Localization in Semiconductor Quantum Wire Nanostructures

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Localization properties of quasi-one dimensional quantum wire nanostructures are investigated using the transfer matrix-Lyapunov exponent technique. We calculate the localization length as a function of the effective mean-field mobility assuming the random disorder potential to be arising from dopant-induced short-range δ-function or finite-range Gaussian impurity scattering. The localization length increases approximately linearly with the effective mobility, and is also enhanced by finite-range disorder. There is a sharp reduction in the localization length when the chemical potential crosses into the second subband.

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An early motivation in developing semiconductor quantum wires was the suggestion that one-dimensional phase space restrictions would severely reduce impurity scattering, thereby substantially enhancing electron mobilities making possible faster transistors and optoelectronic devices. The rationale for this proposed mobility enhancement is the fact that at low temperatures the only possible resistive scattering process in one dimension is the 2k_F-scattering, implying enhanced low temperature mobility as all other scattering processes are suppressed. In real quasi-one dimensional quantum wire systems there would be additional inter-subband scattering processes which are, however, weak in general, and therefore, it was argued that high quality quasi-one dimensional GaAs quantum wires could potentially have low temperature mobilities surpassing those in modulation-doped two dimensional HEMT structures. There is, however, a serious flaw in this phase-space-restriction-induced mobility enhancement argument: Impurity disorder-induced 2k_F multiple scattering leads, in fact, to localization and zero mobility in one dimensional systems. It is well-established that all one electron states in a disordered one dimensional system are exponentially localized, and this Anderson localization phenomenon leads to the inevitable rigorous conclusion that strictly one dimensional quantum wire structures are always zero mobility insulators (because some disorder must always be present in real systems), and cannot carry any current in the thermodynamic limit. In high-quality low-disorder quantum wires, the localization length may be large, and only if the length of the wire is shorter than the localization length, the system can behave as an “effective” metal with non-zero effective mobilities. The important issue for quantum wire transport is then to figure out the localization length for a given realization of disorder, which could be parameterized by the mean-field mobility calculated within the Born approximation which being a single impurity scattering approximation does not lead to localization (localization being a purely multiple scattering-induced interference phenomenon).

In this paper, we carry out a calculation of the quantum wire localization length as a function of disorder using the mean-field Born approximation mobility as the relevant parameter characterizing the impurity scattering strength. We find that in reasonable high-quality GaAs quantum wires the localization length may be several microns, making it possible to fabricate current carrying quantum wires for nanoelectronic or even microelectronic applications.

Our goal is to calculate the zero temperature quantum wire localization length in the presence of random impurity disorder. We model the impurities as randomly distributed point scattering centers with the electron-impurity interaction as short-range δ-function or finite-range Gaussian potentials. The mean field mobility of the quantum wire is calculated using the first order Born approximation, which should be roughly the same as the corresponding two dimensional mobility of the GaAs material from which the quantum wire is made. The electronic localization length at the Fermi level is determined by calculating the Lyapunov exponent of the transfer matrix for the system. We find that the localization length increases linearly with the mobility of the wire at low electron density (i.e. when only the lowest subband is occupied). Other things being equal (i.e. the same mobility) finite-range of the scattering potential tends to increase the localization length. We also find a sharp reduction in the localization length when the electrons start to fill the second subband.

The quantum wire is modeled as a two-dimensional strip along the x direction with a length L and a width w along the y direction with randomly distributed scattering centers along the strip. Without any loss of generality, we ignore the third direction (i.e. the z axis) completely because the thickness of real GaAs quantum wires is often much less than their width. For a perfect quantum wire with an infinite rectangular confining potential well along the y direction, the energy spectrum and the electron wavefunction can be written as:
\[ E_{nk} = \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 n \pi^2}{w^2}, \]  
\[ \phi_{nk} = \frac{1}{\sqrt{L}} e^{ikx} \sqrt{\frac{2}{w}} \sin \left( \frac{n \pi}{w} y \right). \]

The impurity potential centered at \((x_i, y_i)\) is taken to be:

\[ V_{im}(x, y) = v_o \delta(x - x_i) \delta(y - y_i) \]  
(2a)

or

\[ V_{im}(x, y) = \frac{v_o}{\pi s^2} e^{-\frac{(x-x_i)^2}{s^2}} e^{-\frac{(y-y_i)^2}{s^2}}. \]  
(2b)

The infinite potential well confinement is obviously an idealization which, for our purpose, should be a good approximation because choosing a different model confinement will only change the impurity potential matrix elements \(i.e.\) the disorder strength \(v_o\), which we are parameterizing. While our choice for the impurity potential in Eqs. (2a) and (2b) is mainly a matter of convenience, we have explicitly verified that screened Coulomb impurity potential in a GaAs quantum wire may be reasonably approximated by a Gaussian potential. We also make a one- or two-subband approximation for our calculations which should be accurate for low electron densities. Including more (than two) subbands should not change our results qualitatively.

The localization length is calculated using the transfer matrix technique. We first divide the wire of length \(L\) into small segments of length \(a\) (which is taken to be much less than the average inter-impurity distance). The system can then be effectively described by the two-channel (corresponding to two subbands) Anderson model with nearest neighbor hopping, \(i.e.\)

\[ \mathcal{H} = \sum_i \sum_{n,m=1,2} (E_n \delta_{nm} + V_{nm}) |ni><mi| - \sum_i \sum_{n=1,2} t(|ni><ni+1| + |ni+1><ni|) \]  
(3)

where the hopping term \(t = \hbar^2/2m^*a^2\), and \(V_{nm}\) are the random on-site scattering matrix elements which can be calculated from the impurity potential and the electron wavefunction. A transfer matrix formalism can be easily set up for such a Hamiltonian. The localization length is then given by the inverse of the smallest Lyapunov exponent of the transfer matrix.

The mean field mobility of the wire, which is used to parameterize the strength of disorder, is calculated using the first order Born approximation. If only the lowest subband is occupied, an electron can only be scattered from \(k_F\) to \(-k_F\) or vice versa. The transport scattering rate is then given by:

\[ \frac{1}{\tau} = \frac{2m^* N_i}{\hbar^3 k_F} \frac{1}{|V_{11}(2k_F)|^2}, \]  
(4)

with the mobility \(\mu = e\tau/m^*\), where the matrix element \(V_{11}\) of the impurity potential \(V_{im}\) is taken entirely within the lowest subband \(n = 1\). The mobility calculation for the 2-subband scattering problem is discussed below. Because of the exact one to one correspondence between the random disorder and the mean-field mobility, \(\mu \propto N_i < |V|^2 >\), as defined in Eq. (4), the impurity potential \(V_{im}\) may be uniquely parameterized by the mean field mobility \(\mu\) provided the average impurity density \(N_i\) is known. We take \(N_i\) to be equal to the average electron density (again with no loss of generality) in the quantum wire, which is taken to be \(10^6 cm^{-1}\) for all our calculations.

\[ FIG. 1. \] The relation among the localization length(\(\lambda_L\)), mobility(\(\mu\)) and the range of the impurity potential(\(s\)) for a 500\(\mu m\) long and 100\(\AA\) wide wire. The impurity concentration is \(1 \times 10^6 cm^{-1}\) (the same as the electron density).

Our one-subband localization calculation results in the lowest subband are shown in Fig 1. The short-range scattering model corresponds to the \(s = 0\) limit. The mean field mobility in Fig. 1 is calculated neglecting inter-subband scattering, which we discuss below. As shown in Fig. 1, the localization length increases approximately linearly with the mobility of the wire. Finite-range scatterers also tend to increase the localization length. It is well known that the Lyapunov exponent takes a long time to converge in the Anderson model, particularly for finite range disorder. The results shown in Fig. 1 involve up to \(10^7\) iterations. It is noteworthy that we still have fluctuations in our results for high mobility (and finite potential range) samples even after \(10^7\) iterations! In general, the localization length is found to be larger than the elastic mean free path extracted from the mean-field mobility.

As can be seen from Eq. (4), the electron mobility can be increased by increasing the electron density which is proportional to \(k_F\) (assuming, of course, that \(N_i\) is fixed). This is true when electrons only occupy the lowest subband. As electrons start to occupy the second subband, enhanced inter-subband scattering is introduced at the Fermi level which could result in a sharp reduction of the localization length. For example, an electron with momentum \(k_{F1}\) in the lowest subband could be scattered...
into either the $-k_F$ state in the same subband or the $\pm k_F$ states in the second subband. The two-subband generalization of Eq. (4) is straightforward. The scattering time for the first subband $\tau_1$ is different from that for the second subband $\tau_2$. Using the Boltzmann equation and first order Born approximation, it is straightforward to show that in the most general two-subband model including inter-subband scattering processes:

$$\frac{1}{\tau_1} = \frac{2m^*N_i}{\hbar^2k_{F1}}<|V_{11}(2k_{F1})|^2 >$$

$$+ \frac{m^*N_i}{\hbar^2k_{F2}}\left[ (1 - \frac{k_{F2}\tau_2}{k_{F1}\tau_1}) <|V_{12}(k_{F1} - k_{F2})|^2 >
+ (1 + \frac{k_{F2}\tau_2}{k_{F1}\tau_1}) <|V_{12}(k_{F1} + k_{F2})|^2 > \right],$$

$$\frac{1}{\tau_2} = \frac{2m^*N_i}{\hbar^2k_{F2}}<|V_{22}(2k_{F2})|^2 >$$

$$+ \frac{m^*N_i}{\hbar^2k_{F1}}\left[ (1 - \frac{k_{F1}\tau_1}{k_{F2}\tau_2}) <|V_{21}(k_{F1} - k_{F2})|^2 >
+ (1 + \frac{k_{F1}\tau_1}{k_{F2}\tau_2}) <|V_{21}(k_{F1} + k_{F2})|^2 > \right].$$

The mobility is then easily calculated once we get $\tau_1$ and $\tau_2$. It is interesting to note that when the second subband just starts to be occupied (i.e. $k_{F2}$ is very small), both $\tau_1$ and $\tau_2$ are small leading to a mobility reduction due to enhanced inter-subband scattering. This causes a sharp decrease in the localization length as $E_F$ enters the second subband.

We present our two-subband localization results in Fig. 2 for a 200 Å wide quantum wire. The impurity concentration is fixed at $10^6$ cm$^{-1}$. We use a fixed impurity strength $v_o$ which is normalized to the results presented in Fig. 1 with $\delta$-function impurity and a mobility value of $1 \times 10^5$ cm$^2$V$^{-1}$s$^{-1}$. Both the mobility and the localization length drop sharply when electrons start to fill the second subband. It is interesting to note that (similar to Fig. 1) the localization length is almost an order of magnitude larger than the effective mean free path obtained from the Born approximation mobility values.

FIG. 2. The variation of density of states(a), electron mean free path(b), mobility(c), and localization length(d) as the Fermi energy (measured in units of $\Delta$) increases. ($\Delta$ is the energy difference between the bottom of the lowest two subbands.) The wire is 500 $\mu$m long and 200 Å wide. Results for three different impurity potential ranges are shown: 0(solid line), 2nm(dashed line), and 5nm(dotted line). The impurity concentration is $1 \times 10^6$ cm$^{-1}$. The impurity potential strength is normalized to that of the wire presented in Fig. 1 with $\delta$-function impurity and $1 \times 10^5$ cm$^2$V$^{-1}$s$^{-1}$ mobility.

In summary, we have calculated the localization length for a quasi-one dimensional quantum wire within the two-subband model. We find that the localization length increases linearly with the mobility of the wire at low electron density (i.e. only the lowest subband is occupied). Finite-range scatterers also tend to increase the localization length. The sharp drop in the localization length seen in Fig. 2 may be difficult to observe experimentally because of finite thermal and collisional broadening ef-
fects which may affect the one dimensional density of states singularities of Fig.2(a). The localization length, in general, is found to be much larger than the elastic mean free path calculated on the basis of the Born approximation.

Our most important result is that the localization length in semiconductor quantum wires could be many microns long even in modest quality (i.e. mean-field $\mu < 10^6{\text{cm}^2\text{V}^{-1}\text{s}^{-1}}$) samples. Thus, the physics of Anderson localization is unlikely to adversely affect operation of microelectronic devices fabricated by using semiconductor quantum wires.

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