Wigner Function Model of Quantum Transport in an Electron Waveguide

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A Wigner function model is successfully formulated for the first time to simulate the quantum mechanical transport in an ideal electron waveguide. The temperature dependence of the two terminal conductance of a perfect electron waveguide and the static and dynamic behavior of an electron waveguide with a potential barrier(well) are presented. For an abrupt switching to a certain well potential, an oscillatory current transient is observed due to the resonance of electron.

1. INTRODUCTION

An electron waveguide is a wire that is so clean and so small that electron waves can propagate in guided modes. It is now possible to make it using molecular beam epitaxy in conjunction with high resolution electron beam lithography. The two terminal electrical conductance of a perfect electron waveguide is quantized as a function of the width. Furthermore, the conductance is expected to be controlled by the potential barrier(well) formed inside the wire as shown in Fig. 1, where the barrier height is varied by an external gate voltage. In this paper, the Wigner function model, that has been a promising tool for quantum transport modeling of quantum well electronic and optical devices[1-3], is successfully formulated for the first time to simulate the quantum mechanical transport in an ideal electron waveguide. The static and dynamic behavior of an electron waveguide with a potential barrier(well) are discussed. In the static analysis, the Wigner function model is compared with the Landauer formula. For an abrupt switching of a barrier potential, the current transient response is discussed.

2. WIGNER FUNCTION MODEL FOR AN ELECTRON WAVEGUIDE

In the electron waveguide model with the potential barrier(well) shown in Fig. 1, the barrier height \( eV_B \) is varied as a function of external gate voltage. For the confinement of electron waves in the transverse(depth and width) directions, the infinite potential barriers are assumed. In the depth direction, only the fundamental mode is considered. The contacts to the wire are assumed to be the reservoirs characterized by the thermal equilibrium distribution of electrons. In this simple model, the three dimensional quantum Liouville equation with respect to the Wigner function is transformed into the following one dimensional equation.

\[
\frac{\partial F_W}{\partial t} = -\frac{\hbar k \partial F_W}{m^* \partial z} - \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{dk'}{2\pi} V(z, k-k') F_W(z, k'),
\]

where \( V(z, k-k') \) is the Fourier transform of the potential energy function for electrons and \( F_W(z, k) \) is the Wigner function integrated over the transverse momenta and coordinates. Using \( F_W(z, k) \), the total current \( J(z) \) is found represented by

\[
J(z) = e \int_{-\infty}^{\infty} \frac{dk}{2\pi m^*} F_W(z, k),
\]
For an electron waveguide with the dimensions of $L_2$, $L_y$, and $L_z$, the boundary conditions for the Wigner function at the left and right boundaries are given by

$$F_W(0, k) = \sum_n 2f_{FD}(k, k_n^0, k_z^0), \quad k > 0 \quad (3)$$

$$F_W(L_z, k) = \sum_n 2f_{FD}(k, k_n^0, k_z^0), \quad k < 0 \quad (4)$$

where $f_{FD}$ is the Fermi-Dirac distribution function characterized by the Fermi level $E_F$, the temperature $T$, $k_n^0 = n\pi/L_y$, where $n$ is the mode number, and $k_z^0 = \pi/L_z$. The Fermi level is assumed 10meV throughout the paper.

Eq.(1) is solved numerically based upon the finite difference method. However, since the results of the Wigner function simulation depend critically on the numerical method used, the discretization of eq.(1) must be performed carefully. Essentially, the finite difference approximation must be consistent with the analytic forms of equations, not only the quantum Liouville equation but the moment equations derived from it. As a more consistent approximation to the moment equations, the weighting function given by $\sin(k)/k$ multiplied to the discretized Fourier transform of the potential energy function. Particularly, in the analysis of the electron waveguide, the above approximation is useful because the Wigner function is localized near $k = 0$.

3. QUANTUM TRANSPORT SIMULATION IN AN ELECTRON WAVEGUIDE

First, to verify the validity of our model, the two terminal conductance of a perfect waveguide is studied. The applied bias voltage $V$ is 50μV and the electron effective mass is assumed 0.067$m_0$ throughout the device, where $m_0$ is the free electron mass. Fig.2 shows the temperature dependence of the conductance as a function of the width. Note that the curves other than $T = 0$ are illustrated by shifting 30nm each to the right not to overlap. The clearly quantized steps of $2e^2/h$ at $T = 0$ are found to become ambiguous with temperature. Thus, it is essential for the quantization of conductance that the temperature is much smaller than the separation between transverse energy levels. For example, at $T = 4K$ the quantized steps become ambiguous over the fourth step, where the fundamental transverse energy $E_{kT} = \hbar^2\pi^2/2mL_y^2$ becomes comparable to the thermal energy $k_BT = 0.34meV$.

Next, the variation of the two terminal conductance of a wire with the configuration shown in Fig.1 is studied. Fig.3 shows the variation of the conductance as a function of barrier(well) potential $eV_B$ for $L_B = 5.1nm$. Since the width of the wire is fixed 30nm in this example, only one width mode can propagate in the wire. In the figure, the solid and the dashed lines correspond to the Wigner function model and the so-called Landauer formula, respectively. In the Landauer formula, the intensity transmission probability of the guided mode with different electron energy is summed assuming the distribution function given at the reservoirs. On the other hand, in the Wigner function model the distribution function excited at one reservoir is found spread in the $k$(wave number) space as it travels through the wire due to the barrier(well) potential repulsion as shown in Fig.4. Such a nonlocal effect of the potential in the Wigner function model, which seems to be more practical, causes the discrepancy of the two curves in Fig.3.
shown in Fig. 5(a). After such a initial current response, the current approaches to the steady state value. On the other hand, for the negative barrier potential switchings, the remarkable current oscillation continues till about 2.0ps as shown in Fig. 5(b). This current oscillation is considered due to the resonance of electron in the potential well. In fact, as is seen in Fig. 3, the conductance decreases abruptly at $V_B = -50$mV, because electrons are trapped in the well due to resonance. Consequently, this current oscillation is observed only for the potential switching to $V_B = -50$mV.

4. CONCLUSION

The Wigner function model has been successfully formulated for an ideal electron waveguide for the first time. After showing the validity of the formulation, it is applied to the simulation of the static and transient behaviors of an electron waveguide with a potential barrier(well). In this paper, the self-consistent calculation in the electrostatic potential is not performed. Since the space charge may affect the transport characteristics of electron waveguides, we will have to study the quantum transport model incorporating self-consistent space charge effects. Further, we will extend our model to electron waveguides in two spatial dimensions to make it more applicable to practical devices.

5. REFERENCES