Self-consistent calculation of ionized impurity scattering in semiconductor quantum wires

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We calculate the electron elastic mean free path due to ionized impurity scattering in semiconductor quantum wires, using a scheme in which the screened ionized impurity potential and the electron screening self-consistently determine each other. By using a short-range-scattering potential model, we obtain an *exact* solution of the self-energy within the self-consistent Born and "noncrossing" approximations. We find that, compared to the mean free path for the bare unscreened potential $\ell_{\rm bare}$, the calculated mean free path including self-consistent screening $\ell_{\rm sc}$ is *substantially larger*, going as $\ell_{\rm sc} \sim \ell_{\rm bare}[\ln(\ell_{\rm bare})]^2$ for large $\ell_{\rm bare}$.

Advances in nanofabrication technology now make it possible to fabricate semiconductor quantum wires in which the motion of the electrons is confined to be in one spatial direction. Quantum wires have the potential for many microelectronics applications, such as novel optoelectronic devices and transistors, and many experiments probing the electronic properties of these quantum wires have been performed.[1] It is, of course, experimentally desirable to make these wires as clean as possible. However, to populate the wires with carriers, it is necessary to place ionized dopants close to the wire, and these dopants scatter the free carriers in the wire. Thus, elastic impurity scattering cannot be avoided in conducting quantum wires. A quantitative understanding of ionized impurity scattering in quantum wires is thus important from both technological and fundamental viewpoints.

Sakaki[2] made the striking prediction that in quantum wires that are remotely doped, the electrons should have extremely high mobilities because elastic ionized impurity scattering for Fermi surface electrons is greatly suppressed. This is due to the fact that at low temperatures, the only allowed resistive scattering in a one-dimensional system is the $2k_F$ scattering. However, in Sakaki's calculation, and in some subsequent calculations by others,[3] the interaction between the ionized donors and the conduction electrons was assumed to be the *bare* unscreened Coulomb potential. This ignores screening effects of the electrons in the quantum wire. In this paper, we show, using many-body techniques, that the inclusion of screening effects in the wire *substantially enhances* the mean free path of electrons at the Fermi surface. The mean free path for electrons at the Fermi surface is particularly important because this is the quantity which determines the low field transport properties in these structures. Furthermore, it has been shown that the mean free path and the localization length of electrons in strictly one-dimensional systems are essentially equivalent,[4] and thus the mean free path of electrons is the maximum length over which a quantum wire can be considered metallic. This gives added impetus for an accurate calculation of the electronic mean free path in quantum wires.

The simplest approximation taking screening into account is one which assumes that disorder has no effect on the screening properties of the one-dimensional electron gas.[5] Unfortunately, in the $T = 0$ limit, this approximation gives meaningless results for the mean free path of electrons at the Fermi surface, for the following reason. At the Fermi surface, the only elastic scattering that can occur is the transfer of electrons from one side of the Fermi surface to the other, with momentum transfer of $2k_F$. To the lowest order, this depends on the $2k_F$ component of the screened impurity potential. However, as is well known, the $2k_F$ screening at $T = 0$ in a pure one-dimensional wire is *perfect* (i.e., the $2k_F$ screening diverges), and hence within this approximation, the scattering rate at the Fermi surface is always zero for any impurity concentration. Clearly one needs a better (and more physical) approximation.

The key point is that disorder affects screening which will no longer be perfect at $2k_F$ in the presence of impurities. The extent to which screening in the presence of scattering is modified from the pure wire case depends on the strength of the disorder created by the ionized impurities, but the strength of disorder in turn depends on the strength of screening. Thus, we are faced with a problem in which both the scattering potential and the screening properties self-consistently determine each other. In this paper, we carry out this self-consistent scheme in one-dimensional wires, which has been previously applied to two-dimensional systems in a large magnetic field,[6] but to the best of our knowledge, has not yet been applied to one-dimensional systems.

In our model, we assume that (1) the electrons are confined to a one-dimensional quantum wire in the strip geometry with a finite width w in infinite square well confinement and (2) the ionized donors are placed randomly along a line a distance d away from the wire. (One could quite easily use a distribution of distances d to simulate a more realistic configuration of impurities, but we find the quantitative effect of doing so is small.) The set of equations which must be solved for this calculation is shown schematically in Fig. 1. For a given screened impurity potential, the Green's function is computed. In this paper, we employ both the Born approximation and what we denote the "noncrossing approximation," which excludes all diagrams that have impurity lines crossing

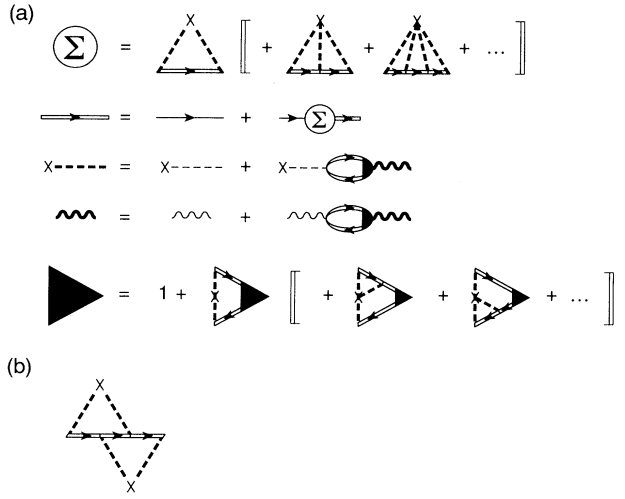

FIG. 1. (a) Set of diagrams which are solved to calculate the electron Green's function in the self-consistent Born approximation (excluding diagrams in parentheses) and noncrossing approximation (including diagrams in parentheses). The thin (thick) dashed (wavy) lines are the bare (dressed) electron-impurity (electron-electron) interactions. The screened electron-impurity interaction and the Green's function are numerically iterated until self-consistency is obtained. (b) Second-order contribution to self-energy, which we ignore in the self-consistent loop.

one another. (In fact, as we show below, for experimentally relevant parameters we find that Born and noncrossing approximations give essentially indistinguishable results.) Then, with these Green's function, one computes the polarizability, including the ladder vertex corrections (which are necessary to satisfy the Ward identities and ensure, *inter alia*, that particles are conserved). This gives the dielectric function,[7] which is used to screen the disordered impurity potential, yielding a new screened impurity potential. This loop is iterated until convergence is complete.

The actual bare electron-impurity interaction should of course be the long-ranged Coulomb interaction, and ideally, the exact interaction should be used in the calculation, but the numerical task in performing the iteration to self-consistency is formidable. Therefore, as a first attempt, we find it expedient to approximate the screened interaction to be of the short-ranged form $U_0\,\delta(x-x_0)$ (i.e., a constant in momentum space). This approximation is valid because the actual screened interaction in quantum wires is short ranged due to screening by the conduction electrons. Our primary motivation in using the short-range scattering potential model is that we are able to obtain physically meaningful analytical results whereas the Coulomb case is necessarily completely numerical in the self-consistent scheme.

The short-ranged impurity potential approximation yields simple expressions, both in the Born and noncrossing approximations, for the self-energy Σ and the static random phase approximation (RPA) polarizability $\Pi(q)$ with vertex corrections.[7,8] For both approximations, the self-energy is k independent and is given, for arbitrary temperature, by [in this and subsequent equations, to obtain the result for the Born (noncrossing) approximation, the terms within $[\![\ ]\!]$ should be excluded (included)]

$$\Sigma(\omega) = N_i U_0^2 \int_{-\infty}^{\infty} \frac{dq}{2\pi}\, G(q,\omega) \times \left[\!\!\left[+N_i U_0 \sum_{n=2}^{\infty} \left\{ U_0 \int_{-\infty}^{\infty} \frac{dq}{2\pi} G(q,\omega) \right\}^n \right]\!\!\right],$$

$$G(q,\omega) = \frac{1}{\hbar\omega - \xi_q - \Sigma(\omega)}. \tag{1}$$

Here N_i is the impurity concentration, m is the band electron mass, and $\xi_q = \hbar^2 q^2/(2m) - \mu$, where μ is the chemical potential (which is computed self-consistently). This implies that $\Sigma(z)$ can be obtained from the following cubic equation:

$$(x^2 + \mu + \hbar\omega)\left(x\left[\!\!\left[-\frac{U_0 k_F}{2} \right]\!\!\right]\right) - \frac{\hbar\gamma}{2} = 0, \qquad \Sigma = x^2 + \hbar\omega + \mu, \tag{2}$$

where $\gamma = 2N_i U_0^2 m/(\hbar^3 k_F)$ is the Born approximation scattering rate for electrons at the Fermi surface. The proper choice for the correct solution from the three roots of Eq. (2) is dictated by the requirement that $\mathrm{Im}[\Sigma(\omega)] \lesseqgtr 0$ for $\mathrm{Im}[\omega] \gtreqless 0$. In Fig. 2, we show the self-energy for both approximations with $\hbar\gamma/E_F = 0.5$. Note that the magnitude of $\mathrm{Im}[\Sigma(\omega)]$ is *smaller* in the noncrossing approximation than in the Born approximation, because the Born approximation overestimates the scattering of a particle from a δ-function potential.

The static RPA polarizability with the ladder vertex corrections (Fig. 1) in a one-dimensional electron gas is found to be

$$\Pi(q) = 2k_F k_B T \sum_{i\nu_n} \left\{ E_F^{1/2} \sqrt{\Sigma(i\nu_n) - i\hbar\nu_n - \mu}\, \left(\frac{\hbar^2 q^2}{2m} + 4\{\Sigma(i\nu_n) - i\hbar\nu_n - \mu\} \right) \right.$$

$$\left. -\hbar\gamma E_F \left[\!\!\left[\times \{1 + N_i^{-1} U_0^{-1} \Sigma(i\nu_n)\} \right]\!\!\right] \right\}^{-1}, \tag{3}$$

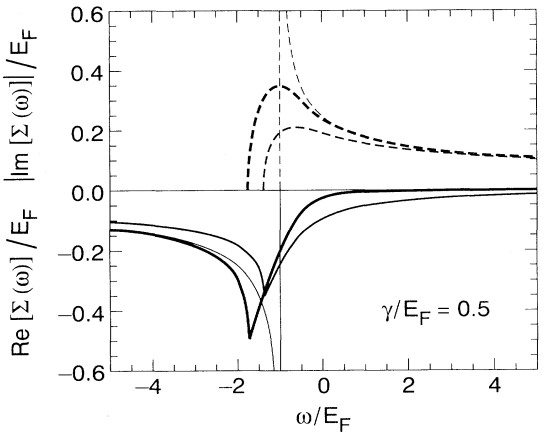

FIG. 2. Real (solid lines) and imaginary (broken lines) parts of the electron self-energies for impurity scattering, as a function of frequency, for $\hbar\gamma/E_F = 0.5$, in the self-consistent Born (thick bold lines) and noncrossing (medium bold lines) approximations. For comparison, we also show the Σ for the non-self-consistent Born approximation (thin lines), in which the bare (instead of dressed) Green's function is used.

where the summation is over the "fermion frequencies" $i\hbar\nu_n = (2n+1)\pi k_B T$. While the above equations are valid for finite temperature, henceforth, we specialize to the case of $T = 0$, where the effects of self-consistent screening are most pronounced. In Fig. 3, we show the calculated $\Pi(q)$ for various values of the strength of disorder in both the Born and noncrossing approximations. The suppression of the Kohn anomaly in $\Pi(q = 2k_F)$ is larger in the Born approximation than in the noncrossing approximation, which is consistent with the fact that the Born approximation overestimates scattering.

We incorporate the δ-function screened potential approximation into our iteration scheme by adjusting the potential strength U_0 at each iteration to match the Born approximation scattering rate at the Fermi surface. The self-consistent scattering rate γ_{sc} is calculated as follows. For a set of parameters (doping density, etc.), we pick an initial U_0 to match the scattering rate of the bare Coulomb interaction at the Fermi surface. The polarizability is then calculated for that U_0 (for both the separate cases of the Born and noncrossing approximations). This allows us to recalculate the scattering rate for the screened Coulomb potential at the Fermi surface. The U_0 is then adjusted to reproduce this scattering rate, and the polarizability is recomputed. This procedure is repeated until convergence is complete, which typically takes 10–50 iterations. The chemical potential is also adjusted to ensure that the density of electrons is constant, as shown in the inset of Fig. 3.

The results are shown in the Fig. 4, for the wire density $n = 10^6\,\mathrm{cm}^{-1}$ and wire width $w = 100\,\text{Å}$. We show the mean free path $\ell = v_F/\gamma$, for both the bare and the self-consistently screened Coulomb interactions with both approximations, as a function of the distance d of the impurities from the wire. The mean free path for the bare Coulomb interaction ℓ_{bare} is a reproduction of Sakaki's result[2] generalized to take into account the finite width of the wire. As can be seen from Fig. 4, both Born and noncrossing approximations give essentially indistinguishable results for self-consistently screened mean free paths ℓ_{sc}, indicating that multiple

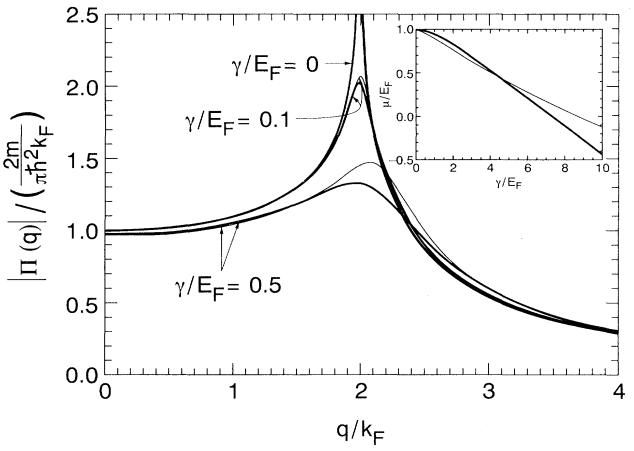

FIG. 3. Static one-dimensional polarizabilities $\Pi(q)$ within the RPA with short-ranged impurities (including vertex corrections) at $T = 0$ for $\hbar\gamma/E_F = 0, 0.1, 0.5$. The bold lines are for the self-consistent Born approximation and the thin lines are for the noncrossing approximation. There is a larger suppression of the $2k_F$ peak in the Born approximation as compared to the noncrossing approximation, due to the fact that the Born approximation overestimates the scattering. The inset shows the chemical potential as a function of disorder in both approximations.

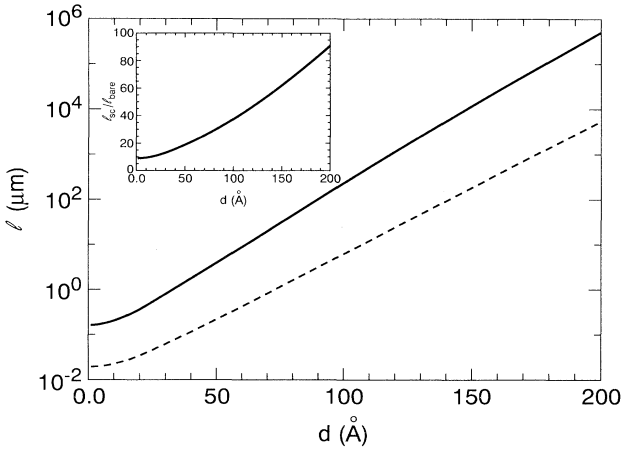

FIG. 4. Elastic mean free paths ℓ as a function of distance of charged impurities d from a quantum wire. The parameters used were for GaAs, with an electron density of $10^6\,\mathrm{cm}^{-1}$ and a wire width of 100 Å. The solid line is for the self-consistently screened potentials and the broken line is for the bare Coulomb interaction. On this plot, the result for noncrossing approximation is essentially indistinguishable from that of the self-consistent Born approximation. In the inset, we show the ratio of the self-consistently screened to bare mean free paths, as a function of d.

scatterings from the same impurity do not play an important role in the transport properties of these systems. Also note that the self-consistently calculated mean free paths are significantly longer than the unscreened mean free paths. The large enhancement is a result of the Kohn anomaly in $\Pi(q = 2k_F)$ (see Fig. 3), which diverges logarithmically as the scattering goes to zero. Thus, the self-consistent scattering rate γ_{sc}, in the limit where the bare scattering rate γ_{bare} is small, goes as $\gamma_{sc} = \gamma_{bare}/|\epsilon(2k_F)|^2 \sim \gamma_{bare}/|\ln(\gamma_{sc})|^2$, which implies that the self-consistent mean free path should go (to lowest order) as $\ell_{sc} \sim \ell_{bare}\,|\ln(\ell_{bare})|^2$. We have explicitly verified this asymptotic behavior in our numerical calculation.

This result seems to indicate that semiconductor quantum wires will be very good conductors, and will be metallic over very large length scales, because the elastic mean free path is essentially a measure of the localization length in one-dimensional systems. Experimentally, however, the opposite seems to be true. Attempts to fabricate quantum wires using electrostatic confinement with a split gate generally fail if the length of the wire is more than a few micrometers,[9] and it has been theoretically shown[10] that these wires tend to become disjointed before single channel occupation is achieved. The reason for this extreme sensitivity to impurities in the electrostatically confined wires is that the confinement potential is very shallow,[11] and therefore perturbations due to ionized impurities have a very large effect. However, recently, wires of GaAs in $Al_xGa_{1-x}As$ have been fabricated,[12] where the confinement potential is much stronger, and these wires are more robust against the effects of the ionized dopant potential. These wires should show dramatically long mean free paths at the Fermi surface, as calculated in this paper. Our theory is only applicable to the situation with weak disorder, where $\hbar\gamma/E_F \lesssim 1$.

Before concluding, we discuss the validity of our assumptions and approximations, and possible extensions of this calculation. It is natural to ask if multiple scattering diagrams we have left out of our self-consistent iteration scheme, such as the one shown in Fig. 1(b), are important. We have evaluated this diagram explicitly, assuming a δ-function interaction, and a k-independent self-energy in the Green's function, and we obtain

$$\Sigma_2(k,\omega) = \frac{3E_F}{4}\,\frac{(\hbar\gamma)^2}{[\hbar\omega + \mu - \Sigma(\omega)]\{\hbar^2k^2/(2m) - 9[\hbar\omega + \mu - \Sigma(\omega)]\}}. \tag{4}$$

Comparing Eqs. (2) and (4), one can see that Σ_2 is smaller by a factor of $\hbar\gamma/E_F$ than the Born and noncrossing approximation Σ's, and therefore since $\hbar\gamma/E_F < 0.1$ in our self-consistent calculation, Σ_2 makes a negligible contribution. We find that the results for the calculated self-consistently screened mean free paths are relatively insensitive to the criterion used for the adjustment of U_0 to match the actual screened Coulomb interaction. However, it is probable that the scheme we have used somewhat overestimates the effect of self-consistent screening, since we are looking at the scattering rates where the effect of screening is the strongest (i.e., at the Fermi surface). On the other hand, we have neglected the effect of electron-electron vertex corrections in the polarizability, which have been shown to *increase* the divergence at $2k_F$.[13] To extract the true scattering rate, one must use the actual Coulomb interaction for the bare electron–ionized-impurity interaction. This considerably complicates the iteration task, due to the lack of any analytic results and the strong k dependence of the self-energy, and work on this is currently in progress. We expect our short-ranged results to be at least semiquantitatively valid. The issue of the applicability of Fermi liquid theory to disordered interacting one-dimensional systems is complicated and has been discussed previously.[14] Finally, we note that our calculation can easily be extended to include effects of finite temperature and occupancy of several subbands. The finite temperature will serve to cut off the $2k_F$ divergence of screening, and therefore the maximum polarizability at $2k_F$ will be on the order of $\ln[\max\{k_BT, \hbar\gamma\}]$.

To conclude, using a self-consistent screening scheme, we have calculated the elastic mean free path of electrons in a quantum wire which are scattered by remote ionized impurities. We have shown that the mean free paths of electrons at the Fermi surface is significantly enhanced by the self-consistent screening. The calculated mean free paths provide a direct measure of the length scale over which the electrons in quantum wires are expected to exhibit metallic behavior due to the peculiarity of Anderson localization in one-dimensional disordered systems.

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