Electron transmission through the impurity band of a mesoscopic semiconductor quantum wire

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The overlap between the states of electrons bound to different shallow impurities randomly distributed along the center of a semiconductor quantum wire leads to an impurity band. The $T=0$ electron transmission probability through such a band is calculated for a finite length of this disordered quantum channel sandwiched between perfect conductors. For comparison, a density-of-states calculation is made for the finite portion of disordered wire. It is found that transmission probability, in the region of the impurity band, increases both with increasing concentration of donors and decreasing confinement, and decreases with increasing length. It exhibits typical conductance fluctuations, which are also studied as a function of concentration and the length and width of the confining well. In the metallic regime of large concentrations, the fluctuations become independent of impurity concentration and sample length, as the universal conductance fluctuations. It can be thought that a somewhat poorly defined metal-insulator crossover takes place with increasing concentration, for a given fixed length of the quantum wire. We estimate, for example, that a 300×300 Å^2 wire of GaAs doped with 0.5×10^{18} Si atoms/cm^3 should show no impurity conductance when longer than 0.4 μm.

INTRODUCTION

The possibility to confine electrons spatially in a controlled way with semiconductor heterostructures has been responsible for important developments in both basic and applied physics. Two-dimensional electron gas at semiconductor interfaces forms the basis of most of today's electronic devices and allowed the discovery of phenomena like the quantum Hall effect and weak localization. With different techniques, one can further confine the electrons and make a quantum wire;[1,2] a structure in which the electrons are confined in two spatial dimensions and free to move along the third. Much attention has been given recently to the quantum transport in these systems. The actual samples are in general either intentionally or unintentionally doped with shallow impurities, which introduce disorder and drastically affect the electronic transport.

Depending on the density of impurities and on the size of the sample, the bound states can form a band with both localized and delocalized states, which have, respectively, localization length smaller and larger than the size of the sample.[3] For a given energy in this impurity band, corresponding initially to a delocalized state, an Anderson-type metal-insulator crossover is expected to occur by either increasing the size of the sample or decreasing the impurity concentration. In order to understand such a crossover we have investigated how the energy-dependent conductance, proportional to the transmission probability T as given by the two-terminal conductance equation[4] $G=(e^2/h)T$, in the impurity band of these quasi-one-dimensional systems, depends on the size of the sample, on the impurity concentration, and on the degree of confinement. The independent electron approximation is used.

Notice that this is not a phase transition since it depends on the size of the sample. It is well known that an infinite one-dimensional disordered system is always an insulator. According to the scaling theory of localization, a metal-insulator phase transition can only occur in three dimensions.[5,6] We show here that, in these quantum wires, the size-induced metal-insulator crossover in the impurity band is not abrupt nor well defined. For a small number of impurities (small sample and impurity concentration), we obtain smooth transmission spectra, which are highly dependent on the impurity configuration. And on the other hand, for larger samples and impurity concentration, we observe large fluctuations in the transmission probability. The crossover, in this case, is of a mesoscopic character.

The study of conductance fluctuations has been extensive since their observation in small metallic samples.[7,8] The theory has been developed mainly for metallic samples in the weakly localized regime, using the more usual models of disorder.[9–12] In our case, by changing the impurity concentration, we can go from the strictly localized to the metallic regime, passing through the metal-insulator crossover. It is only in the limit of large concentrations that we find conductance fluctuations which are independent of sample length and concentration, as the universal conductance fluctuations.[9–12]

For sufficient long or dilute systems the transmission is obviously zero and it approaches one in the opposite limit. For different concentrations, we estimate the critical sample length, beyond which there is no impurity conductance.

It is also interesting to notice that, due to a much larger binding energy for the bound electrons, the impurity band in these quasi-one-dimensional systems is much more separated from the conduction (sub)band than in the bulk.[13] Although some recent evidence for a metal-insulator transition in the impurity band exists, the question of whether this transition in the bulk occurs at the impurity band or on the conduction-band tail, with the

impurity band already merged, is still open.[14] In this work, we study the crossover occurring in the impurity band of a quantum wire.

We first present the model for an impurity band in a semiconductor quantum wire, next we describe the calculation of the transmission coefficient, and finally discuss the results. We also show results on the behavior of the conductance fluctuations close to the metal-insulator crossover in this model for the impurity band.

MODEL FOR AN IMPURITY BAND IN A QUANTUM WIRE

We consider the transmission of an electron through a finite quantum wire of length d along its axis, which is oriented in the z direction. In order to describe the semiconductor quantum wire, we use a model very similar to that used in Ref. 15. We consider a wire with square cross section of side L. In the plane perpendicular to the wire, the electrons are confined by infinite walls at $x=\pm L/2$ and $y=\pm L/2$. This is a very good approximation whenever the binding energy and the impurity bandwidth are much smaller than the depth of the confining potential, as is usually the case.

We assume the wire is doped with donor impurites distributed randomly along its z axis with position vectors $\mathbf{r}_i=z_i\hat{z}$ and linear concentration n. We neglect the influence of excited and conducting states and start with the following one-electron tight-binding Hamiltonian:

$$H=\sum_{i,j} H_{ij}|i\rangle\langle j| \ , \tag{1}$$

where $\langle \mathbf{r}|i\rangle=\psi(\mathbf{r}-\mathbf{r}_i)$ is the ground-state wave function of an electron bound to an impurity at $\mathbf{r}_i$. With effective Bohr radius $a^*=4\pi\epsilon_0 k_{sc}\hbar^2/m^*e^2$ and effective Rydberg $1\ \mathrm{Ry}^*=\hbar^2/2m^*a^{*2}$, where m^* is the effective mass and k_{sc} is the dielectric constant of the semiconductor, as units of length and energy, respectively, the matrix elements are given by

$$H_{ij}=\left\langle i\left|-\nabla^2+v(x,y)+\sum_l u_l\right|j\right\rangle \ , \tag{2}$$

where $u_l=-2/|\mathbf{r}-\mathbf{r}_l|$ is the unscreened Coulomb potential due to impurity l, $v(x,y)$ is the confining potential described above, and the sum runs over all the impurities.

By choosing the bound ground-state energy

$$E=\langle i|-\nabla^2+v(x,y)+u_i|i\rangle \tag{3}$$

as the origin of energy, the matrix elements become $H_{ij}=\langle i|\sum_{l\neq i}u_l|j\rangle$. We now, as usual, neglect multicenter integrals of the types $\langle i|u_l|j\rangle$, with i, l, and j all different, and $\langle i|u_l|i\rangle$, with $i\neq l$, and keep only the largest term, which gives the following hopping:

$$H_{ij}=V(z=|z_i-z_j|)=\langle i|u_j|j\rangle \ . \tag{4}$$

Finally, one can neglect the overlap between second (and higher) -nearest neighbors and arrive at a tridiagonal Hamiltonian with purely off-diagonal disorder.

The off-diagonal elements depend on the random distance between the neighbor impurities and on the confining length L. Using, as in Ref. 15, a Gaussian-type trail wave function for ψ we find the following expression for the z-dependent hopping:

$$V(z)=(E-E_0-\alpha+\alpha^2z^2)e^{-\alpha z^2/2} \ , \tag{5}$$

where α is the variational parameter, which is obtained by minimizing E, and $E_0=\langle\psi|-\nabla^2_{xy}+v(x,y)|\psi\rangle$. This is just the Fourier transform of $V(k)$ obtained in Ref. 15. Figure 1 shows how $V(z)$ varies with L. It decays faster for stronger confinement.

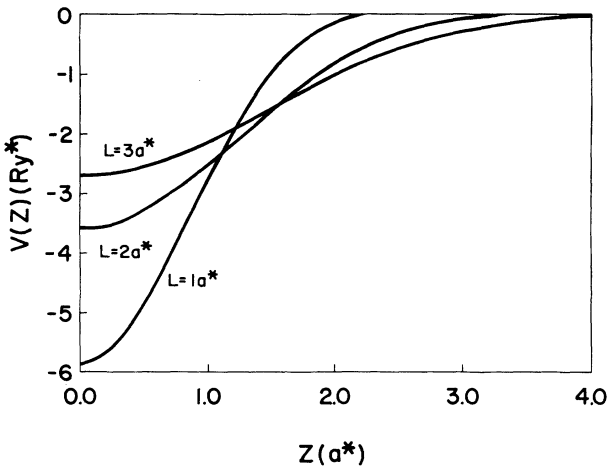

FIG. 1. Hopping parameter as a function of the distance between impurities, as given by Eq. (5), for different values of the confinement length L. Effective units are used through all the figures. Observe that a larger confinement (i.e., smaller L) corresponds to a deeper function for the hopping. The magnitude of the hopping drops off with donor separation.

We should stress that this impurity band model is quite different from the Anderson model for disordered systems, which is used in most theoretical work on localization theory. In this model, disorder enters through the site energies on the diagonal, which are randomly distributed in the interval $[-W/2, W/2]$. In our case, starting from low concentration, adding more impurities means an increase in disorder but also means an increase in conductance. This happens as the magnitude of the hopping increases and fluctuates more. After a certain concentration, there is a decrease in disorder, which corresponds to the flat region of $V(z)$ at small values of z, responsible for small fluctuations in the hopping. We should mention some previous studies of pure off-diagonal disorder, which use, however, models somewhat different from the one investigated here.[16]

TRANSMISSION PROBABILITY CALCULATION

In a tight-binding linear chain described by the equations

$$-t_{l,l-1}c_{l-1}+\epsilon_l c_l-t_{l,l+1}c_{l+1}=Ec_l \ , \tag{6}$$

where the c's are the amplitudes and the t's are the hopping terms, the sites can be eliminated one at a time using a decimation or renormalization of the chain (see Refs.

17–19). This procedure keeps the same form of the equations and is exact. If site l is eliminated there are corrections to the site energies at $l-1$ and at $l+1$ and an effective hopping between them appears. These are given by the following equations:

$$\varepsilon'_{l\pm1}-\varepsilon_{l\pm1}=\frac{t_{l\pm1,l}t_{l,l\pm1}}{E-\varepsilon_l}\ , \tag{7}$$

$$t'_{l-1,l+1}=-\frac{t_{l-1,l}t_{l,l+1}}{E-\varepsilon_l}\ . \tag{8}$$

The primes denote the corresponding elements belonging to the renormalized chain. All others elements are the same as those of the original chain.

Eventually this process reduces our initial disordered chain of impurities to only two sites with energies E_L and E_R connected by an effective hopping $V_{\rm eff}$, which are now energy dependent. In order to calculate the transmission, we connect at the left and right of this effective portion semi-infinite perfect linear chains with hopping parameter V_0. This parameter is that obtained by assuming that the distribution of impurities is uniform, i.e., $V_0=V(n^{-1})$. Therefore, if the equidistributed configuration were realized, a transmission probability equal to 1 is obtained.

Electrons are incident from the left and described by a plane wave e^{ikla}. There is a reflected portion re^{-ikla} and a transmitted portion te^{ikla}. Since the decimated disordered chain is reduced to only two sites and an effective interaction, one can write two tight-binding equations, each centered at one of the two sites:

$$-V_0c_{-1}+E_Lc_L-V_{\rm eff}c_R=Ec_L\ , \tag{9}$$

$$-V_{\rm eff}c_L+E_Rc_R-V_0c_1=Ec_R\ . \tag{10}$$

The site -1 is at the left of L and the site 1 is at the right of R, as in Fig. 2. In terms of r and t, the amplitudes are

$$c_L=1+r\ , \tag{11}$$

$$c_{-1}=e^{-ika}+re^{ika}\ , \tag{12}$$

$$c_R=t\ , \tag{13}$$

$$c_1=te^{ika}\ . \tag{14}$$

Therefore, two equations are obtained for r,t and $T=t^*t$ is calculated. The energy is varied between the limits $[-2V_0,2V_0]$ to cover the entire region which is transmitting if the whole infinite chain were ordered.

The following results for $T(E)$, and hence for the conductance $G(E)=(e^2/h)T(E)$, are obtained using this method and assuming a random distribution of nd shallow donors in the interval $[0,d]$. The hopping parameters are generated as described in the preceding section.

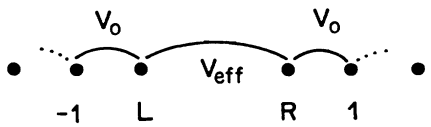

FIG. 2. Scheme of the decimated chain, connected to perfect conductors on both sides with constant hopping parameter V_0.

Using the same parameters, a configuration averaged calculation is made of the density of states for the finite portion of disordered quantum wire. Although this information is quite different from the transmission probability, it is useful for the purpose of making an analysis of the results. A direct diagonalization of the Hamiltonian corresponding to different configurations was performed, and the energies were collected into a histogram with 50 intervals of energy.

RESULTS

Figure 1 shows the hoppings parameter $V(z)$ as a function of the separation between two consecutive donors. The magnitude of the hopping is seen to drop off with donor separation. A low donor concentration then leads to small hopping parameters and only a very narrow impurity band centered at $E=0$. This band can be seen either in the density of states or in the transmission probability at low concentrations. Figure 3 shows the density

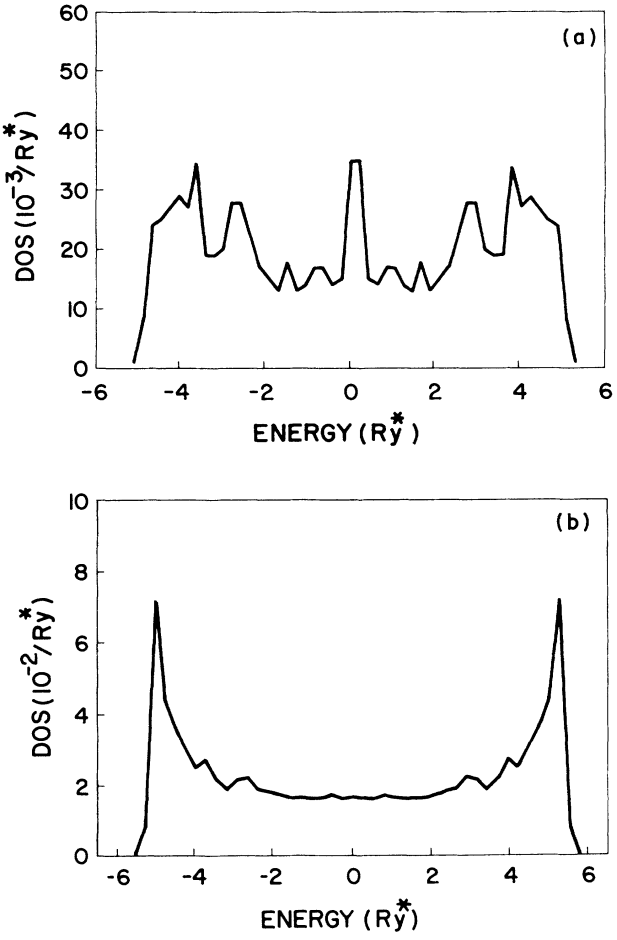

FIG. 3. Ensemble-averaged density of states (DOS) for the finite disordered portion of the wire, averaged over 50 configurations. In (a) the calculation is for a sample length $d=20a^*$ and concentration $n=1a^{*-1}$. In (b), with the same length and $n=3a^{*-1}$, we see a DOS typical of a one-dimensional metal. The origin of energy corresponds to the bound-state energy in the case of an isolated impurity.

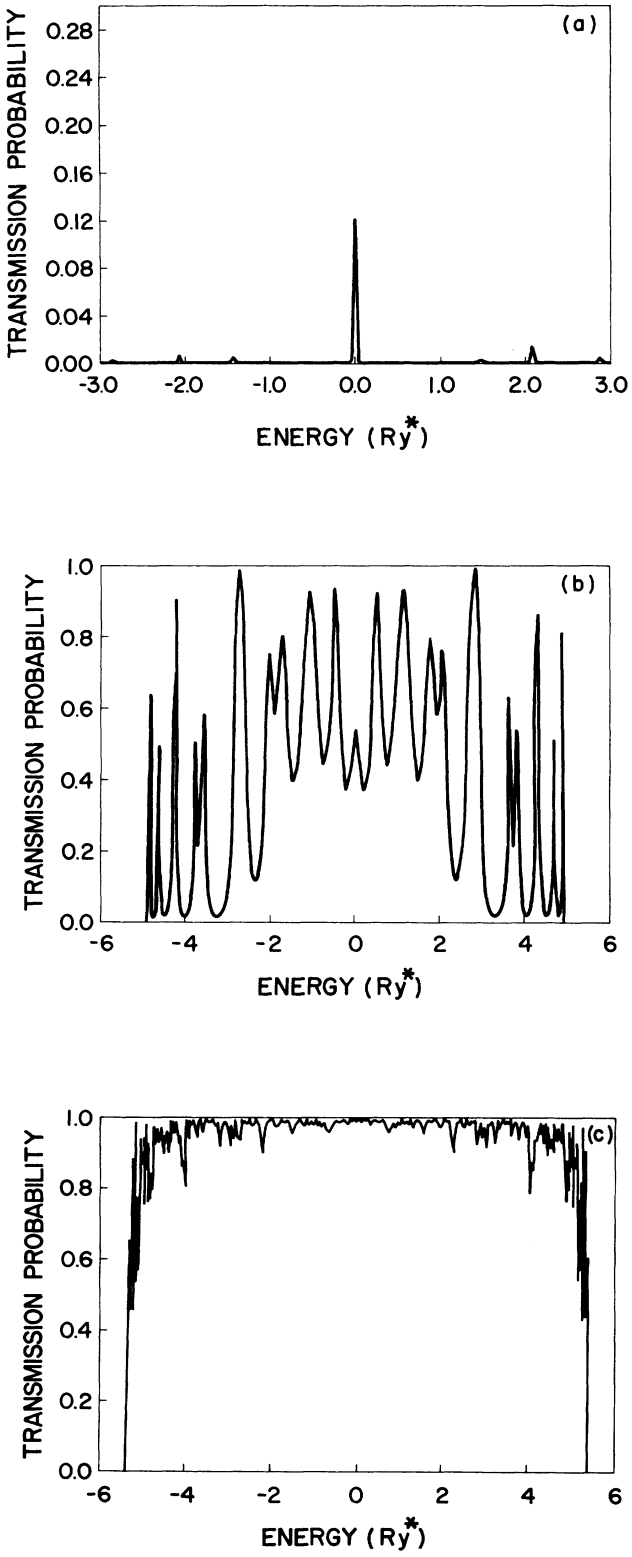

FIG. 4. Transmission probability $T(E)$ as a function of energy in the interval $[-2V_0, 2V_0]$ for a sample size $d = 20a^*$ and for typical cases of small, intermediate, and high impurity concentration. (a) has concentration $n = 1a^{*-1}$, (b) has concentration $n = 2a^{*-1}$, and (c) has concentration $10a^{*-1}$. The width of the quantum wire is $L = 3a^*$. Additional details are given in the text.

of states for the isolated chain, averaged over 50 configurations. For small concentrations we see the peak just mentioned [Fig. 3(a)]. This peak becomes dominant at lower concentrations. For higher concentrations the average density of states attains its typical one-dimensional form [Fig. 3(b)].

In the high impurity concentration limit, two effects neglected here start to play a role. When the impurity band merges with the first conduction subband, the hybridization between the two bands affects the upper part of the impurity band.[20] We expect, however, that our model will still give good results for the center and lower part of the band, even when some overlap exists. The unperturbed first conduction subband starts at the energy $E_B(L)$, corresponding to the binding energy of an electron bound to a donor inside the wire. An idea about the mixing of the bands can be obtained by comparing $|2V_0|$ with $E_B(L)$. $|2V_0|$ increases with concentration and $E_B(L)$ ranges approximately from 2 to 5 Ry* when L goes from 3 to $1a^*$.[13] From Fig. 1 we see that, in a wire with $L = 1a^*$, for example, the bands start merging at concentrations close to $1a^{*-1}$.

Unless the impurities are intentionally placed around the center of the wire, other complications appear, in the high concentration limit, since the hopping dependence on the transverse distance between the impurities and its related diagonal disorder cannot be neglected.[21] We believe, however, that accounting for these complications will not add significantly to our understanding of the physics of the problem.

Next we show the results for the transmission coefficient. In Fig. 4 one sees that a sequence of increasing concentrations broadens the region of nonzero transmittance, starting from a rather narrow band at $E = 0$. Intermediate values of concentration show oscillations typical of conductance fluctuations. These are shown for a particular distribution of impurities in the interval $[0, d]$, and the result is strongly dependent on configuration. For example, if in a particular

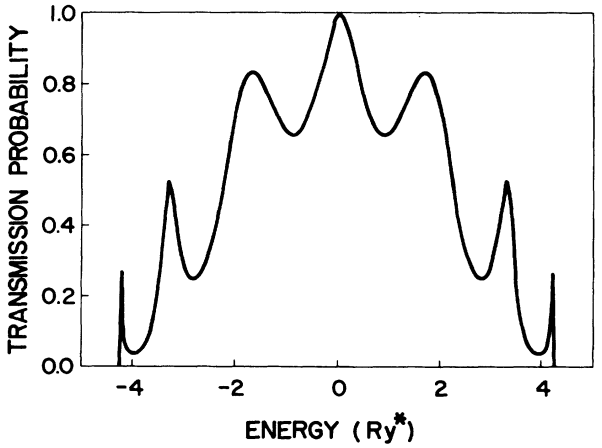

FIG. 5. Transmission probability $T(E)$ in the interval $[-2V_0, 2V_0]$ for a relatively short chain ($d = 10a^*$) showing a relatively smooth function of energy. The width of the quantum wire is $L = 3a^*$.

configuration, there is a particular large separation between consecutive donors, the transmission probability T of that sample will be very small. On the other hand, a high concentration of donors will lead to a small separation between consecutive donors. In this situation there will be only small fluctuations in the hopping parameter according to Fig. 1, and the transmission will be close to 100%. For $d=20a^*$, small, intermediate, and large concentrations of impurities are shown in Figs. 4(a), 4(b), and 4(c), respectively. In each case, $T(E)$ is plotted in the range $[-2V_0,2V_0]$. As a proviso, we must indicate that we do not necessarily probe the transmittance of all states using this method, but only those which happen to lie in our natural interval $[-2V_0,2V_0]$. Particularly for intermediate values of concentration, there are states which lie outside of this interval. It is, however, expected that these are localized states with extremely small values of conductance.

For shorter lengths and similar concentrations the results appear to be rather smooth. This is shown in Fig. 5, which shows the result for $T(E)$ in the case of $d=10a^*$. The resonances do not occur at the same values as the eigenvalues of the isolated chain. However, broader resonances occur for shorter chains, in which the influence of the semi-infinite metallic portion is much stronger. This, added to the fact that there are fewer eigenvalues for the shorter chains, makes the result much smoother.

We study the fluctuations in the transmission coefficient at the center of the impurity band ($E=0$) by performing an ensemble average over 90 configurations. Both $\langle T\rangle$ (dashed line) and the root-mean-square (rms) fluctuation $\sqrt{\langle T^2\rangle-\langle T\rangle^2}$ (solid line) are plotted in Fig. 6, as a function of length for different concentrations. The results show how both drop off with length and how both also increase for larger concentrations. They give some idea of the kind of metal-insulator crossover we have, occurring either as a function of length or as a function of impurity concentration. As a rough cri-

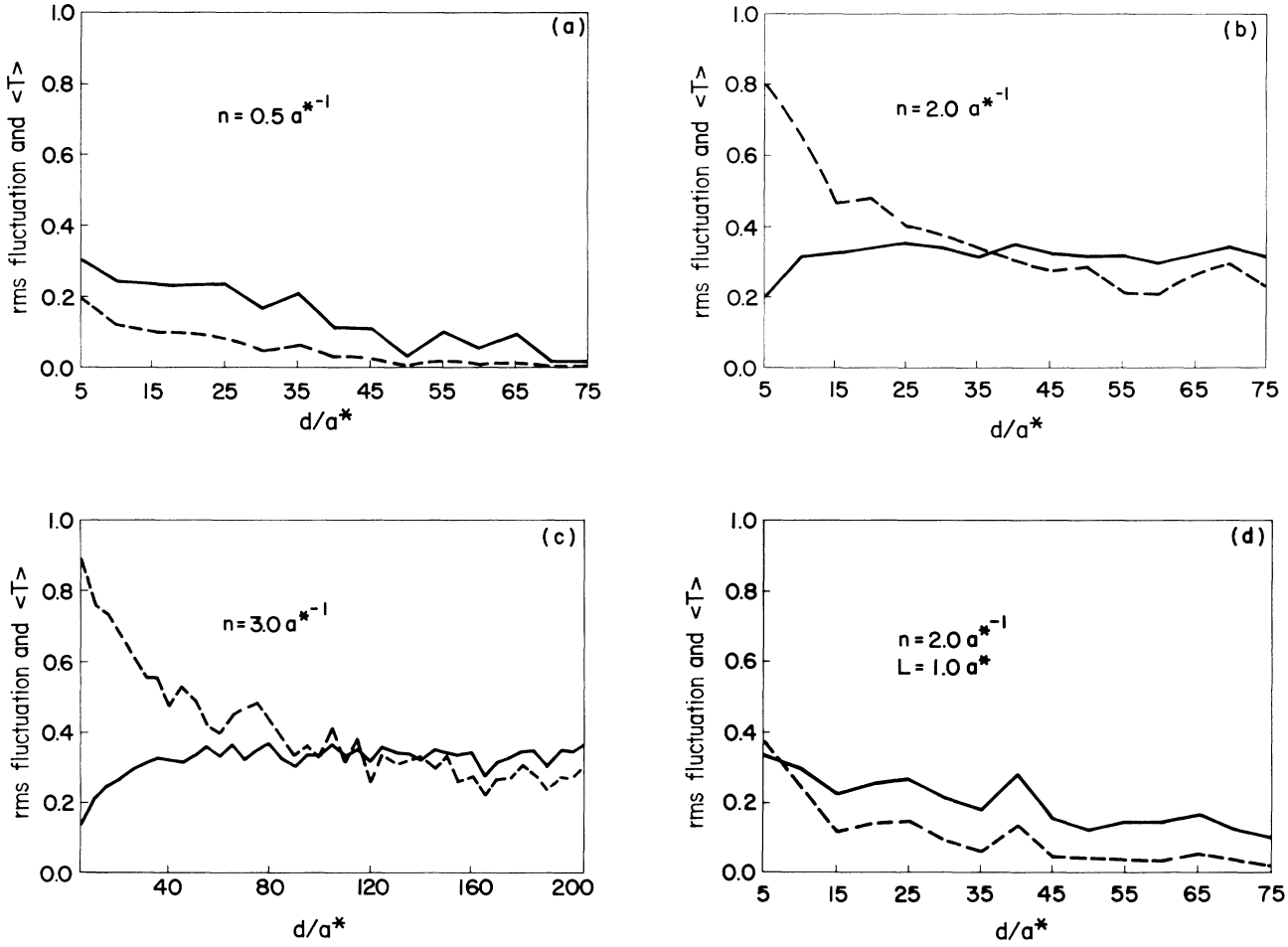

FIG. 6. This figure shows an ensemble-averaged transmission probability ($\langle T\rangle$) (dashed line) and the ensemble-averaged root-mean-quare (rms) fluctuation of T, $\sqrt{\langle T^2\rangle-\langle T\rangle}$ (solid line), as a function of sample length d, for various concentrations. (a)–(c) all have $L=3a^*$ and impurity concentration $n=0.5$, 2, and $3a^{*-1}$, respectively. The point where the average transmittance gets smaller than the rms fluctuation defines the critical sample length for impurity conductance. Observe that the rms fluctuation in (b) and (c) stays almost constant from the crossover throughout the metallic regime. (d) shows the results for a smaller confinement length ($L=1a^*$) with concentration $n=1a^{*-1}$, when both the average transmittance and its fluctuations drop to zero faster as the sample size d increases.

terion, one can take the crossover point at which $\langle T \rangle$ becomes smaller than the noise (rms) fluctuation as defining the length of a device over which there is metallic conductance within the impurity band.

The conductance fluctuations, in the limit of large impurity concentrations, have a magnitude which is independent of concentration and sample length. This is in agreement with the concept of universal conductance fluctuation in small metallic systems.[9-12]

CONCLUSIONS

We have shown that a small piece of a doped semiconductor quantum wire, sandwiched between metallic leads, carries an impurity band with increasing transmission probability for increasing impurity concentration and/or decreasing length. Conductance fluctuations are seen and are very dependent on the particular configuration of the impurities. At high concentrations, it becomes sample size and concentration independent, as the universal fluctuations in small metallic samples. The results represent an extension of previous calculations,[5,6] either in three dimensions or in an infinite one-dimensional chain to the important case of a finite length quantum wire. In particular, the impurity conductance through such a device has been calculated and explained, and the results are in accord with all the expectations one has about such a situation.

We have estimated the critical length for a metallic regime in the impurity band, as a function of impurity concentration and degree of confinement. One can see from our results, for example, that a 300 Å$\times$300 Å GaAs ($a^* \sim 100$ Å) quantum wire, 0.4 μm long, becomes metallic in the center of the band at concentrations near 0.5×10^{18} cm^{-3}; all experimentally realizable values.[2]

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