

## Numerical Study of the Interference Effects of the Electron Waves Scattered by Impurities in the Quasi One-Dimensional System

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We present a numerical method to investigate transport phenomena through a region, where the obstacles are placed, in a quantum wire. Using the method, the interference effects between the incident electron wave and the electron wave scattered by the impurity have been investigated. Transport phenomena through slits in a quantum wire have also been studied.

### 1. INTRODUCTION

There have been increasing interests in the ballistic transport phenomena in quasi one-dimensional systems.<sup>1-3)</sup> In these systems, the positions of impurities play an essential role in the quantum conduction, because of the interference effects of electron waves. Recent advances in the STM and nanolithography techniques have made it possible to place impurities on various positions in the sample with dimensions smaller than the mean free path. There has been a great interest in the possibility of realizing electron devices based on the quantum mechanical behavior of electron, where the interference of electron waves plays an important role in their operation principles. Several researchers have numerically investigated the interference effects in quantum wires with various structures and potentials.<sup>4,5)</sup>

In this paper, we show a useful method for studying the electron conduction through a region containing a small number of impurities in the quasi one-dimensional system by solving the Lippmann-Schwinger equation. We have also studied the interference effects of electron waves around slits.

### 2. MODEL

We consider a quantum wire consisting of three regions, as shown in Fig. 1, and introduce the following tight-binding model:

$$H = H_0 + V, \tag{1}$$

$$H_0 = t \sum_n \sum_{m=1}^{M-1} (C_{n,m+1}^\dagger C_{n,m} + C_{n,m}^\dagger C_{n,m+1}) + t \sum_n \sum_{m=1}^M (C_{n+1,m}^\dagger C_{n,m} + C_{n,m}^\dagger C_{n+1,m}) + \sum_n \sum_{m=1}^M U_m C_{n,m}^\dagger C_{n,m}, \tag{2}$$

$$V = \sum_{n=1}^N \sum_{m=1}^M v_{n,m} C_{n,m}^\dagger C_{n,m}, \tag{3}$$

where  $C_{n,m}$  is the annihilation operator at the lattice site  $(n,m)$ ,  $t (< 0)$  the hopping integral between the nearest neighbors,  $U_m$  the confinement potential in the  $y$ -direction and  $v_{n,m}$  the potential of the obstacle. The eigenfunctions and the eigenvalues of unperturbed Hamiltonian  $H_0$  can be written as

$$|\phi_{l,k}\rangle = \sum_{n,m} \alpha_{l,m} \exp(ikan) |n,m\rangle, \tag{4}$$

$$E_{l,k} = \epsilon_l + 2t \cos(ka). \tag{5}$$

Here,  $|n,m\rangle$  is an atomic orbital at  $(n,m)$ ,  $a$

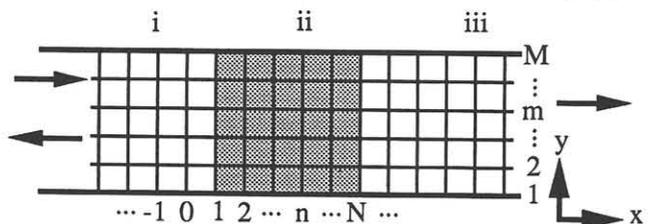


Fig. 1 Schematic illustration of the system. The impurities exist only in region ii. The parameters  $M$  and  $N$  are the lattice numbers for the  $y$ -direction of the wire and for the  $x$ -direction of the region ii, respectively.

the lattice constant,  $l(=1,2,\dots)$  the mode of the subband, and  $k$  the wave vector in the  $x$ -direction. The coefficients  $\alpha_{l,m}$  and the subband energy  $\varepsilon_l$  can be obtained from the Schrödinger equation;

$$t\alpha_{l,2} + U_1\alpha_{l,1} = \varepsilon_l\alpha_{l,1},$$

$$t(\alpha_{l,m+1} + \alpha_{l,m-1}) + U_m\alpha_{l,m} = \varepsilon_l\alpha_{l,m} \quad (2 \leq m \leq M-1), \quad (6)$$

$$t\alpha_{l,M-1} + U_M\alpha_{l,M} = \varepsilon_l\alpha_{l,M}.$$

Following the Lippmann-Schwinger equation, the wave function can be expressed as

$$\langle n,m | \psi \rangle = \langle n,m | \phi_{l,k_l} \rangle + \sum_{n'=1}^N \sum_{m'=1}^M \langle n,m | G_0(E) | n',m' \rangle v_{n',m'} \langle n',m' | \psi \rangle, \quad (7)$$

where the wave vector  $k_l (>0)$  is given by  $E = \varepsilon_l + 2t\cos(k_l a)$ . Green's function for the unperturbed part  $H_0$  can be straightforwardly calculated as

$$\langle n,m | G_0(E) | n',m' \rangle = \langle n,m | \frac{1}{E + i0 - H_0} | n',m' \rangle = \sum_{j=1}^M \frac{i\alpha_{j,m}\alpha_{j,m'}}{2t\sin(\kappa_j a)} \exp(i\kappa_j |n-n'|a). \quad (8)$$

The quantity  $\kappa_j (>0)$  equals  $(1/a)\cos^{-1}[(E - \varepsilon_j)/(2t)]$  for the propagating mode and  $(1/a)\cosh^{-1}[(E - \varepsilon_j)/(2t)]$  for the evanescence mode. The total number of modes (sum of the propagating and evanescence modes) is set to the total number of the  $y$  sites,  $M$ . For simplicity, we consider the case where the impurities possess an infinitely strong potential ( $V=1000|t|$ ) and  $U_m = 2|t|$ .

### 3. RESULTS AND DISCUSSION

#### (1) Transport phenomena through a quantum wire containing two impurities

First, we consider a quantum wire containing two impurities which locate at the center of the wire. The number of the propagating mode is set to unity ( $E_F = -1.99|t|$ ). Figure 2 shows the conductance calculated with the use of Landauer's formula.<sup>1)</sup> As can be seen from Fig. 2, the conductance oscillate as a function of a distance between the two impurities. When the distance between the two impurities equals  $29a + 85an/2$  ( $n = 0,1,2,\dots$ ), a

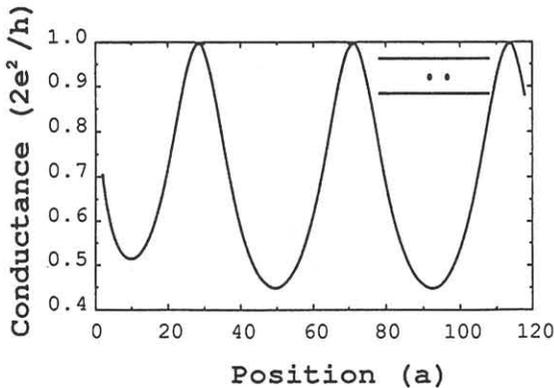


Fig. 2. Conductance plotted as a function of distance between the two impurities. The two impurities are located at the center of the wire. The Fermi wavelength is  $85a$ . The width of the wire is  $51a$ .

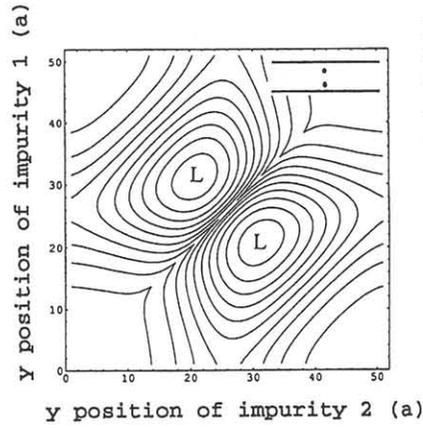


Fig. 3. Contour plot of the conductance for the two impurities system, where the  $x$  position of the two impurities are  $1a$ . L denotes the lowest value of conductance. The width of the wire is  $51a$ . The Fermi wavelength is  $85a$ .

resonant tunneling can be observed. The conductance behavior is analogous to that calculated analytically in the one-dimensional system containing two impurities possessing weak potentials.

Next, we discuss transport phenomena for the case where the two impurities are located at the same  $x$  position and the number of the propagating mode equals unity. Figure 3 shows the dependence of conductance on the  $y$  positions of the two impurities as a contour plot. The conductance is minimized when the distance between the two impurities is  $10a$ , and the distance between the impurity and the edge is  $20a$ . The positions of the minima of the conductance are unchanged in the range of  $-1.996$  to  $-1.986|t|$  for the Fermi energy, where the number of the propagating mode equals unity. This constancy is considered to indicate enough stability for device applications, since a device will be insensitive to changes in the Fermi energy within this range.

#### (2) Quantum conduction through slits in a quantum wire

Okada *et al.* reported the measurement of the angular distribution of electron injected through a quantum point contact using the two Schottky split gates system in the presence of a magnetic field  $B$ .<sup>6)</sup> In this study, we have considered the quantum mechanical effects for the double slit system, using our numerical method, and calculated results have been attempted to compare with the experimental results.<sup>6)</sup> We consider the quantum wire possessing two slits which are sequentially arranged along the  $x$ -direction, and the first and second slits act as injector and detector, respectively. In our geometry, the effects of the reflected waves scattered by the edges can also be found, although the width of the wire in the experiment is regarded to be infinite. Since we have considered the case of  $B=0$ , we have calculated the conductance as a function of the  $y$  position of the lower end of the detector in order to compare these results with the experimental findings in which the conductance was observed as a function of the magnetic field strength.

Figure 4A shows the calculated conductance for the double slit system, where one propagating mode is allowed to exist in the injector. When the difference of the  $x$  position between the injector and the

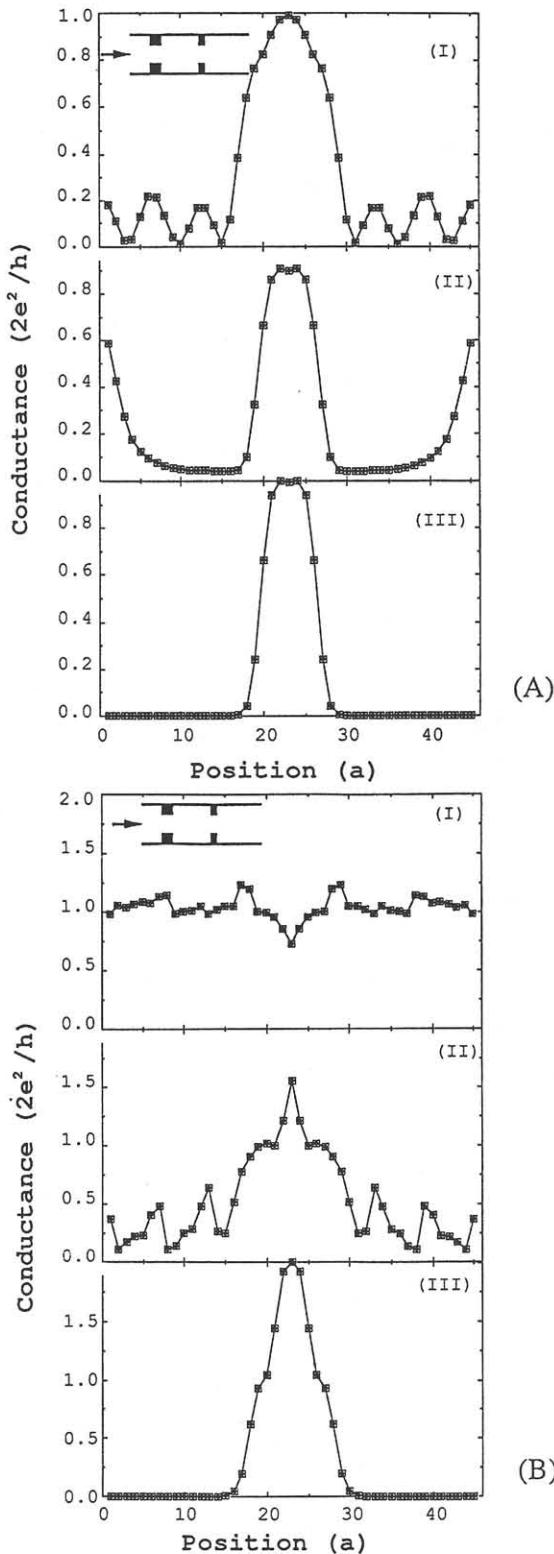


Fig. 4. Dependence of the quantum wire conductance on detector location. The widths of the wire, injector, and detector are  $50a$ ,  $6a$ , and  $6a$ , respectively. The difference of the  $x$  position between the two slits is  $8a$  (I),  $5a$  (II), and  $2a$  (III). The Fermi energy is  $-1.60 \text{ t}$  (A) and  $-0.61 \text{ t}$  (B).

detector equals  $2a$ , the calculated conductance shows a single peak structure. When the difference of  $x$  position between the two slits becomes  $5a$ , the edges of the conductance curve rise. This is due to the interference among the incident wave and the scattered waves. We can easily notice the interference effects in Fig. 4AI. When two propagating modes are allowed to exist in the injector (Fig. 4B), the interference effects are pronounced, compared with the single mode case. This is because the magnitude of momentum for the  $y$ -direction in the double mode case is larger than that in the single mode case. We can find a shoulder structure around the center peak in Figs. 4BII and 4BIII. As the distance between the two slits increases, the center peak gradually disappears and the double peak structure is found (Fig. 4BI). The aspects in Figs. 4AI and 4BI are considered to be analogous to those in the experiment in both single and double mode cases. Although it is necessary to discuss the magnetic field dependence of the conductance for precise comparison of the calculation with the experiment, the interference effects are correctly taken into account in our calculations.

#### 4. CONCLUSION

We have presented a numerical method to study transport phenomena through a quantum wire with various potentials in the ballistic transport regime. We have calculated the conductance for the two impurities and two slits systems precisely. Our formulation can also be extended to treat cases in which magnetic field is present.

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