Tr. J. of Physics
23 (1999) , 559 – 564.

Exchange-Correlation Effects in the Impurity-Limited Mobility of GaAs Quantum Wires

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Received 01.03.1999

Abstract

We study the many-body effects described by the local-field corrections on the mobility of quasi-one dimensional electron systems. The low temperature mobility due to remote-impurity doping and interface-roughness scattering is calculated within the relaxation time approximation. We find that correlation effects significantly reduce the mobility at low density.

1. Introduction

Recent advances in microfabrication techniques have provided the realization of quasi-one-dimensional (Q1D) electronic structures[1] in which the free motion of electrons take place in only one spatial direction. Such systems are thought to offer interesting device possibilities because of the reduced phase space available to the charge carriers. At the same time, the Q1D electronic structures can also be used as a testing ground for our understanding of the many-body interactions[2] in low-dimensional systems, since most experimental efforts[3] are devoted to measure these effects. In this work, we study the effects of exchange and correlation on the mobility of quantum wire systems due to impurity scattering. Impurity effects are important for device applications.

Mobility limits for charged impurity scattering in Q1D systems have been considered by Sakaki,[4] Fishman,[5], Lee and Spector,[6] and Gold and Ghazali[7] within various approximation schemes. Numerical calculations for the mobility of Q1D electron systems are also provided.[8] Screening effects play an important role in the transport properties of low-dimensional electronic structures. They are usually treated within the random-phase approximation (RPA). Our aim is to explore the density dependence of the mobility for different impurity scattering mechanisms in a theoretical model which goes beyond the RPA. We have shown that the correlation effects significantly reduce the low density

mobility of quantum wires.[9] This paper summarizes our main results and discusses further developments.

2. Model and Theory

We use a model of the Q1D electron gas consisting of a cylindrical quantum wire of radius R with infinite potential barrier. The Coulomb interaction among the electrons assumed to be in the lowest subband is calculated by

$$V(q) = (2e^2\epsilon_s) \int d^2r \int d^2r' \, |\phi(r)|^2 \, K_0(q|r-r'|) \, |\phi(r')|^2 \, , \tag{1}$$

where $\phi(r)$ is the ground-state wavefunction and $K_0(x)$ is the modified Bessel function of the second kind. The many-body effects are described by the screening function $\varepsilon_t(q,\omega) = 1 - V(q)[1-G(q)]\chi_0(q,\omega)$, where $G(q)$ is the so-called local-field correction[10] and χ_0 is the dynamic susceptibility of the noninteracting system. For instance, the collective excitations (plasmons) of the system are calculated from the solution of $\varepsilon_t(q,\omega) = 0$. When we set $G(q) = 0$, we recover the familiar random-phase approximation (RPA). In this work we employ the local-field corrections numerically obtained by Calmels and Gold[11] for an extensive range of radius and density values. In general, the disorder effects will modify the screening function but we neglect them in the lowest order approximation. We shall later discuss the possible improvements of including the correlation and disorder effects on an equal footing.

Gold and Götze[12] have developed a self-consistent theory of electron dynamics which take the exchange-correlation and disorder effects into account. Within this approach, the relaxation time defined as the imaginary part of the memory function at zero frequency, is given by

$$\frac{1}{\tau(\omega=0)} = \frac{1}{nm} \sum_q q^2 \, \frac{\langle |U(q)|^2 \rangle}{\varepsilon_t(q)^2} \, \phi_0^{''}(q,0) \, , \tag{2}$$

from which the the mobility may be calculated using $\mu = e\tau(0)/m$. This expression is a special case of the mode-coupling approximation to the more general memory function describing the relaxation phenomena.[12] Using the lowest order relaxation function $\phi_0(q,z) = [\chi_0(q,0) - \chi_0(q)]/z$, where $\chi_0(q,z)$ and $\chi_0(q)$ are the dynamic and static susceptibilities, respectively, we obtain $\phi_0^{''}(q,0) = 2\pi\rho_F m k_F \, \delta(q-2k_F)/q^2$. Here $\rho_F = 2m/\pi k_F$ is the density of states on the Fermi level of a 1D electron gas. Finally, the momentum relaxation time takes a simple form

$$\frac{1}{\tau} = \frac{k_F}{E_F} \, \frac{\langle |U(2k_F)|^2 \rangle}{\varepsilon_t(2k_F)} \, . \tag{3}$$

In our calculations we use the finite temperature formalism[2, 13] so that $\varepsilon_t(2k_F)$ does not have any divergent behavior.

3. Results and Discussion

We use the material parameters appropriate to GaAs (i.e. the effective mass of electrons is $m = 0.067m_e$, where m_e is the bare electron mass and the static dielectric constant is $\epsilon_s = 13$) in the subsequent calculations. For the scattering by remote impurities, we assume that the impurities are located randomly at some distance R_i from the axis of the quantum wire of radius R. The averaged random potential is written as $\langle |U(q)|^2 \rangle = N_i V_{\rm imp}^2$, where N_i is the linear impurity density. $V_{\rm imp}(q)$ is evaluated at the impurity positions R_i using

$$V_{\rm imp}(q) = -(2e^2/\epsilon_s) \int d^2r \, |\phi(r)|^2 \, K_0(q|r - R_i|) \, . \tag{4}$$

The mobility for remote doping finally takes the form

$$\mu_{\rm RD} = \left(\frac{e a_B^2}{\hbar} \right) \frac{\pi}{16} \frac{N}{N_i} \frac{\varepsilon_t(2k_F)^2}{F_{\rm imp}(2k_F)^2} \, , \tag{5}$$

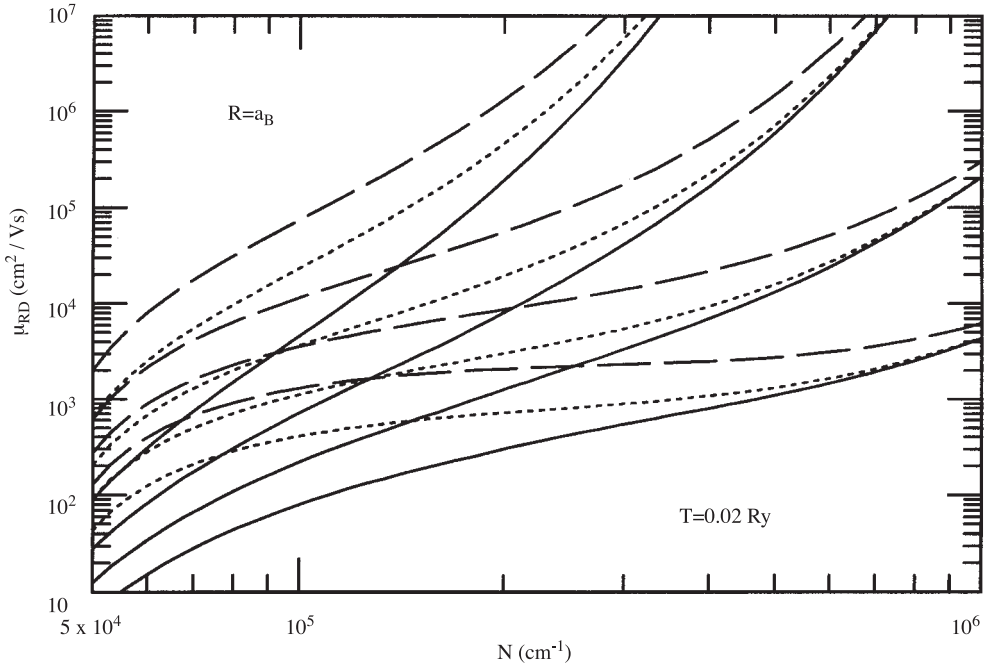

Figure 1. Mobility for remote doping as a function of electron density. The solid and dashed lines represent calculations with and without the local-field corrections, respectively. Curves from bottom to top are for $R_i = 0$, 1, 2, and $4R$. The dotted lines correspond to HF approximation.

where we have used $V_{\rm imp} = (2e^2/\epsilon_s) F_{\rm imp}$. In Figure 1 we show the mobility due to remote-impurity doping with (solid lines) and without (dashed lines) the local-field correction

for various impurity locations. The local-field factor G enters the calculation through ε_t and in the case of RPA we set $G = 0$. We take the impurity density to be $N_i = 10^6\,\mathrm{cm}^{-1}$ and the quantum wire radius $R = a_B$. The low density ($N < 5 \times 10^5\,\mathrm{cm}^{-1}$) mobility decreases substantially when the local-field effects are taken into account. Densities lower than $5 \times 10^4\,\mathrm{cm}^{-1}$ are unrealistically low and the form of the local-field factors we use may not be applicable. As the electron density increases mobility approaches to the RPA limit indicating that the local-field corrections are no longer important. The dotted lines show μ_{RD} calculated within the Hartree-Fock (HF) approximation which includes only the exchange effects. This means the screening function ε_t is evaluated within the HF approximation. We observe that exchange effects already reduce the mobility from its RPA value. Correlation effects result in a further reduction.

Interface-roughness scattering is known to be the dominant scattering mechanism for 2D electrons in thin quantum wells. We expect similar behavior in quantum wire systems. Adopting the model of Gaussian decay of the roughness fluctuations[14] we obtain for the random potential $\langle U(q)|^2\rangle = (dE_1/dR)^2\eta\delta^2\pi^{1/2}e^{-q^2\eta^2/4}$, where δ and η are the height and range parameters, respectively of our model, and $E_1 \sim 1/R^2$ is the first subband energy. The mobility due to interface-roughness becomes

$$\mu_{\mathrm{IR}} = \left(\frac{ea_B^2}{\hbar}\right)\frac{\pi^{1/4}}{4}\,\frac{R^6 N e^{k_F^2\eta^2}}{\beta_1^4\eta\delta^2 a_B^2}\,\varepsilon_t(2k_F)^2\,. \tag{6}$$

The mobility due to interface-roughness scattering as a function of the electron density for a GaAs quantum wire of radius $R = a_B$ and average roughness fluctuation size $\delta = 3\,\text{Å}$ is in Figure 2. The solid and dashed curves indicate results with and without the local-field corrections, respectively. The upper and lower curves are for the range parameters $\eta = 20\,\text{Å}$ and $\eta = 60\,\text{Å}$. We observe that μ_{IR} is strongly reduced for $N < 3 \times 10^5\,\mathrm{cm}^{-1}$ when the correlation effects are included.

Recently, Thakur and Neilson[15] have considered an improvement of our method of calculating the impurity-limited mobility. They have considered the interaction effects in the relaxation function $\phi(q, z)$ which is approximated by the free-particle value ϕ_0. This allowed them to treat the correlation and disorder effects on an equal footing within a self-consistent scheme. They have found situations where the mobility drops toward zero and the mean free path becomes of the order of the average electron spacing corresponding to strong localization. This opens new possibilities to study the localization effects, especially in relation to strong correlations, in low-dimensional systems. Recent observation of a metal-insulator transition in 2D electron systems at zero magnetic field[16] indicates interesting directions to pursue.

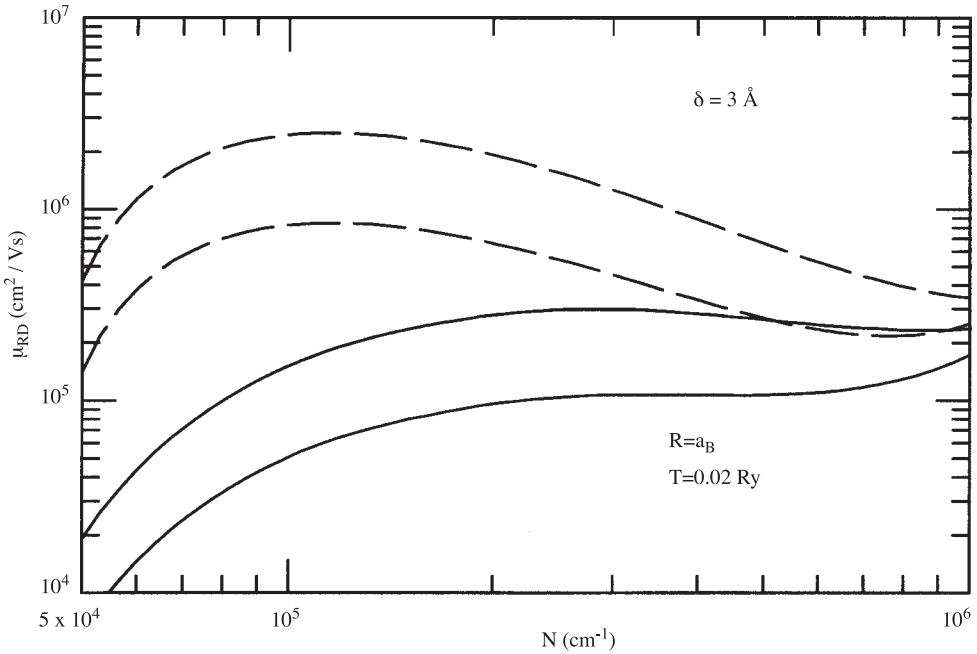

Figure 2. Mobility for interface-roughness scattering as a function of electron density. The solid and dashed lines represent calculations with and without the local-field corrections, respectively. Top and bottom curves are for $\eta = 20\,\text{Å}$ and $\eta = 60\,\text{Å}$, respectively.

In this work we have studied the influence of many-body effects on the impurity-limited mobility of semiconductor quantum wire systems. The local-field corrections embodying the exchange-correlation effects are used to calculate the mobility due to remote doping and interface-roughness scattering. In contrast to the usually employed RPA, we found that correlation effects significantly reduce the mobility at low densities.

This work was supported by the Scientific and Technical Research Council of Turkey (TUBITAK) under Grant No. TBAG-1662.

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