Transport properties of an electron gas on the surface of silicon (111): the importance of a density dependent effective mass

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Abstract. For zero temperature we study transport properties of a two-dimensional electron gas on the surface of silicon (111). We obtain good agreement with recent experimental results if we take into account a strongly density dependent effective mass and the existence of a metal-insulator transition, both taken from experiment. We discuss the effect of the density dependent effective mass on the critical electron density of the metal-insulator transition as predicted by the mode-coupling theory. A reentrant metallic phase is predicted at low density.

1. Introduction
For three decades the transport properties of the two-dimensional electron gas (2DEG) have been a very exciting research area in connection with the metal-insulator transition (MIT) [1]. Recently, some very interesting experiments were made in the low-electron-density range of the 2DEG. It was found that, besides the existence of a MIT in silicon (100) and discussed since a long time [1], also a strong mass enhancement occurs, with a trend to diverge at a critical density $N_{cm}$, which is near to the density of the MIT $N_{cm} = N_{MIT}$ [2,3]. This mass enhancement was first measured using a parallel magnetic field [3]. The origin of this mass divergence is not known and was confirmed with other experimental techniques, for instance with the Shubnikov-de Haas (SdH) effect [2].

Low temperature transport properties of the 2DEG on the surface of silicon (111) have been measured recently and a mass divergence has been reported [4]. We have analyzed these experimental results within a mode-coupling approach and we found a surprisingly good agreement between theory and experiment [5]. In this paper we present additional results.

2. Model and theory
Two scattering times determine transport experiments: the transport scattering time $\tau_t$, accessible in transport measurements in zero magnetic field, and the single-particle relaxation time $\tau_s$, accessible in SdH measurements [1] in a perpendicular magnetic field. For weak and short-range disorder the two scattering times should be finite and behave similar. However, near the MIT the transport scattering time becomes small and vanishes at the transition point. We describe the mobility with a mode-coupling approach [6], where multiple scattering...
effects lead to the MIT. Weak-localization corrections are neglected. The single-particle relaxation time is related to the Dingle temperature [1] and \( \tau_s \) represents a measure how disorder modifies the density of states in the presence of disorder in the limit of a vanishing magnetic field. At the MIT with a finite density of states \( \tau_s \) is also finite. Multiple scattering effects only give small modifications to \( \tau_s \) [7], if compared to the contribution of multiple scattering effects to \( \tau_s \).

In lowest order (\( O \)) of the disorder one finds that \( 1/\tau_s^e \) and \( 1/\tau_s^o \) are proportional to the random potential \( \langle |q| \rangle^2 \) created by the disorder. In our transport theory screening effects are described within the random-phase approximation [1,6] and many-body effects are treated in using the local-field correction in Hubbard approximation. Charged-impurity scattering, important at low electron density, and interface-roughness scattering, important at high electron density, have been taken into account. For details of the calculation, see Ref.5.

When the effective mass is enhanced, the effective Bohr radius \( a_B^* \approx 1/m^* \) decreases and approaches zero when the effective mass diverges. This means that the screening properties are strongly improved when mass enhancement occurs. For low electron density one finds \( 1/\tau_s^o \propto 1/\varepsilon_f q_s^2 \propto m^* a_B^2 \propto 1/m^* \). Therefore we conclude that \( \tau_s^o \propto \tau_s^o \propto m^* \) [5] and a divergence of the effective mass \( m^* \) implies a divergence of both scattering times, calculated in lowest order of the disorder.

For the transport scattering time we take into account multiple scattering effects, described by the parameter \( A \). They are very important near \( N_{MIT} \) and are the origin for the MIT [6]. The mobility in the metallic phase is given \( \mu(N) = \mu_0 (N) (1 - A) = e\tau / m^* \) [8]. In the insulating phase the mobility vanishes \( \mu(N) = 0 \). \( \mu_0 (N) = e\tau^o / m^* \) represents the mobility calculated in lowest order of the random potential. The critical density \( N_{MIT} \) of the MIT is characterized by \( A = 1 \). In most cases one can use as approximation \( A = N_{MIT} / N \). For the single-particle relaxation time one can show that multiple scattering effects give a small effect and the lowest order result is an excellent approximation. In fact one finds \( \tau_s^o > \tau_s^o \) while \( \tau_s^o < \tau_s^o \).

3. Transport properties and critical density of the metal-insulator transition
For the effective electron mass \( m^* \) of the 2DEG at the surface of silicon (111) we use, for \( N > N_{crit} \), the form \( m^*/m_e = 0.47/(1 - N_{crit}/N) \) with \( N_{crit} = 2.2 \times 10^{11} \text{cm}^{-2} \) as the critical density of the divergent mass, which fits the experimental result [4]. \( m_e \) is the free electron mass. In the following we discuss two models. One where the electron mass is kept constant, independent of the electron density, and the other where the effective electron mass is density dependent. For the model with a density dependent mass we use the following parameters: charged impurity density at the Si/SiO\(_2\) interface \( N_i = 1.45 \times 10^{11} \text{cm}^{-2} \) and interface-roughness parameters \( \Delta = 3.2 \text{Å} \) and \( \Lambda = 57 \text{Å} \). For the constant mass model we use: impurity density at the Si/SiO\(_2\) interface \( N_i = 1.6 \times 10^{11} \text{cm}^{-2} \) and interface-roughness parameters \( \Delta = 3.6 \text{Å} \) and \( \Lambda = 56 \text{Å} \).

In Ref.5 we have shown that the measured [4] mobility versus electron density can be well fitted by the constant effective mass model but equally well by the density dependent effective mass model. A MIT at \( N_{MIT} = 3.1 \times 10^{11} \text{cm}^{-2} \) was taken into account. We mention that \( N_{MIT} = 1.4 N_{crit} \) and we conclude that the mobility vanishes at \( N_{MIT} \) due to the MIT. We concluded that by fitting the mobility versus the electron density data no valuable information can be obtained concerning a possible density dependence of the effective mass. This was a very important result [5].
Figure 1. Scattering times $\tau_t$ and $\tau_s^0$ as function of electron density for the 2DEG on silicon (111). The solid dots ($\tau_t$) and triangles ($\tau_s^0$) are experimental results of Ref.4. The solid lines represent our calculation where a density dependent effective electron mass is taken into account. The dashed-dotted lines represent the calculation with a constant electron mass.

In figure 1 we compare the transport scattering time $\tau_t$ as function of the electron density with experimental results. For low density the experimental results for the transport scattering time show a tendency to decrease, in agreement with our theory taking into account a MIT and a density dependent mass, see the solid line. With a constant mass we cannot find agreement between theory and experiment, see the dashed-dotted line. The calculated single-particle relaxation time $\tau_s^0$ is also in reasonable agreement with experiment when a density dependent effective mass is used in the calculation, see the solid line.

In order to fit the mobility [5] we used the critical electron density of the MIT $N_{\text{MIT}} = 3.1 \times 10^{11} \text{cm}^{-2}$, obtained from experiment [4]. Within the mode-coupling theory [6] one can calculate the critical density for the MIT. Our theoretical results for $N_t$ versus the critical electron density $N_{\text{MIT}}$ are shown in figure 2. The calculation for $N_t = 1.45 \times 10^{11} \text{cm}^{-2}$, used in Ref.5 to fit the mobility data [4], gives $N_{\text{MIT}} = 2.98 \times 10^{11} \text{cm}^{-2}$. This value is in very good agreement with the experiment and confirms the predictive power of our theory. For the constant mass model $N_{\text{MIT}}$ is lower than in experiment, see the dashed-dotted line in figure 2.

In order to obtain more information for low density we used for $N < N_{\text{cm}}$ the form $m^* / m_e = 0.47 / (1 - N / N_{\text{cm}})$. The results for the critical density of the MIT are shown in figure 2 as the dashed line. We conclude that the theory predicts a MIT for $N_t > 5.8 \times 10^{10} \text{cm}^{-2}$ if the electron density decreases. We find a metallic reentrant behavior for $N_t < 5.8 \times 10^{10} \text{cm}^{-2}$: if the electron density decreases one expects a MIT, then an IMT and then again a MIT. We mention that for the reentrant metallic phase the parameter $A$ is large $0.8 < A < 1$ and the mobility is low in the metallic phase, the phase underneath the dashed line in figure 2.

Our calculation of $N_{\text{MIT}}$ was made for a total degeneracy of 4, two for the spin and two for the valleys. In Ref.5 we argued that the effective mass divergence might be due to a Bloch instability, where the degeneracy factor is two if $N < N_{\text{cm}}$. We have calculated $N_{\text{MIT}}$ also in this
case and found similar numbers. The degeneracy factor also is reduced to two in the fully spin-polarized 2DEG [2]. For a degeneracy of two and $N_i = 1.45 \times 10^{11} cm^{-2}$ we get $N_{mit} = 3.62 \times 10^{11} cm^{-2}$, which corresponds to an increase of 21% compared to the result found for a degeneracy of 4. We conclude that the region of the metallic phase decreases slightly with decreasing degeneracy. The reason is the reduced screening for the lower degeneracy.

![Figure 2](image_url)

**Figure 2.** Charged impurity density versus critical electron density of the MIT for the 2DEG on silicon (111). The solid line represents the calculation for a density dependent electron mass and the dashed-dotted line is for a constant electron mass. The solid dot represents the values of $N_i$ and $N_{mit}$ used for the fit of the mobility versus electron density [5]. The dashed line represents a calculation with a density dependent electron mass for $N < N_{cm}$.

4. Conclusion

We evaluated transport properties of a 2DEG on the surface of silicon (111) by assuming a divergent effective mass at $N_{cm}$ and a metal-insulator transition at $N_{mit} = 1.4 N_{cm}$. Near $N_{cm}$ the single-particle relaxation time strongly increases ($\tau_x \to \infty$) due to screening, in agreement with experimental results. We claim that this screening effect is also relevant for heavy-fermion systems. The phase-diagram of the metal-insulator transition has been studied in detail and we predict, for low impurity density, a reentrant behavior of the metallic phase.

References

[1] Ando T, Fowler A B and Stern F 1982 Rev. Mod. Phys. 54 437
[2] Kravchenko S V and Sarachik M P 2004 Rep. Prog. Phys. 67 1; Shashkin A A 2005 Phys. Usp. 48 129
[3] Shashkin A A, Kravchenko S V, Dolgopolov V T and Klapwijk T M 2001 Phys. Rev. Lett. 87 086801
[4] Shashkin A A, Kapustin A A, Deviatov E V, Dolgopolov V T and Kvon Z D 2007 Phys. Rev. B 76 241302
[5] Gold A 2007 J. Phys. : Condens. Matter 33 2495
[6] Gold A and Götze W 1986 Phys. Rev. B 33 2495; Gold A 1991 Phys. Rev. B 44 8818
[7] Gold A 1988 Phys. Rev. B 38 10798
[8] Belitz D, Gold A and Götze W 1981 Z. Phys. B Condensed Matter 44 273