Time-dependent transport in two-dimensional quantum-wire structures

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We present a time-dependent calculation of electron transport in two-dimensional quantum-wire-based devices: the electron waveguide coupler, the quantum modulated transistor, and a quantum wire with a narrow double constriction. We follow the propagation of electron wave packets through the systems and determine the temporal behavior of the device operation by calculating various time scales.

Recently there has been considerable interest in the properties of ballistic electron transport in confined semiconductor geometries.[1] This is due partly to the potential applications to ultrafast electronic devices. Indeed, devices with their operation principle entirely based on quantum interference have been proposed and fabricated.[2,3] On the theory side, a thorough understanding of quantum transport including the ballistic regime is an urgent task. So far, much theoretical effort has been focused on analyzing the transmission pattern of electrons propagating through various ultrasmall one- and two-dimensional quantum systems where electron waves maintain phase coherence. A particularly interesting system is the T-shaped quantum wire investigated by Sols *et al.*[4] as they argued that such a structure can operate as a transistor. Another interesting structure is the electron waveguide coupler (EWC) proposed by del Alamo and Eugster[5] and Tsukada, Wieck, and Ploog.[6] This is an electronic analog of the optical directional coupler and it switches electrons from one quantum wire to another. In these quantum devices, switching is provided not by tuning a current, but rather by tuning the phase of the electron waves.

Although quantum interference effects provide new ideas for device application, many technical aspects have yet to be understood both theoretically and experimentally. One of them is concerned with the operation time of a device, such as the switching time of electrons in the directional coupler mentioned above. While various estimates can be made, a time-dependent calculation of quantum transport is clearly needed to make a quantitative theoretical prediction. While switching time of a one-dimensional structure has been studied thoroughly,[7] less attention has been paid to two-dimensional quantum wires.[8] It is the purpose of this paper to provide an extensive study of several two-dimensional quantum-wire structures. In particular we numerically solve the time-dependent two-dimensional Schrödinger equation in the ballistic regime and investigate the temporal response of the quantum-wire structures to an input of electron wave packet. We have studied three structures: EWC, a wire with narrow double constriction, and the quantum modulated transistor.[4] Relevant time scales for the transport are computed numerically. For example, we found that the switching time (dwell time) τ_d for electron transfer from one wire to the other in EWC depends on the energy of incident electron E_0. τ_d varies from 0.12 to 0.27 ps for $E_0 = 217$ meV and $E_0 = 58$ meV, respectively. Hence the structure studied here can achieve a rather high switching frequency.

The electron waveguide coupler, modeled as a four-terminal device,[9] is shown in Fig. 1(a). The two quantum wires, parallel to the x axis, are coupled through a potential barrier. Assuming that the electron coherence length is longer than the size of the device, we treat the transport of electrons ballistically within each wire, but include scattering of the electrons due to the presence of the junction, i.e., the regions V, VI, and VII. Such scattering, due to geometric junctions in two dimensions, affects transmission much more significantly than in one dimension. The quantum wires are modeled in a fashion similar to those of Sols *et al.*[4] We assume, for simplicity of the calculation, that the boundaries are hard walls, i.e., the potential energy $V = \infty$. Inside the wires, i.e.,

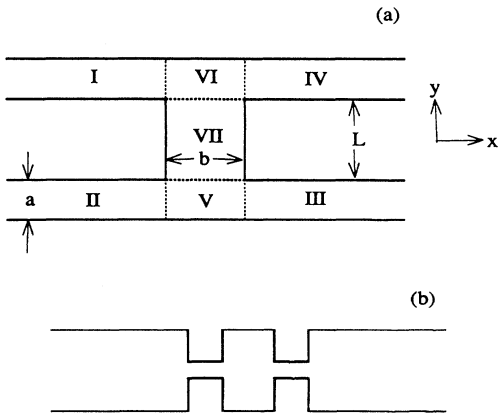

FIG. 1. (a) Schematic view of the four-terminal electron waveguide coupler where regions VI, VII, and V form the interaction region. (b) Schematic view of a quantum wire with a narrow double constriction.

regions I, II, III, IV, V, and VI, the potential is zero. In the coupling region VII a potential $V = V_0$ is added which may be controlled by a voltage. Both quantum wires have the same width a and are separated by a distance L. The coupling region, region VII, has a width b.

The static properties of this structure have been studied in detail in Refs. 9 and 10. It is shown that for certain electron energies, the transmission coefficient from lead III to lead I reaches unity, i.e., total electron switching is achieved. Our plan here is to follow in time an electron wave packet as it propagates from lead III. Depending on the average energy of the wave packet, it may decide to turn the corner and switch to the other quantum wire. The time it takes to switch can then be measured.

The time evolution of the electron wave function is governed by the time-dependent Schrödinger equation written as

$$i\hbar\frac{\partial\psi(x,y,t)}{\partial t} = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2\psi(x,y,t)}{\partial x^2}+\frac{\partial^2\psi(x,y,t)}{\partial y^2}\right) + V(x,y)\psi(x,y,t). \quad (1)$$

We choose the initial condition to be a Gaussian wave packet in the first subband located inside lead III:

$$\psi(x,y,t=0) = \frac{1}{(\pi\sigma^2)^{1/4}}e^{[ik_0x]}e^{[-(x-x_0)^2/2\sigma^2]}\frac{1}{(2a)^{1/2}}\sin\left(\frac{\pi}{a}y\right). \quad (2)$$

Here $\hbar k_0$ gives the initial average momentum [the initial average energy is $E_0 = \hbar^2(k_0^2 + \pi^2/a^2)/2m^*$], x_0 gives the location of the peak at $t = 0$, σ determines the spatial spread of the wave packet and gives an energy width $\delta E = \sqrt{2\hbar^2E_0/m^*}(1/\sigma)$, and $m^* = 0.067m_0$ is the isotropic effective mass for gallium arsenide. Equation (1) is solved using a typical Crank-Nicholson-type algorithm[11–14] on a 2000×60 grid with a typical spatial mesh size of 5 Å and a time step less than 0.23 fs. As confirmed previously[9] in a static calculation, given the structure parameters there is an electron momentum which gives total electron transfer from lead III to lead I. For example, for $a = L = 100$ Å, $b = 440$ Å, and $V_0 = 4.54$ meV, a plane wave with $k_0a = 0.8$ will totally transfer to lead I.

The time evolution of the Gaussian wave packet is plotted in Fig. 2 for every 1000 time steps (with time step of 0.23 fs). As the wave packet travels through the scattering region, two reflected (in lead III) and transmitted (in lead II) wave packets with small amplitudes have been generated. This behavior is different from the usual one-dimensional resonant tunneling through a double-barrier structure[12] where the buildup of electron density inside the quantum well is via multiple reflections (Fabry-Pérot-type mechanism). In that case only one reflected and transmitted wave packet is obtained. This is easily understandable: for EWC the scattering of the incoming wave is due to the geometric junction, hence the electron wave packet is propagating through the structure continuously rather than resonant tunneling, and there are essentially two T-shaped junctions in the structure which leads to the two reflected and transmitted wave packets with amplitudes large enough to be seen.

For the transfer of waves from one wire to the other, we note that the Gaussian wave packet consists of plane waves with an average momentum k_0 and the component with exactly k_0 can transfer through completely from lead III to I as mentioned above. Reflected and transmitted waves with small amplitudes are generated due to plane-wave components with momentum off k_0. Obviously as we increase the spatial spread of the wave packet σ or equivalently decrease the incident energy width, more wave will be transferred.[15] The transfer is measured by a transfer coefficient T, which is the total probability of electrons in lead I. For instance, T is increased from 0.69 to 0.71 and 0.75 as σ is increased from 400 Å to 500 Å and to 600 Å, where the calculation is performed at $k_0a = 0.6$.

The switching time τ of the electron transfer from one wire to the other cannot be defined uniquely and a reasonable prescription is needed. We computed this quan-

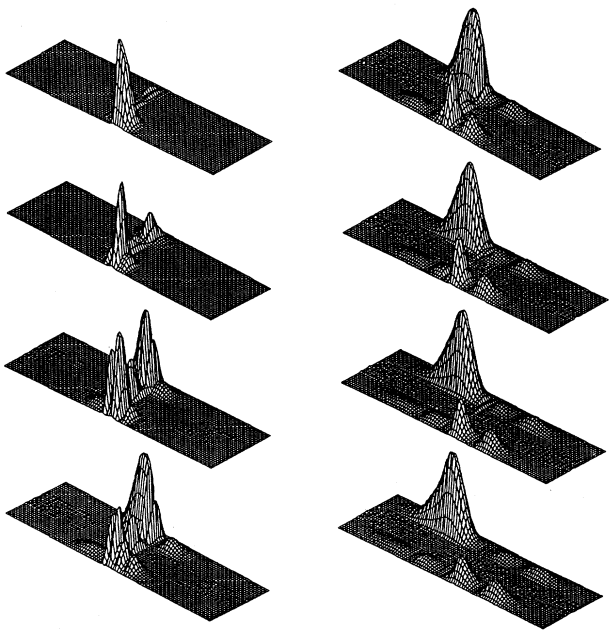

FIG. 2. Time evolution of the electron wave packet for every 1000 time steps on the electron waveguide coupler. The figures are ordered according to time from up to down and left to right. Over 60% of the electron wave has been transferred. Parameters: $a = L = 100$ Å, $b = 440$ Å, $\sigma = 300$ Å, $k_0a = 0.8$, $V_0 = 4.54$ meV, and the time step is 0.23 fs.

tity by monitoring the electron probability density $\rho(t)$ in the junction region Ω, i.e., region Ω=VI+VII+V such that we can follow the electron transfer in time:

$$\rho(t) = \int_{\Omega} |\psi(x,y,t)|^2 dx\, dy. \tag{3}$$

In Fig. 3, we plot the electron probability density ρ versus time t (solid line) for $k_0a = 0.6$, $a = L = 100$ Å, $b = 440$ Å, $\sigma = 800$ Å, $V_0 = 4.54$ meV, and a time step of 0.174 fs. The density ρ increases from zero as the electron begins to transfer, reaches a peak value, and then decreases, indicating the completion of the process. The dwell time[7] τ_d is defined as

$$\tau_d = \int \rho(t) dt. \tag{4}$$

From Fig. 3, we obtain $\tau_d = 0.267$ ps. Notice that $\rho(t)$ is approximately a Gaussian-like curve; we can fit $\rho(t) = p_{\max}\exp[-(t-t_0)^2/\alpha^2]$ where $p_{\max}$ and α are the peak value and spread of $\rho(t)$. Using this fit, $\tau_d = \alpha p_{\max}\sqrt{\pi} = 1.065\tau p_{\max}$, where we have introduced the full width at the half maximum τ. From Fig. 3, we have $\tau = 1.133$ ps and $p_{\max} = 0.2117$, resulting in $\tau_d = 0.255$ ps, which is in reasonable agreement with $\tau_d = 0.267$ ps. For $\sigma = 600$ Å (dotted line) and 500 Å (dashed line) plotted in Fig. 3, we have $\tau_d \approx 0.265$ ps for both σ's, indicating that τ_d is not sensitive to this parameter.

Another time scale of interest is the transit time[16] defined as $\tau_t \equiv 2b/v$. This time scale corresponds to the electron traveling through a distance $2b$ with velocity v. Taking the average initial velocity of the electron wave packet inside the junction, $v = 5 \times 10^5$ m/s and $b = 440$ Å, one obtains $\tau_t = 0.17$ ps, which is not too far from the value of $\tau_d = 0.267$ ps. This is understandable since our system is quite transmissive thus the dwell time should be close to the transit time. Note that for one-dimensional resonant tunneling through a double-barrier system where a classically forbidden region is present, the two times are usually considerably different[12] and τ_d is usually much larger than τ_t. It is known that the tunneling process is mediated by quasibound states inside the junction region. Hence the lifetime of a quasibound state τ_q can be another relevant time scale. If we view the transfer of electrons from one wire to the other as through a resonance process, then the nature of the quasibound state which mediates the resonance can be inferred from a static calculation.[9] For instance, using the transfer coefficient T as a function of the incident energy E, the half-width at half maximum of the peak of $T(E)$, Δ, is related to τ_q: $\tau_q = \hbar/\Delta$. For $k_0a = 0.6$ (corresponding to Fig. 3) we have $\Delta = 1.5$ meV or $\tau_q = 0.4$ ps from a static calculation.

We have also examined different structural parameters. For $a = L = 100$ Å, $b = 520$ Å, and $V_0 = 3.4$ meV, a static calculation[9] indicates that the transfer coefficient $T(E)$ reaches unity at a larger momentum $k_0a = 5.32$, which is just below the threshold of the second subband $k_0a = 5.44$. Dynamically, we use a wave packet with $\sigma = 400$ Å and time step of 0.116 fs about 63% of the wave transfers. In this case we found that the dwell time $\tau_d = 0.119$ ps (see Fig. 4), which can be compared with the transit time $\tau_t = 0.11$ ps. Again, these two time scales are essentially the same. As before, the lifetime of the quasibound state is estimated from a static calculation where we found $\Delta = 5.5$ meV, thus $\tau_q \sim 0.114$ ps, which happens to be close to the other two times.

Another interesting situation which we studied is the propagation in a quantum wire in which a narrow double constriction is put in place. See Fig. 1(b). In this structure the energy of the propagating electron in the first subband in the wider region may be lower than the propagation threshold of the constrictions. This leads to a classically forbidden region where electrons can only tunnel through. For certain energies resonant tunneling is observed.[17] The temporal behavior of this structure has been studied using the same method as above. In particular, for a variety of system parameters where resonant tunneling occurs, the dwell time as defined above is considerably larger than the transit time, similar to the case of one-dimensional resonant tunneling. Typi-

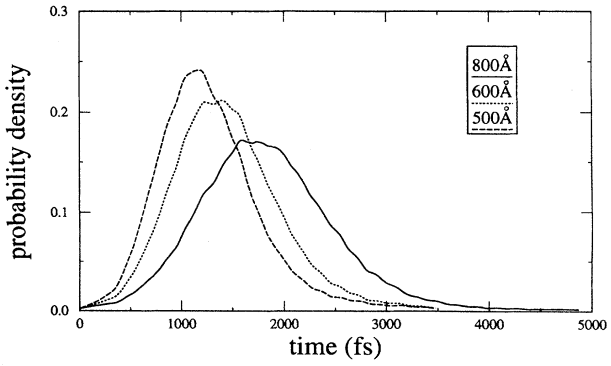

FIG. 3. The electron density ρ inside the junction region Ω=VI+VII+V vs time t (fs). Parameters: $a = L = 100$ Å, $b = 440$ Å, $k_0a = 0.6$, and $V_0 = 4.54$ meV. Here the solid line, dotted line, and dashed line correspond to the spatial spread of incoming electron wave packet $\sigma = 800$ Å, 600 Å, and 500 Å, respectively.

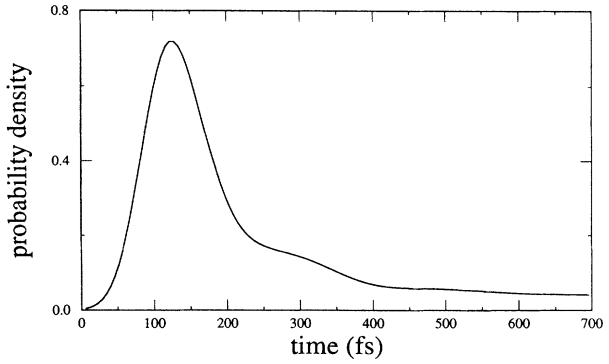

FIG. 4. The electron density ρ inside the junction region Ω vs time t (fs). Parameters: $a = L = 100$ Å, $b = 520$ Å, $\sigma = 400$ Å, $k_0a = 5.32$, and $V_0 = 3.4$ meV.

cally, we found $\tau_d/\tau_t \sim 5$. For instance, for "barrier" width $w = 60$ Å, well width $l = 140$ Å, the width of the wire $a = 600$ Å, and $k_0 a = 0.66$ the dwell time is found to be $\tau_d = 0.383$ ps while the transit time is $\tau_t = 0.072$ ps. This difference in the two time scales is understandable since the resonant tunneling process leads to a time delay, such as what happens in one-dimensional tunneling diodes. Finally, we have also studied the temporal response of the T-shaped quantum modulated transistor proposed by Sols *et al.*[4] In this case, the wave propagation is continuous and thus the switching time is comparable to the transit time.

In summary, we have presented an extensive investigation on the temporal behavior of ballistic transport in two-dimensional quantum-wire structures. In particular, results for two useful time scales were presented for the electron waveguide coupler and quantum wire with narrow double constriction. The dwell time of the former is ranging from 0.12 to 0.27 ps for typical system parameters and is of the same order as the corresponding classical transit time. For the latter case, the two time scales are quite different due to the resonant tunneling nature.

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