Effect of an applied electric field upon one-dimensional localization

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The transmission coefficient of an electron interacting with a one-dimensional chain of variable length L is calculated using a variation of standard transfer-matrix techniques. The potential energy with which the electron interacts consists of a random potential and a fixed static electric field. In this study, the random potential is modeled as a potential step on a lattice. Using the zero-temperature Landauer formula, the dimensionless resistance and, hence, the localization length are obtained. It is found that the presence of the electric field causes delocalization of the electron for all applied fields F.

I. INTRODUCTION

Recently, there has been a great deal of theoretical and experimental interest in understanding the conductance of metal-oxide-semiconductor field-effect transistors (MOSFET's) at low temperatures[1,2] and the transport properties of multiple quantum wells.[3-6] This interest stems from attempting to observe the spatial localization of electrons in the device or the quantum well. In such a device, the conduction channel is essentially one dimensional and resembles a quantum wire or chain containing random impurities. In the quantum-well case, the potentials are fixed, but the spatial lengths of the well and barrier layers vary. Previously, Landauer established a connection between the dimensionless resistance and the transmission coefficient of the chain.[7] Hence, the resistance of the device is determined immediately upon computation of the transmission coefficient of the chain. It is the dependence of the transmission coefficient upon applied field that we explore here.

The problem of determining the transmission coefficient of a chain of length L with random impurities has been studied extensively.[8-10] As a result of the random potentials, the electronic wave function becomes spatially localized. In the limit of weak localization, Landauer's result reduces to Ohm's law; in the limit of strong localization, it leads to an exponential dependence of the resistance upon the length of the disordered region. However, in the presence of an applied electric field, such as that found in the conduction channel of a MOSFET, the nature of the electronic states is not well understood. Previous calculations of the transmission coefficients have been performed in which the random potential is taken to be a δ function.[11-13] Here we study the case in which the random potential is taken to be a step of fixed width, but varying strength. It is found that at small applied electric fields a smooth transition between localized and delocalized states occurs as one qualitatively expects.

Similiar calculations have been reported recently by Cota, José, and Azbel.[14] The model potential used in this communication is similar to that of Ref. 14, and our numerical results confirm their predictions. However, these authors use an approximation that we avoid: They employed a "ladder approximation" to the actual potential that is accurate at low fields, but expected to be inaccurate at high fields. This ladder approximation consists of ignoring the continuous variation of the linear potential term and adjusting the potential in each well (barrier) to account for the mean potential drop in that region. This leads to considerable algebraic simplification and allows relatively easy numerical calculations using standard transfer-matrix techniques. In the present work, we sacrifice the algebraic simplicity gained by employing the ladder approximation and, as a result, obtain exact expressions for the various quantities needed. As will be seen later, the transmission coefficient must be evaluated numerically in any event, and there is little additional numerical cost if the exact expressions are retained. In contrast to the technique employed by Cota *et al.* which requires numerous matrix multiplications, we have adapted a recursive technique introduced by Azbel and Soven.[8] The advantages of this method, as will be seen below, are that it is numerically stable and that it is recursive in nature. Rather than dealing with the amplitudes of left- and right-going waves, this technique represents the amplitude by a complex phase. It is then straightforward to show that the real and imaginary parts of this complex phase can be propagated from adjacent regions recursively. The method, as originally applied by Azbel and Soven, was restricted to regions of constant potential. In this work we extend the method to regions in which the potential is a linear function of the coordinate.

Our numerical results confirm and supplement the results of Cota *et al.* We also find that the localization length is a universal function of an appropriate dimensionless parameter apart from sudden jumps. Hence, we are able to confirm that the jumps do not arise from the "ladder approximation" nor the numerical difficulties associated with the transfer-matrix technique. In addition, the numerical parameters we have chosen allow for parti-

cles with energies greater than, less than, and approximately equal to the mean barrier height so that there is significant tunneling between adjacent wells.

II. NUMERICAL GENERATION OF THE TRANSMISSION COEFFICIENT

We now describe the technique used to calculate the transmission coefficient and five further details of the potential energy. We begin with the latter. A one-dimensional disordered chain of length L is assumed to exist along the z axis. The disorder is represented, in this case, by a random step potential of spatial extent b in the unit cell of length a and is given by

$$V(z)=\begin{cases}0, & z<0\ ,\\ V_n-eFz, & na<z<na+b\ ,\\ -eFz, & na+b<z<(n+1)a\ ,\\ -eU, & L<z\ ,\end{cases} \tag{1}$$

where the V_n are chosen at random, $F=U/L$ is the electric field associated with application of a voltage U to the chain, the electron charge is $-e$, and we require $b<a$. The case is representative of the conduction channel of a MOSFET. Alternatively, one could fix the potentials in each cell and vary the spatial lengths b and a to represent a multiple-quantum-well structure. As noted previously, the ladder approximation of Cota *et al.*[14] consists of replacing the portion of the potential that arises from the applied bias by a constant, which is different for each cell. This implies that in each cell the solution of the Schrödinger equation is given by plane waves.

The Schrödinger equation obtained at energy E, as a result of potentials with the structure of Eq. (1), can be solved exactly in terms of Airy functions. To this end, we introduce the auxiliary variables,

$$k_e^3=\frac{2meF}{\hbar}\ , \tag{2}$$

$$\zeta_n=k_e[(V_n-E)/eF-z]\ , \tag{3}$$

$$\gamma_n=-k_e(E/eF+z)\ , \tag{4}$$

so that the general solution to the Schrödinger equation is

$$(z)=\begin{cases}A_0\exp(ikz)+B_0\exp(-ikz), & z\le 0\ , \quad (5a)\\ A_n[\mathrm{Ai}(\zeta_n)-i\,\mathrm{Bi}(\zeta_n)]+B_n[\mathrm{Ai}(\zeta_n)+i\,\mathrm{Bi}(\zeta_n)], & na<z<na+b\ , \quad (5b)\\ C_n[\mathrm{Ai}(\gamma_n)-i\,\mathrm{Bi}(\gamma_n)]+D_n[\mathrm{Ai}(\gamma_n)+i\,\mathrm{Bi}(\gamma_n)], & na+b<z<(n+1)a\ , \quad (5c)\\ t\exp(ik'z)+t'\exp(-ik'z), & (n+1)a<z\ , \quad (5d)\end{cases}$$

where Ai and Bi are the usual Airy functions[15] and $k\,(k')$ corresponds to free particle motion at energy $E\,(E+eU)$.

To determine the transmission coefficient, we employ continuity of the wave function and its first derivative at all interfaces. For simplicity, we ignore any effective-mass differences in the various regions. Our procedure parallels that of Azbel and Soven[8] in that we seek relationships between $A_{n+1}(B_{n+1})$ and A_n and B_n, and then introduce auxiliary variables that allow for stable numerical propagations. Using the continuity of the wave function and its first derivative at $z=na+b$ and $z=(n+1)a$, we obtain the following relationships:

$$A_n[\mathrm{Ai}(\zeta_n^2)-i\,\mathrm{Bi}(\zeta_n^2)]+B_n[\mathrm{Ai}(\zeta_n^2)+i\,\mathrm{Bi}(\zeta_n^2)]=C_n[\mathrm{Ai}(\gamma_n^1)-i\,\mathrm{Bi}(\gamma_n^1)]+D_n[\mathrm{Ai}(\gamma_n^1)+i\,\mathrm{Bi}(\gamma_n^1)]\ , \tag{6a}$$

$$A_n[\mathrm{Ai}'(\zeta_n^2)-i\,\mathrm{Bi}'(\zeta_n^2)]+B_n[\mathrm{Ai}'(\zeta_n^2)+i\,\mathrm{Bi}'(\zeta_n^2)]=C_n[\mathrm{Ai}'(\gamma_n^1)-i\,\mathrm{Bi}'(\gamma_n^1)]+D_n[\mathrm{Ai}'(\gamma_n^1)+i\,\mathrm{Bi}'(\gamma_n^1)]\ , \tag{6b}$$

$$A_{n+1}[\mathrm{Ai}(\zeta_{n+1}^1)-i\,\mathrm{Bi}(\zeta_{n+1}^1)]+B_{n+1}[\mathrm{Ai}(\zeta_{n+1}^1)+i\,\mathrm{Bi}(\zeta_{n+1}^1)]=C_n[\mathrm{Ai}(\gamma_n^2)-i\,\mathrm{Bi}(\gamma_n^2)]+D_n[\mathrm{Ai}(\gamma_n^2)+i\,\mathrm{Bi}(\gamma_n^2)]\ , \tag{6c}$$

$$A_{n+1}[\mathrm{Ai}'(\zeta_{n+1}^1)-i\,\mathrm{Bi}'(\zeta_{n+1}^1)]+B_{n+1}[\mathrm{Ai}'(\zeta_{n+1}^1)+i\,\mathrm{Bi}(\zeta_{n+1}^1)]=C_n[\mathrm{Ai}'(\gamma_n^2)-i\,\mathrm{Bi}'(\gamma_n^2)]+D_n[\mathrm{Ai}'(\gamma_n^2)+i\,\mathrm{Bi}'(\gamma_n^2)]\ , \tag{6d}$$

where the definitions of the arguments of the Airy functions occurring in Eqs. (6) are

$$\zeta_n^1=k_e[(V_n-E)/eF-z]\ , \tag{7a}$$

$$\zeta_n^2=k_e[(V_n-E)/eF-na-b]=\zeta_n^1-k_eb\ , \tag{7b}$$

$$\gamma_n^1=-k_e(E/eF+na+b)\ , \tag{7c}$$

$$\gamma_n^2=-k_e[E/eF+(n+1)a]\ . \tag{7d}$$

Equations (6) can be recast into matrix form so that the relationship between the coefficients A_0, B_0, and t,t' is ultimately given by

$$\begin{pmatrix}t\\ t'\end{pmatrix}=\prod_{i=0}^{N}\underline{m}_i\begin{pmatrix}A_i\\ B_i\end{pmatrix}=\underline{M}\begin{pmatrix}A_0\\ B_0\end{pmatrix}\ . \tag{8}$$

Here the $\underline{m}_i$ are the transfer matrices that correspond to the solution of Eqs. (6) in each layer. Hence, evaluation of the transmission coefficient requires the solution of two simultaneous equations subject to the boundary conditions $A_0=1$ and $t'=0$. However, the evaluation of the matrix $\underline{M}$ requires many matrix multiplications, which often lead to numerical instability. Within the ladder approxima-

tion, Cota *et al.*[14] have taken this route to determine $\underline{M}$ and the transmission coefficient.

While formally exact, the technique described above often is not numerically tractable. To circumvent this numerical difficulty, we use an alternative technique to obtain the transmission coefficient. We begin by introducing the auxiliary variables G_n and ϕ_n in the manner of Azbel and Soven:[8]

$$A_n = \exp(G_n + i\phi_n) \ , \tag{9a}$$

$$B_n = \exp(G_n - i\phi_n) \ . \tag{9b}$$

The advantage of this transformation is that rather than dealing with large (small) numbers such as the A_n and B_n, which are characterized by a phase and an exponent, we deal with the exponent and phase directly. Using Eqs. (9) in Eqs. (6) after considerable algebra transforms the matrix multiplication to a recursive relationship between the exponents G_{n+1} and G_n and the phases ϕ_{n+1} and ϕ_n. This is particularly advantageous when the energy of the particle is less than the barrier height and the barrier is wide. In this situation, numerical instabilities easily occur in Eq. (8), but in this technique they are completely avoided.

To obtain the transmission coefficient $D(E) = (k'/k)|t|^2$, we propagate two independent solutions of the Schrödinger equation. The first solution has $A_0 = B_0 = \frac{1}{2}$ and corresponds to propagating $\cos(kz)$; the second solution $A_0 = -B_0 = i/2$ and corresponds to propagating $\sin(kz)$. Let $G(G')$ and $\phi(\phi')$ correspond to propagating the cosine and sine solutions from $z = 0$ to $z = L$. It is then straightforward to show that the transmission coefficient is given by

$$D = \frac{(k/k')}{|it_s' - t_c|^2} \ , \tag{10}$$

where t_s' and t_c correspond to the amplitudes of a left-going wave arising from propagating the sine and a right-going wave arising from propagating the cosine, respectively. Note that Eq. (10) has the same structure as the result given by Azbel and Soven[8] in the absence of an applied field. We now write the transmission coefficient as $D = \exp(-\alpha L)$, where α is the inverse of the localization length L_0.

III. NUMERICAL RESULTS

To investigate the role of an applied electric field F upon the localization length, we have evaluated Eq. (9) using a potential of the form given by Eq. (1) for fixed-unit-cell length $a = 3.0$ Å and potential extent $b = 2.0$ Å. The random potential step V_n was chosen by using a random-number generator such that $V_n = fV_{\max}$ with $V_{\max} = 1.3$ eV and $0 < f < 1$. The $\{f\}$ were obtained using a uniform random-number generator. Notice that in the absence of any applied field, we employ energies such that the electrons are randomly in a situation in which their local wave vector corresponds to exponential growth or decay. As noted previously, this condition often introduces numerical instabilities into Eq. (7), but the technique employed in this work avoids this difficulty. Electrons with three incident energies ($E = 1.100$, 1.436, and 1.772 eV) and several electric fields ranging from $0 < F < 4.2 \times 10^4$ eV/cm were considered. The chains consisted of 100, 200, 400, 600, 800, 1000, 2000, and 4000 cells. For each parameter set, 50 random chains were generated and the average transmission coefficient was extracted. We note in passing that all the numerical calculations were performed on a Cary Research Inc. XM-P. Figure 1 summarizes the results of this calculation and demonstrates the dependence of the inverse localization length as a function of dimensionless variable $x = eFL/E$ for the various parameters detailed above.

Figure 1 shows that the inverse localization length is a monotonically decreasing function of applied field so that the localization length is monotonically increasing. This implies that the electronic wave function is merely spreading out throughout the whole chain, which is qualitatively expected as a result of applying a static electric field. Furthermore, Fig. 1 suggests that the behavior of $\alpha(x)$ as a function of x is universal, except for jumps that occur in each curve. These jumps are attributed to tuning the electron's energy to the energy of a localized state allowed by the parameters.[16]

In Fig. 2 we plot $\alpha(x)/\alpha(0)$, where $\alpha(0)$ is obtained by extrapolation from Fig. 1 and depends only upon the energy of the electron. From Fig. 2 we see that the behavior of $\alpha(x)/\alpha(0)$ is apart from numerical jumps and noise, a universal function of x. As noted above, the jumps correspond to tuning the electron into a localized state. In fact, Cota *et al.*[14] have suggested, based upon the analysis

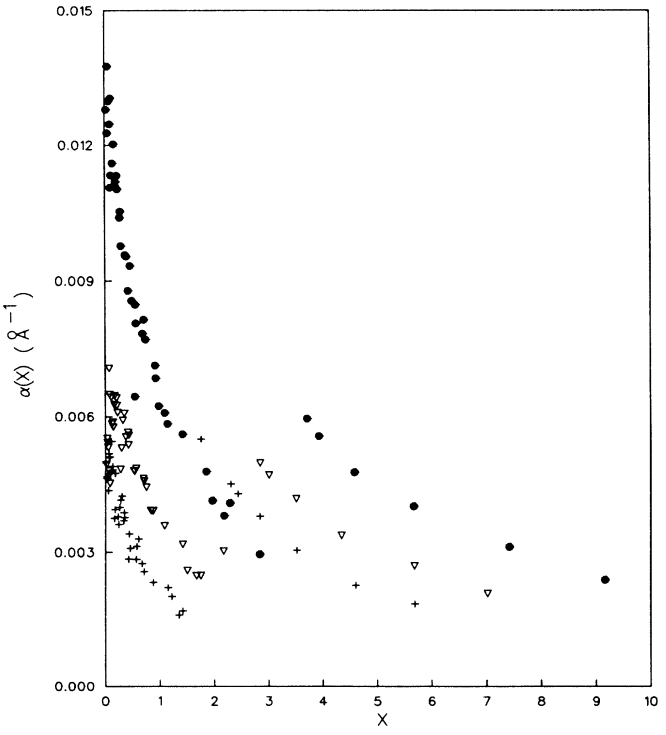

FIG. 1. Variation of the inverse localization length α in units of Å^{-1} as a function of the dimensionless variable $x = eFL/E$. The symbols ●, ▽, and + denote results obtained with energies $E = 1.1$, 1.436, and 1.772 eV, respectively.

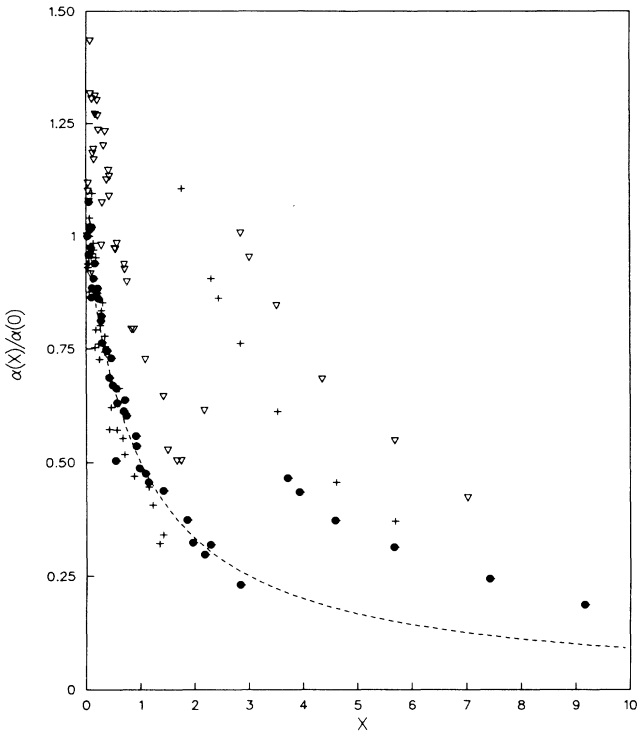

FIG. 2. Variation of $\alpha(x)/\alpha(0)$ using the data shown in Fig. 1. The theoretical result $\alpha=(x)/\alpha(0)=1/(1+x)$ is shown as the broken line.

presented below, that at large x this ratio is a universal function; our numerical calculations tend to confirm this suggestion.

For any nonzero value of x, the electron continuously gains energy from the electric field associated with the applied potential. Hence, for long chains the electron has local energy $E > V_{\max}$. In this case, the electron has near-unity probability of traversing the potential step. Letting r_n denote the probability of traversing the nth random step, the transmission coefficient is then given by

$$D=\prod_i^N (1-r_n)=\exp\left[-\sum_i r_i\right] \tag{11}$$

if multiple scattering is ignored. The presence of multiple scattering is responsible for the localized states. Using the Wentzel-Kramers-Brillouin (WKB) approximation, it can be shown that

$$r_i=0.125\frac{\langle V_i^2\rangle}{(E+eFai)^2}\ , \tag{12}$$

which for large x leads to

$$\alpha=-\frac{\ln D}{L}=\frac{\alpha_0}{1+x} \tag{13}$$

so that $\alpha(x)/\alpha(0)=1/(1+x)$. This result is plotted in Fig. 2 as the dashed line and yields semiquantitative agreement with our results. The analysis presented above cannot yield the discontinuous jumps seen in the numerical calculations because they are the result of multiple scattering, an effect which is neglected in obtaining Eq. (13).[16]

IV. CONCLUSIONS

The primary results of this paper are twofold and consist of the results presented in Figs. 1 and 2. In these figures, the dependence of the inverse localization length upon applied electric field is explored, as well as the extension of the method of Azbel and Soven[8] to other than constant potentials. In fact, we have used this new formulation to consider several problems in optics.[17] With regard to localization from the figures, we see two primary effects: (1) The behavior of the localization length is a universal function of the variable $x=eFL/E$ and (2) there is a smooth transition from localized to delocalized states as expected. The results of this study confirm and validate the earlier numerical results, predictions, and conclusions of Cota *et al.*,[14] which are obtained using a different numerical method and with additional approximations to the potential.

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