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Born approximation versus the exact approach to carrier-impurity collisions in a one-dimensional semiconductor: Impact on the mobility

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We study the collision of a one-dimensional (1D) electron with a screened Coulomb impurity in a single-subband GaAs quantum wire. The exact reflection probability is calculated and shown to drastically differ from the reflection probability in the Born approximation. As a result, both models also give completly different 1D electron mobilities. Further, we introduce the exact mean-field screening and show that except for high electron densities it leads to a quite different reflection probability than the linear mean-field (Lindhard) screening. Finally, we show that the Boltzmann 1D mobility concept has to be replaced by a more general semiclassical theory, if in a typical collision the backward reflection occurs with probability close to unity. [S0163-1829(99)50716-9]

Electrons in a semiconductor quantum wire can be viewed as a one-dimensional (1D) electron gas.[1] In the diffusive limit, the mobility of such 1D electron gas is usually evaluated[1,2] from the semiclassical Boltzmann transport equation which regards the scattering of a 1D electron on impurities like successive collisions with individual impurities. Usually, the collisions are treated in Born approximation[1,2] and the impurities are screened by the linear mean-field (Lindhard) screening.[3]

In this work the Schrödinger equation for the 1D electron-impurity collision problem is solved exactly and the Born approximation is found to fail. We also introduce the exact mean-field screening and find that the linear mean-field screening is only justified at high electron densities. Finally, we show that the Boltzmann 1D mobility concept has to be replaced by a more general semiclassical theory if in a typical collision the backward reflection occurs with probability close to unity.

We consider an infinite GaAs wire buried in $Al_xGa_{1-x}As$. The wire axis is associated with the x axis, the wire cross section in the y-z plane is $L_y \times L_z = 14 \times 14$ nm. We assume that only the lowest energy subband is occupied by electrons. The electron wave function is taken as $\xi(x,y,z) = \Psi_{11}(y,z) e^{ikx}/\sqrt{L_x}$, where L_x is the normalization length, k is the wave vector, and $\Psi_{11}(y,z) = \sqrt{2/L_y}\cos(\pi y/L_y)\sqrt{2/L_z}\cos(\pi z/L_z)$.

In semiclassical limit the classical motion of electron wave packet is interrupted by quantum collisions with individual impurities. In a 1D system this limit can only be justified in presence of some phase-breaking process,[4] otherwise the impurity disorder causes the Anderson localization of the 1D electron wave function. We do not consider the phase-breaking processes[4] explicitly but we assume that they are efficient enough to justify the semiclassical limit. In that limit one usually applies the Boltzmann equation, which gives the 1D electron mobility[1,2]

$$\mu = -\frac{e\hbar^2}{N_L m^2}\int_{-\infty}^{\infty}\frac{dk}{\pi}k^2\tau(k)\frac{\partial}{\partial\varepsilon}f[\varepsilon(k)], \tag{1}$$

where $\varepsilon(k) = \hbar^2 k^2/2m$ is the electron energy, m is the electron effective mass, N_L is the 1D electron density, $f[\varepsilon(k)]$ is the Fermi distribution, and $\tau(k)$ is the momentum relaxation time. For impurities, for simplicity positioned with density $N_{\rm imp}$ on a line parallel to the wire, we have

$$\frac{1}{\tau(k)} = N_{\rm imp}\int_{-\infty}^{\infty}\frac{dk'}{2\pi}W(k,k')\frac{k-k'}{k}, \tag{2}$$

where $W(k,k')$ is the probability of scattering from k to k'. In Born approximation

$$W(k,k') = \frac{2\pi}{\hbar}|U(k-k')|^2\delta[\varepsilon(k)-\varepsilon(k')] \tag{3}$$

(Fermi's golden rule), where

$$U(q) = \int_{-\infty}^{\infty}dx e^{ixq}V(x-x_0,y_0,z_0) \tag{4}$$

is the interaction matrix element—the Fourier transform of the electron-impurity interaction energy

$$V(x-x_0,y_0,z_0) = -e\int dy\int dz|\Psi_{11}(y,z)|^2 \times\varphi(x-x_0,y,z,y_0,z_0), \tag{5}$$

and $\varphi(x-x_0,y,z,y_0,z_0)$ is the potential at point (x,y,z) due to the impurity positioned at (x_0,y_0,z_0).

The linear mean-field theory of screening gives in 1D (Ref. 3)

$$U(q) = \mp\frac{G_{11}(q,y_0,z_0)}{1+\chi(q)G_{11,11}(q)}, \tag{6}$$

where the plus (minus) sign holds for the repulsive (attractive) interaction,

$$\chi(q) = \sum_k\frac{f(k)-f(k+q)}{\varepsilon(k)-\varepsilon(k+q)} \tag{7}$$

is the Lindhard polarizability function,

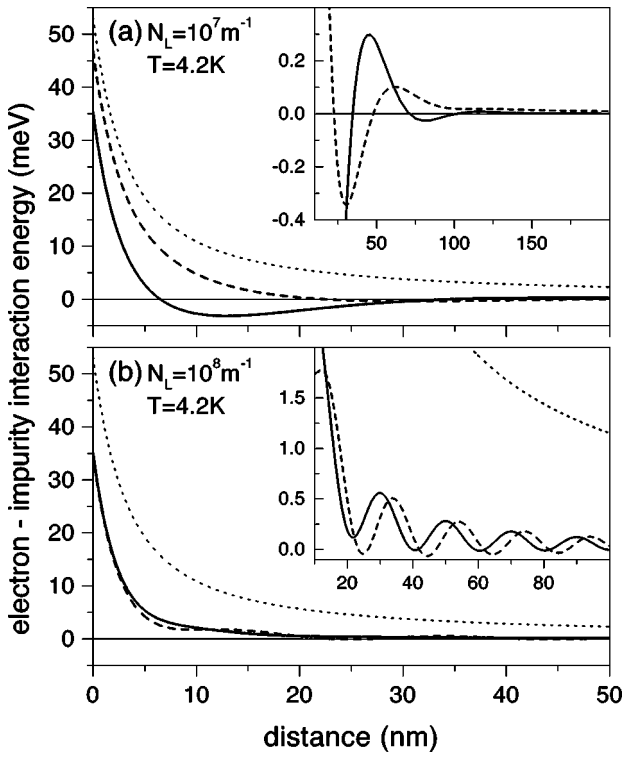

FIG. 1. Electron-impurity interaction energy versus electron-impurity distance (the inset shows the same on a different scale) for a repulsive impurity positioned in the center of the quantum wire. The electron density (N_L) and temperature (T) used in the calculations are indicated. The dotted line shows the unscreened interaction and the full line shows the interaction screened by the Lindhard polarizability. When multiplied by -1, both results hold for the attractive interaction. The dashed line shows the repulsive interaction screened by exact mean-field screening (see the text).

$$G_{11,11}(q)=\int dy_0 \int dz_0 |\Psi_{11}(y_0,z_0)|^2 G_{11}(q,y_0,z_0), \tag{8}$$

$$G_{11}(q,y_0,z_0)=\frac{e^2}{2\pi\epsilon_s}\int dy \int dz |\Psi_{11}(y,z)|^2 \times K_0[|q|\sqrt{(y-y_0)^2+(z-z_0)^2}] \tag{9}$$

is the unscreened interaction, $K_0[X]$ is the modified Bessel function, and ϵ_s is the material permittivity.

The full lines in Fig. 1 show $V(x-x_0,y_0,z_0)$ as a function of $|x-x_0|$, calculated by Fourier transforming Eq. (6) back into x space. The results are obtained for an impurity positioned at $y_0=z_0=0$. The inset to Fig. 1 shows the Friedel oscillations.

If the scattering is not weak, instead of using Eq. (3) one has to solve exactly the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x-0,y_0,z_0)\right]\Phi_k(x)=\frac{\hbar^2k^2}{2m}\Phi_k(x), \tag{10}$$

where $\Phi_k(x)$ is the scattered 1D wave function. For an electron arriving say from the left-hand side,

$$\Phi_k(x\to-\infty)=e^{ikx}+r_k e^{-ikx}, \tag{11a}$$

$$\Phi_k(x\to\infty)=t_k e^{ikx}, \tag{11b}$$

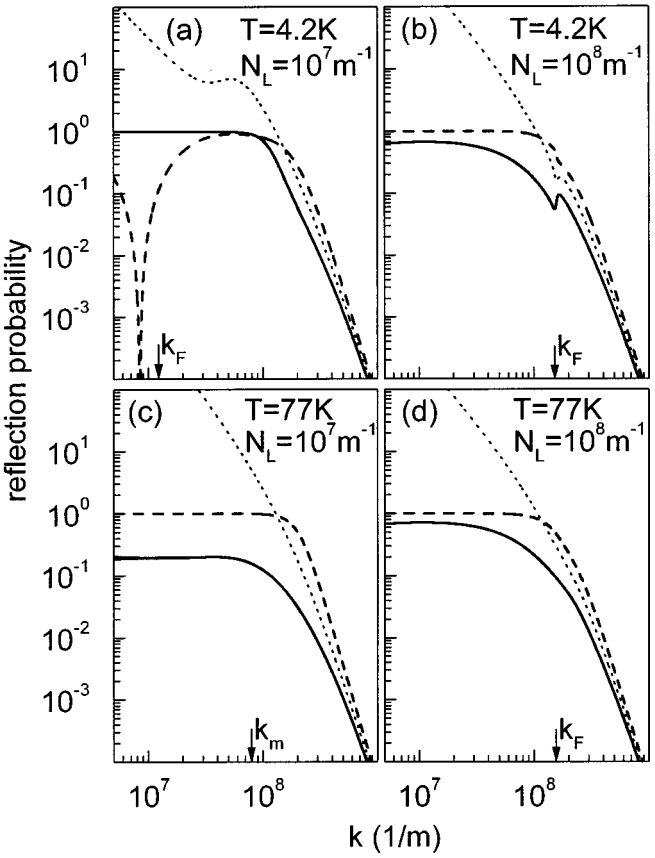

FIG. 2. Reflection probability versus electron wave vector at various temperatures (T) and electron densities (N_L). We assume that the impurity is positioned in the center of the quantum wire and the impurity potential is screened by the Lindhard polarizability. The exact reflection probability is shown in a full line for the attractive interaction and in a dashed line for the repulsive interaction. The Born result is shown in a dotted line. Arrows indicate the Fermi wave vector k_F or (if k_F is not defined) the mean-energy wave vector k_m.

where $R(k)=|r_k|^2$ and $T(k)=|t_k|^2$ are the reflection and transmission probabilities. To obtain exact $R(k)$, we solve (10) numerically with boundary conditions (11).

We want to compare the exact $R(k)$ with the $R(k)$ in Born approximation. In that approximation

$$\Phi_k(x)=e^{ikx}+\int_{-\infty}^{+\infty}dx'\frac{im}{\hbar^2k}e^{ik|x-x'|}V(x'-0,y_0,z_0)e^{ikx'}. \tag{12}$$

Comparing (12) at $x\to-\infty$ with the boundary condition (11a) one gets the Born reflection probability

$$R(k)=|r_k|^2=\frac{m^2}{\hbar^4k^2}|U(2k)|^2. \tag{13}$$

In Fig. 2 we compare the exact and Born reflection probabilities for an impurity screened by the Lindhard polarizability (see Fig. 1 for the impurity potential at 4.2 K). With decreasing k the Born probability exceeds unity and diverges for $k\to0$, which is obviously not physical. Clearly, the exact reflection probability does not exceed unity and, unlike the Born result, depends on the sign of the impurity potential.

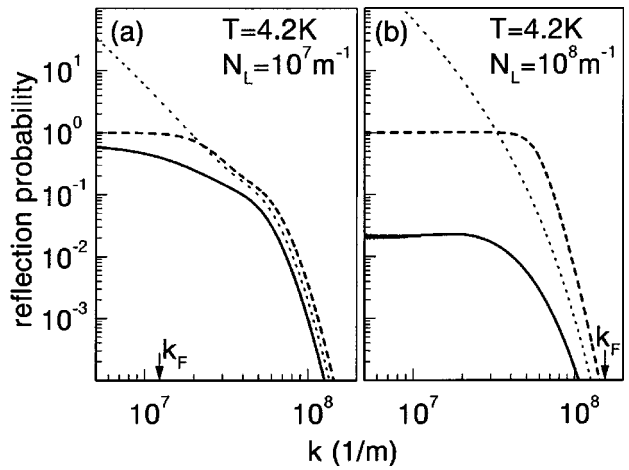

FIG. 3. The same as in Fig. 2, but for a ''remote'' impurity positioned at $x_0=y_0=0$, $z_0=17$ nm.

Only at very large k the Born result approaches the exact one. A small ''saddle'' at $k=k_F$, seen for $N_L=10^8$ m^{-1} and T=4.2 K, is due to the fact that in a degenerate 1D gas the Lindhard polarizability Eq. (7) is peaked at $q=2k_F$ (see Ref. 3 for details). For $N_L=10^7$ m^{-1} the saddle broadens since the degeneracy is weak.

At 4.2 K, a peculiar effect is seen for $N_L=10^7$ m^{-1} in case of the repulsive interaction. The exact $R(k)$ resonantly drops at k slightly below k_F, i.e., the electron resonantly tunnels through the repulsive impurity. The effect can be understood as follows. Figure 1 shows that for $N_L=10^7$ m^{-1} the Lindhard potential exhibits a small ($\sim$0.3 meV) peak about 50 nm apart from the 35-meV central peak. The potential is thus a triple barrier, which can be resonantly transparent for certain low-energy ($\sim$0.05 meV) electrons. No resonant tunneling is seen at 77 K, since the repulsive potential at 77 K (not shown in Fig. 1) does not exhibit Friedel oscillations.

Figure 3 shows the reflection probability for a ''remote'' impurity positioned at point $x_0=y_0=0$, $z_0=17$ nm, i.e., separated from the quantum wire by a 10-nm spacer layer. One sees again that the Born approximation fails except for very large k.

To see how the above findings affect the 1D mobility [Eq. (1)], we rewrite the relaxation time (2) through $R(k)$. Using (3) and (13) we get the equation

$$\frac{1}{\tau(k)}=2N_{\rm imp}\frac{\hbar|k|}{m}R(k), \tag{14}$$

which is more useful than Eq. (2). First, it uses $R(k)$ instead of $W(k,-k)$ and one cannot overlook the failure of the Born approximation [e.g., $R(k)>1$]. Second, the failure can be removed by using Eq. (14) with exact $R(k)$. Table I shows the 1D mobilities for $R(k)$ taken from Fig. 2, Table II shows the same for $R(k)$ from Fig. 3 (for comparative purpose we keep the same $N_{\rm imp}$ as in Table I; we recall that the impurities are distributed with a linear density $N_{\rm imp}$ on a line parallel to the wire axis). One sees that the mobility due to the ''Born'' reflections dramatically differs from the mobility due to the ''exact'' reflections, which additionally strongly depends on the sign of the impurity potential.

TABLE I. Electron mobilities (μ) for the reflection probabilities from Figs. 2(a)–2(d). $N_{\rm imp}=10^6$ m^{-1}. μ_B is the Born result, μ_A is the result for ''exact'' reflections from attractive impurities, and μ_R is the same for repulsive impurities.

	Figure 2(a)	Figure 2(b)	Figure 2(c)	Figure 2(d)
μ_B(m^2/Vs)	3.306	29.0	8.69	30.01
μ_A(m^2/Vs)	27.42	72.04	82.9	75.65
μ_R(m^2/Vs)	2.8×10^8	12.07	8.86	17.34

So far we have relied on the Lindhard screening [Eqs. (6) and (7)]. Now we argue that in a 1D system also the Lindhard screening can fail due to the Born approximation. In the mean-field theory, the impurity at point $\boldsymbol{r}_0$ induces at point x the 1D electron density

$$\rho(x,\boldsymbol{r}_0)=\int\frac{dk}{\pi}f(k)\{|\Phi_k(x)|^2-|e^{ikx}|^2\}, \tag{15}$$

where $\Phi_k(x)$ is given by Eq. (10). The integral form of the Poisson equation for the impurity potential reads

$$V(x-x_0,y_0,z_0)=\mp G_{11}(x-x_0,y_0,z_0)+\int_{-\infty}^{\infty}dx'\,G_{11,11}(x-x')\rho(x',\boldsymbol{r}_0), \tag{16}$$

where $G_{11}(x-x_0,y_0,z_0)$ is the Fourier transform of $G_{11}(q,y_0,z_0)$ and $G_{11,11}(x-x_0)$ is the Fourier transform of $G_{11,11}(q)$. To solve Eq. (16) self-consistently with Eq. (10), the Lindhard model takes $\Phi_k(x)$ in the Born approximation and linearizes $\rho(x,\boldsymbol{r}_0)$ with respect to $V(x-x_0,y_0,z_0)$, which results in Eqs. (6) and (7). We introduce the exact mean-field screening by solving Eqs. (16) and (10) numerically without any approximation.[5] Figure 1 shows such results (dashed lines) for a repulsive impurity[6] at $y_0=0$, $z_0=0$. They significantly differ from the ''Lindhard'' results especially at lower density. Figure 4 shows that for $N_L=10^7$ m^{-1} the exact screening modifies grossly also the reflection probability (e.g., the resonant tunneling below k_F is changed to the perfect reflection).

What remains for discussion is the applicability of the Boltzmann expressions (1) and (14). Let $R(k)=R$, where R is a constant. Equations (1) and (14) then give $\mu=(\pi\hbar RN_LN_{\rm imp}/e)^{-1}f(0)$. For $R=1$ this expression gives a nonzero μ while a correct mobility should be zero because each electron moves back and forth between two impurities. This means that Eqs. (1) and (14) fail to describe the semiclassical transport, if $R(k)$ is close to unity in the vicinity of k_F or k_m. Why is this so?

TABLE II. The same as in Table I, but for the reflection probabilities from Figs. 3(a) and 3(b).

	Figure 3(a)	Figure 3(b)
μ_B(m^2/Vs)	99.7	0.787×10^6
μ_A(m^2/Vs)	673.9	2.63×10^6
μ_R(m^2/Vs)	86.87	0.207×10^6

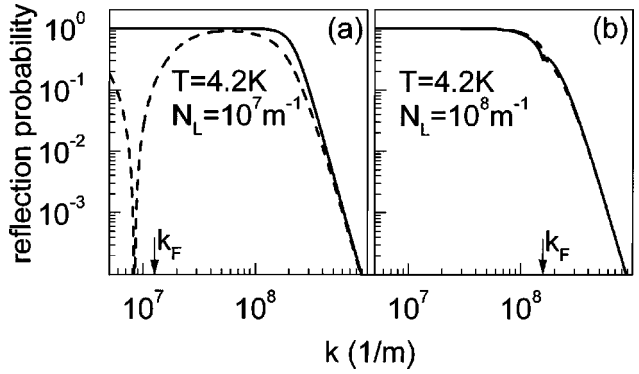

FIG. 4. Exact reflection probability for a repulsive impurity screened by exact mean-field screening (full lines). The corresponding results for the Lindhard screening (dashed lines) are taken from Figs. 2(a) and 2(b).

A general semiclassical description is provided by the following Monte Carlo simulation. The position (including the x coordinate) of each impurity is generated at random and the carriers move classically along the wire. When crossing the x position of an impurity, the carrier is reflected with probability $R(k)$ or transmitted with probability $1-R(k)$. We simulate the mean diffusion distance $(\overline{\Delta x^2})^{1/2}$ during time t, calculate the diffusion coefficient D, and obtain μ from the Einstein relation. For $R\rightarrow 1$ the Monte Carlo simulation gives the expected result $D\rightarrow 0$, $\mu\rightarrow 0$, because the electron is classically localized between two discrete impurities. This effect is not present in the Boltzmann equation, which uses the concept of impurity density rather than the concept of discrete impurities. For $R\leqslant 1/2$ the Monte Carlo simulation gives the same μ as the Boltzmann equation and justifies the latter approach. Details will be given elsewhere, here we give analytical proof for $R=1/2$ in a nondegenerate limit. For $R=1/2$ the diffusion in presence of discrete impurities can be viewed as a random walking with an average step $L=N_{\rm imp}^{-1}$. For N steps one has $\overline{\Delta x^2}=NL^2$, $t=NL/(\hbar|k|/m)$, and $D(k)=\overline{\Delta x^2}/t=L\hbar|k|/m$. Using $D=\langle D(k)\rangle$ and $\mu=eD/k_BT$ we get the result $\mu=(2e/N_{\rm imp})/\sqrt{2\pi m k_B T}$, which can also be obtained from Eqs. (1) and (14).

In summary, we have shown that the collision of a 1D electron with an impurity has to be treated exactly, not in the Born approximation. We have also shown that the exact treatment of the collision needs to be coupled with the exact mean-field screening of the impurity, because the linearized mean-field theory is too inaccurate (except for high electron densities). Finally, the failure of the Boltzmann 1D transport has been demonstrated for $R(k)\rightarrow 1$ and a general semiclassical approach based on the concept of discrete impurities has been proposed. This paper evaluates the above effects for the (often used[1,3]) single-subband model and for impurities positioned on a line. However, there is no good reason why these effects should not be equally important in a realistic impurity distribution (their quantitative impact is simply too huge) or in higher subbands[2] (we see similar effects if we consider just the first excited subband).

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[4] At low temperatures there are two phase-breaking processes in GaAs quantum wires, the acoustic phonon scattering and the electron-electron scattering. In a ''single-subband'' wire the latter process is inelastic due to many-electron collisions [Yu. Sirenko *et al.*, Phys. Rev. B **50**, 4631 (1994); M. Moško and V. Cambel, *ibid.* **50**, 8864 (1994)].

[5] We use the iterative technique similar to the Schrödinger/Poisson solver for inversion Si layers [see p. 463 in T. Ando *et al.*, Rev. Mod. Phys. **54**, 437 (1982)].

[6] The attractive impurity case is complicated by the bound electron states and will be treated elsewhere.