_s, \alpha = 0)$ are also relevant for the temperature dependence

of the conductivity due to interface-roughness and impurity scattering. By taking many-body effects into account the present work extends the validity range of our earlier work [10] to small carrier density.

Our prediction for the temperature dependence for alloy-disorder scattering can be used to study the screening (interaction) and many-body effects in the two-dimensional electron gas. For large electron density we conclude that width effects and many-body effects are important. For very small electron density we find that many-body effects dominate and that the width effects are small.

The experimental finding of a linear temperature dependence of the mobility can, together with our theory, be used to argue that the two-dimensional electron gas behaves as a Fermi liquid.

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