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Analysis of Quantum Waveguide: Effective Width and Height of Potential for Quantum Wires under Split Gates

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In order to apply quantum waveguides to electronic devices, we calculate the electrostatic potential in the split-gate quantum wire and establish the relation between the electrostatic potential and the square well potential which is usually assumed in simulations of these waveguides. The height and width of the square well potential are expressed as simple functions of the gate voltage and their dependencies are clarified. The results may be useful in calculating the characteristics of electronic devices based on quantum waveguides as functions of controllable parameters such as gate voltage.

1 Introduction

Recent progresses in semiconductor fabrication process have made it possible to realize structures in which electrons are confined with low dimensionalities. These structures are called quantum wells or wires and are expected to be useful elements of new electronic devices. As one of such devices, quantum waveguides have been proposed and extensively investigated. The dimensions of quantum waveguides are smaller than the mean free path of electrons and electrons are considered to propagate free from influences of impurities.

The properties of quantum waveguides are determined by its structure and the energy of incident electrons. In order to apply quantum waveguides to electronic devices, its properties have to be changed by external parameters such as bias voltage. For example, it has been proposed to control the waveguide of split-gate type by the applied gate voltage through the change of the width of channel.[1, 2] In this case, we need the information on the relation between gate voltage and the width of the quantum wire.

In the analysis of quantum waveguides, the potentials for electrons are usually assumed to be combinations of, often infinitely high, square well potentials. In our recent investigation, the condition of infinite height has been relaxed and the freedom of geometrical deformation has been taken into account.[3] The shape of the potential, however, is still represented by sharp steps. In realistic waveguides controlled externally electrons are in the potential which resembles but not is equal to the combinations of the square wells.[4, 5] In order to apply the results of theoretical analyses to electronic devices, we have to establish the relation between real potentials and square well potentials.

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In this paper, we analyze the electrostatic potential profile of the split-gate quantum wire and evaluate effective width and depth when this electrostatic potential is represented by a square well potential.

2 Structure and Boundary Conditions

As the simplest case, we consider the two-dimensional system shown in Fig.1 which consists of the gate electronodes, the AlGaAs/GaAs part with the electronode attached to the bottom, and the vacuum part ($\varepsilon = 1$). A quantum well parallel to the x-y plane is located under the gates and electrons form a two-dimensional electron gas when gate electronodes are not biased.

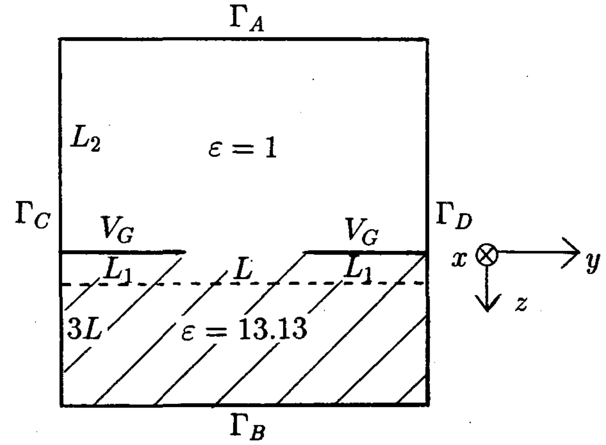

Figure 1: Model of two-dimensional split-gate quantum wire. In z-direction, electrons are confined by band offset in a plane shown by dotted line.

When the bias of the gate is negative, electrons are confined by the electrostatic potential in the y-direction and we have a quantum wire. We obtain the electrostatic potential $V(\mathbf{r})$ solving Poisson's equation

$$-\nabla \cdot [\varepsilon(\mathbf{r})\nabla V(\mathbf{r})] = 4\pi n(\mathbf{r}) \tag{1}$$

by the finite element method. Here $\mathbf{r} = (x, y)$ and $n(\mathbf{r})$ is a charge density. In this paper, we neglect the Hartree potential due to electrons in the quantum wire. In other words, we assume $n(\mathbf{r}) = 0$ except for the gate and bottom electronodes. The boundary conditions are

$$V(\mathbf{r}) = \begin{cases} V_G & \text{on gate,} \\ 0 & \text{on } \Gamma_A,\ \Gamma_B, \end{cases} \tag{2}$$

and

$$\frac{\partial V(\mathbf{r})}{\partial y} = 0 \quad \text{on } \Gamma_C,\ \Gamma_D. \tag{3}$$

The width of the split gate is L. The length of gate electronodes L_1 and the distance between gates and upper boundary L_2 are chosen to be $9L$ and $1800L$, respectively. These length are taken to be sufficiently long in order not to influence the electrostatic potential around gates.

The confinement in the z-direction is provided by the conduction band offset of GaAs and $Al_xGa_{1-x}As$, but we neglect the difference between dielectric constants of two materials (ε(GaAs) = 13.13 and ε(AlAs) = 10.08). We obtain the wave function in the quantum wire by solving one-dimensional Schrödinger equation in the electrostatic potential along the y-direction $V_e(y)$. We show $V_e(y)$ in Fig.2 in the case where the x-y plane is at $0.2L$ from the gates. We denote the amplitude of $V_e(y)$ by V and the wave function and the energy eigenvalue of the ground state by $\psi_e(y)$ and E_e, respectively.

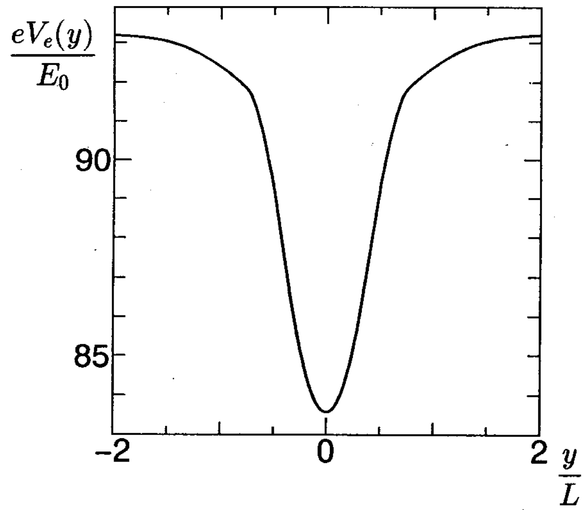

Figure 2: Example of electrostatic potential along y-direction $eV_e(y)/E_0$ at $0.2L$ from gate electronodes when $eV_G/E_0 = 100$, E_0 being $(\hbar^2\pi^2)/(2m^*L^2)$.

3 Evaluation of Effective Width and Height

In order to establish the correspondence between the electrostatic potential and the square well potential, we have to determine the height V_s and width w of the latter. There are two unknowns, V_s and w, to be determined by a given shape of the electrostatic potential and we need some physical consideration.

When the square quantum well has the energy eigenvalue of ground state E_s, the wave number of propagation in the channel is related to $E - E_s$, where E is the incident energy of an electron, and the penetration into the barrier is controlled by $V_s - E$. Since the latter is rewritten as $(V_s - E_s) - (E - E_s)$ by shifting the zero of the energy, we can regard the parameter characterizing the height of the barrier to be $V_s - E_s$.

Based of the above consideration, we calculate the parameters V_s and w for a given electrostatic potential $V_e(y)$ by minimizing $\int |\psi_s(y) - \psi_e(y)|^2 dy$ with respect to the values of V_s and w under the condition that $V_s - E_s = V - E_e$. Here $\psi_s(y)$ is the wave function of ground state in the square well potential.

We show the width of square well potential normalized by L, w/L, as a function of the gate voltage eV_G/E_0 in Fig.3. Here E_0 is $(\hbar^2\pi^2)/(2m^*L^2)$ (m^* is the effective mass of electron). If L and m^* are chosen to be 100Å and $0.067m_e$, respectively, $eV_G/E_0 = 10$ corresponds to $V_G = 0.5$V. The quantum well is located at $0.2L$ from the gates. When $eV_G/E_0 \gtrsim 2$, wave functions decay sufficiently at the boundaries Γ_C and Γ_D.

When $eV_G/E_0 \gtrsim 50$, w/L has the dependency of $V_G^{-0.2}$. We show the fitting function $2.0(eV_G/E_0)^{-0.2}$ in Fig.3. In this case, the energy eigenvalue E_e is less than $0.25V$. Since E_e is relatively low compared with V, $V_e(y)$ can be considered as a parabolic potential. It is well known that the ground state wave function in a parabolic potential is the Gaussian and thus the wave function in the barriers decays rapidly. When $eV_G/E_0 \lesssim 7.0$, on the other hand, w/L has a different dependency on V_G. In this case, E_e is larger than $0.5V$ and is located at relatively higher position than in the former case. The electrostatic potential can be regarded as a constant and the wave function in the barrier may be proportional to $\exp(-|y|/\lambda)$. Therefore the dependence of the width of wire w on V_G is different and more sensitive to V_G.

In Fig.4, we show the height of the square well potential V_s as a function of V_G. We observe that V_s is proportional to V_G in the whole region and approximately expressed by $0.097V_G$. Since V is proportional to V_G (the Poisson's equation is linear), this indicates that V_s is proportional to V. Since we are imposing the condition $V_s - E_s = V - E_e$, the linear dependence of V_s on V is not a trivial result.

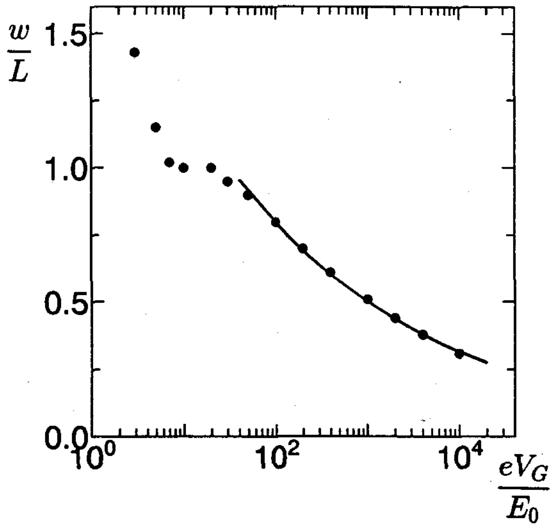

Figure 3: Width of square well potential w/L as function of eV_G/E_0. Solid line represents interpolation formula $2.0(eV_G/E_0)^{-0.2}$.

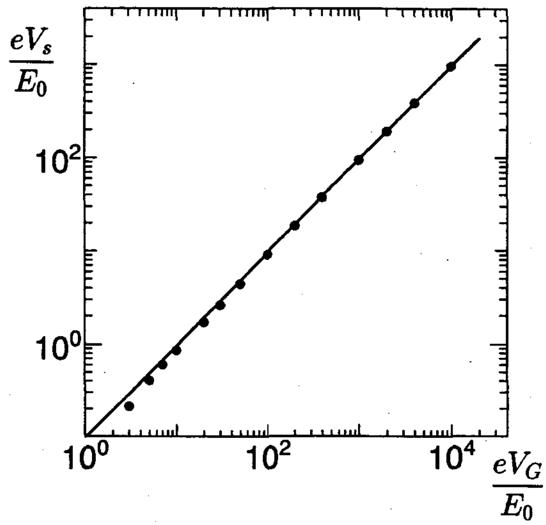

Figure 4: Height of square well potential eV_s/E_0 as function of eV_G/E_0. Solid line represents interpolation formula $0.097eV_G/E_0$.

Based on these results, we can interpret the results of simulations in square well potentials into the characteristics of realistic quantum waveguides realized by split gates. In these low dimensional system of electrons, the effect of electron-electron interactions sometimes play an important role.[6] The analysis of the many electron effects in this kind of structure is in progress and will be reported elsewhere.

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