Electron-correlation effects in the impurity conductance of doped-semiconductor quantum wires

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The effect of electron correlations in the impurity conductance of the shallow-donor impurity band in a semiconductor quantum wire, connected by two ideal leads, is studied by using the Hubbard model in an alloy-analogy approximation. The hopping integral and the intrasite Coulomb interaction energy are estimated numerically from variational wave functions for random impurity configurations. For one electron per impurity, it is shown that there is a considerable reduction in the impurity conduction due to electron correlations. For a given impurity concentration, the disordered wire turns into an insulator at a much shorter sample length than that estimated previously by neglecting correlations.

Fowler *et al.*[1] reported measurements of the near-threshold conductance of a very small metal-oxide-semiconductor structure as a function of carrier concentration at very low temperatures. The conductance was shown to be characterized by strong fluctuations. The observed temperature dependence of the peaks supports the mechanism of resonant tunneling through localized states.[1,2] The states are supposed to be localized around impurities and other defects. Recently, two of us (J.F.W. and E.A.A.S.) (Ref. 3) have investigated, numerically, the zero-temperature conductance of a $GaAs/Ga_xAl_{1-x}As$ channel as a function of the Fermi-energy location within the shallow-donor impurity band, which is separated from the conduction band. In the low-impurity concentration regime, the simulation of this quantum wire, described by a finite one-dimensional disordered tight-binding model, showed peaks similar to those observed experimentally.[1,3] The location of the peaks as a function of Fermi energy (or carrier concentration) varies randomly from sample to sample. They constitute a mesoscopic signal of the actual impurity configuration of the sample. Electron correlations, however, have been neglected in this first study. Because of reduced dimensionality of these semiconductor structures, electron correlations are expected to play a greater role as compared to the effects in bulk semiconductor.

In this work, we consider the effects of electron correlation in the impurity conductance of a semiconductor quantum wire, by regarding this system as a disordered finite Hubbard chain. The intrasite Coulomb repulsion of this Hubbard model is calculated using a variational solution for the electron state bound to shallow donors in quantum wires of different widths. The electron transmission through the Hubbard chain is studied within a simple approximation in which the opposite-spin electrons are treated as quenched site disorder in addition to the underlying hopping disorder. The amount of site disorder is directly related to the intrasite Coulomb repulsion. The results are compared to the electron transmission obtained in the absence of Coulomb interaction. Within this approximation, electron-correlation effects are found to reduce considerably the zero-temperature impurity conductance of small semiconductor quantum wires in an experimentally relevant range of wire widths and impurity concentrations.

Recently, Meir, Wingreen, and Lee[4] have treated the problem of transport through a quantum dot with strong electron correlations, by studying the Anderson model[5] of a single impurity weakly coupled to ideal leads with an on-site Coulomb correlation. Within this model, they were able to explain the anomalous temperature dependence of conductance peaks observed experimentally. In this work, we consider a more complicated problem and study the quantum transport of the shallow-donor impurity band in a semiconductor wire including electron correlations. Here one has to deal with electron-correlation effects in many impurities randomly distributed in a finite semiconductor wire, connected by two ideal leads on both sides. To take electron correlation into account, we extend the tight-binding model studied previously[3] to the Hubbard model described by the Hamiltonian[6]

$$H = E_o \sum_{i\sigma} n_{i,\sigma} + \sum_{i,j,\sigma} V_{ij} a^{\dagger}_{i,\sigma} a_{j,\sigma} + U \sum_{i} n_{i,\sigma} n_{i,-\sigma}, \quad (1)$$

where $a^{\dagger}_{i\sigma}$ and $a_{i\sigma}$ are the creation and annihilation operators of an electron of spin σ at the randomly located impurity site $\mathbf{R}_i$ with energy E_o and $n_{i,\sigma}$ is its number operator. Following Ref. 3, the hopping integral

$$V_{ij} = V(Z = |Z_i - Z_j|) = \int d\mathbf{r}\, \psi^*(\mathbf{r} - Z\hat{\mathbf{z}}) \left(-\frac{e^2}{Kr}\right) \psi(\mathbf{r}), \quad (2)$$

and the intrasite Coulomb interaction energy

$$U = \int d\mathbf{r}_1 d\mathbf{r}_2 |\psi(\mathbf{r}_1)|^2 |\psi(\mathbf{r}_2)|^2 \frac{e^2}{K|\mathbf{r}_1 - \mathbf{r}_2|} \quad (3)$$

are calculated using a variational solution for the bound-state wave function $\psi(\mathbf{r}-\mathbf{R}_i) = \langle \mathbf{r}|i\rangle$. In the above equations, K is the dielectric constant and Z is the separation between the impurities along the wire axis. Here and hereafter we neglect the hopping integral between the second and higher neighbors impurities. It should be noted that the intrasite Coulomb interaction depends only on the geometry of the confining potential.

Figure 1 shows the calculated U for a square wire as a function of its side or wire width W. In the infinite barrier approximation we use, the trial bound wave function reads

$$\psi(\mathbf{r}) = N\cos\left(\frac{\pi x}{W}\right)\cos\left(\frac{\pi y}{W}\right)e^{-\alpha r^2}, \tag{4}$$

where N is the normalization constant and α is the variational parameter. One can see a strong increase in the correlation energy as the wire width is reduced. It approaches the value corresponding to the bulk for wires of cross-section area of the order of $8a_0^* \times 8a_0^*$ (a_0^* is the effective Bohr radius).

In an infinite one-dimensional ordered chain, the Hubbard model has been solved exactly[7] and it has been found that, for one electron per site, the system behaves like an insulator for all values of U. One would expect no electron transmission probability for such an infinite system. However, because the localization length is finite[8] for finite U, the transmission probability can be nonzero for a sufficiently small chain. In this paper we are particularly interested in determining this crossover to finite electron transmission, since it leads to a critical length for metallic behavior. For a finite one-dimensional disordered Hubbard model, described by Eq. (1), exact solutions are not available and one has to resort to some approximation. Here we solve this model by using the alloy analogy,[9] which has the advantage of reducing the problem into an effective disordered one-body tight-binding model that can be treated as before.[3] In the alloy analogy it is assumed that, for the motion of an electron of spin σ, the $-\sigma$ spin electron can be regarded as frozen at the particular sites in a random configuration. In other words, a σ electron can be thought of as moving in an alloy composed of sites of two types. On the sites occupied by $-\sigma$ electrons, it will experience a potential equal to $U + E_o$ with occupation probability $n_{-\sigma}$ and on the empty sites, there will be a potential equal to E_o with occupation probability $1 - n_{-\sigma}$. Here $n_{-\sigma}$ is the average number of $-\sigma$ electrons per site. In a system of randomly distributed paramagnetic impurities with one donor electron, this alloy analogy replaces the Hubbard Hamiltonian (1) by the one-body Hamiltonian

$$H = \sum_i |i\rangle E_i\langle i| + \sum_{i\neq j} V_{ij}|i\rangle\langle j|, \tag{5}$$

where the site energies E_i are distributed randomly with two values E_o and E_o+U with probability $\frac{1}{2}$. It should be noted that for a paramagnetic system with one electron per site $n_{-\sigma} = n_\sigma = 1 - n_{-\sigma} = \frac{1}{2}$.

For an infinite disordered chain described by the Hamiltonian (5), all states are localized.[10] Thus the system behaves as an insulator consistent with the exact results of the one-dimensional ordered Hubbard model.[7] Thus, for our purpose, the alloy analogy can be considered a good approximation to the Hubbard model in Eq. (1). To go beyond the present approximation one has to take into account the effect of the motion of $-\sigma$ electrons on the propagation of a σ electron. As far as the σ spin electrons are concerned, the motion of $-\sigma$ spin electrons is such that a given site energy resonates between E_o and E_o+U. The effect of this resonance is to broaden the two-site energy which in turn can increase the transmission probability. This effect, known as resonance broadening corrections,[9] is complicated to be taken into account. Therefore for the mathematical simplicity we ignore this effect here.

The transmission probability is now obtained with the method described in Ref. 3. In this method a decimation procedure exists that reduces the finite portion of the alloy chain to just two sites connected through an energy-dependent effective interaction. In this decimation or renormalization technique, sites can be removed from the lattice many, or one at a time, leaving invariant the form of the tight-binding equations. We call the final site energies at the left and right E_L and E_R, respectively, and the effective hopping V_{eff}. In order to calculate the electron transmission, we connect at the left and right of this effective portion uncorrelated semi-infinite perfect linear chains. Along the lead, on the left, we assume an incident Bloch wave e^{ikla}, plus a reflected part re^{-ikla}, and on the right a transmitted wave te^{ikla}. Here a is the nearest-neighbor distance of the uniform impurity distribution ($a = n_i^{-1}$, where n_i is the linear impurity concentration), l denotes the impurity position, k is the electron wave vector, r is the reflection coefficient, and t is the transmission coefficient. The wave vector k is such that the incident wave vector has energy $E = -2V\cos(ka)$, so that we can probe the energy interval $[-2V, 2V]$ of the impurity band [$V = V(a)$—note, it

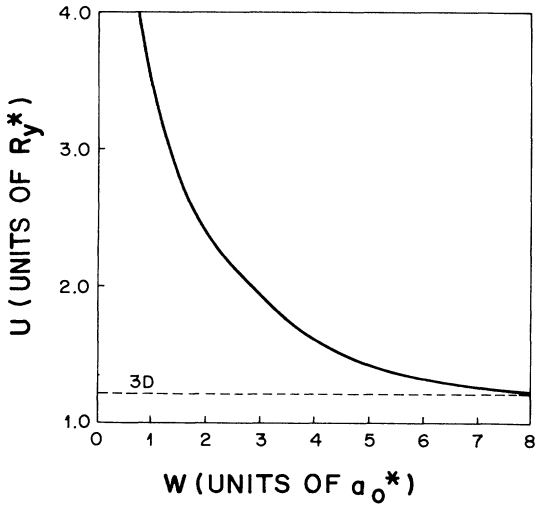

FIG. 1. Intrasite correlation energy U as a function of the width of the square wire W, as given by Eq. (3). Effective atomic units are used and the value for the bulk semiconductor is assigned.

depends on the impurity concentration]. We match the probability amplitudes at the right and left of the finite correlated chain with the Bloch waves, and the two tight-binding equations at E_L and E_R give two equations with two unknowns for r and t. Finally we calculate the transmission coefficient $T = tt^*$. If the entire chain were ordered (no correlation or disorder), we would obtain $T = 1$ for all energies in the above interval.

To measure the effects of the electron correlations we compare in Fig. 2 the critical length, for which the average transmission probability becomes less than 10^{-4}, for a given impurity concentration, when calculated with and without correlation. This critical length can be taken as a measure of the localization length for the infinite quantum wire. The calculation is done by taking the average over impurity configurations as well as the average over the site energies for each configuration in the presence of correlations. The results are shown in atomic units for two wire widths. Typically, 100 realizations were used in each average procedure. Note that the transmission goes bellow 10^{-4} much sooner with correlation as one increases the sample length L with a fixed impurity concentration. One concludes from Fig. 2 that the additional effective site disorder due to the electron-electron correlation reduces significantly the critical length, or alternatively the localization length, of such chains; the reason being that the amount of effective site disorder U, as shown in Fig. 1 and the average hopping energy (see Fig. 1 of Ref. 3), are both of the same order of magnitude (few effective Rydbergs) in this range of wire width and impurity concentration. When the wire width is reduced, further decrease in impurity conductance is observed due to the stronger confinement and smaller hopping between impurity sites.

In summary, we have investigated the effects of electron correlations in the shallow-donor impurity band in a semiconductor quantum wire. A Hubbard model was used in order to access semiquantitatively the effects of electron correlations on the critical sample length for metallic behavior studied previously. The hopping integral and the intrasite Coulomb interaction parameter were estimated numerically and the alloy analogy approximation was used to solve the model approximately. It was shown that electron-correlation effects reduce considerably the average impurity conductance and the critical length, in the case of a half-filled band or one electron per donor.

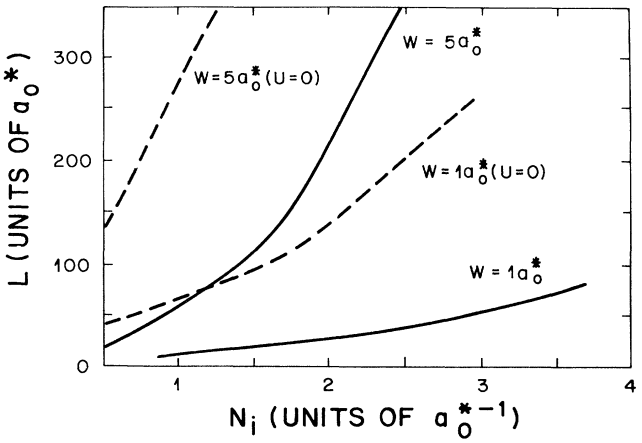

FIG. 2. Critical sample length L for metallic behavior as a function of the impurity concentration n_i, for wires of $5a_0^* \times 5a_0^*$ and $1a_0^* \times 1a_0^*$, with (continuous lines) and without (dashed lines) electron correlations. L can be regarded as a measure of the localization length of the infinite system. The curves give a critical length above which the average electron transmission is negligible (see text) and a metal-to-insulator crossover.

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