Electronic States and Electron Wave Transfer in Coupled Quantum Wires and Its Control by Externally Applied Electric Field

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SYNOPSIS

Quantum mechnical electron wave transfer between two quantum wires which are weakly coupled via a thin potential barrier is considered. The total electronic states are calculated with both analytical (no field case) and numerical methods (under applied electric fields). The transfer efficiency is evaluated for several specified cases of geometrical structures, potential barrier heights and the externally applied electric field. Estimated trasfer time is of the order of one picosecond in typical mesoscopic structures. The model in this paper can be used to determine important structure parameters for experiments on electron directional coupler controled by external elctric field.

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1 Introduction

The quick and great development of recent material growth and microfabrication technologies which are used mainly in producing VLSI enables us not only to observe the quantum mechanical phenomena directly [1] - [3] but also to open a way to apply them to a novel device. Another mesoscopic systems are realized in the field of fine particles etc.

One of primary points of these mesoscopic systems is that the mean free path of electrons is the same order or even large than the system size at low temperatures. Thus the wave nature of electrons appears directely and various characteristic phenomena based on the phase coherency of electron wave functions have been observed [4]. For examples, the Aharonov-Bohm effect (AB), the universal conductance fluctuation (UCF) and the Altshuler-Aharonov-Spibak effect (AAS) are a few typical examples of them [5] - [7].

These effects are important because they are the manifestation of quantum nature of a single electron which is related to the observation problem still remained to be unsoled in the quantum mechanics.

Similarly, quantum beat treated in this paper is one of another typical quantum effects occurring in such mesoscopic system [1]. Let us consider a structure consisting of parallel two quantum wires which are weakly coupled via a thin potential barrier. If the barrier is infinite, the electronic states are completely independent and the energy levels are calculated by solving the Schrödinger equation for each wire separately. In the case of finite barrier height, the transfer integral (Hamiltonian matrix element) between two wires does not vanish and it is necesarry to solve the Schrödinger equation for a total system of two wires.

As long as the coupling between two wires is not so strong [8], the perturbational treatment of the complete system is still possible. In this case, the ground state and the first excited state may be well approximated by the symmetric and the antisymmetric linear combination of the lowest states of each wire, respectively : The coefficients of linear combination depend not only on the energy eigenvalues calculated under the independent wire approximation but also on the matrix element via the thin finite potential barrier [8].

Suppose that we have an electron localized in one of wires in such a system. This state is not the eigenstate of total system but is a superposition of the ground state and the higher energy levels. For example, the superposition of the symmetric and antisymmetric states (the ground state and the first excited state) in the case of equal width wires gives the almost localized state in one of wires. Hence, the probability amplitude in one wire shows an oscillatory modulation (quantum beat) as obtained by solving the time dependent Schrödinger equation under the initial condition of a localized electron in one of wires. Experimentally, this has been observed in an

exciton system of coupled quantum wells [9]-[11].

Recently, one of authors (N.T) and his collaborators have treated this problem in two parallel quantum wires based on the perturbational approach under the independent wire approximation and proposed an electron wave directional coupler using this quatum beat effect [12]. Similar idea has been proposed in the other works independently [13] and in a later work [14] : The direct analog of an optical directional coupler has played an important role in their works. This type of problems has also been theoretically treated in several works for coupled quantum wells, for example, in [15], [16].

Previous treatment, however, is rather qualitative and particularly is lacking the quantitative calculation with respect to *the controling performance evaluation of the quantum beat effect by an externally applied electric field.* Furthermore, their approach becomes less valid, when the structure difference becomes larger or the coupling of two wires becomes stronger, and/or when one introduces an external electric field including the graded potential variation inside of wires as well as the barrier region. The purpose of this work is to give a non-perturbational and quantitative description of this problem, particularly the effect of an externally applied electric field. The results may be useful to choose the structural parameters in preparing an experiment.

2 Model of Weakly Coupled Two Quantum Wires

2.1 The Eigenvalue Equation as Total System

Structures of two parallel wires considered in this paper are shown in Fig.1. We try to describe this system by a model in which two wires with a thin potential barrier of finite height between them are surrounded by an infinitely high potential wall. As shown in the figure, an external electric field can be applied perpendicularly to the thin barrier between wires.

It is possible to consider the case that the potential barrier height surrounding the two wires is finite. However, in that case, we must resort to the numerical treatment to solve the Schrödinger equation as total system. Then the investigation of separating barrier effect becomes rather difficult and tedious. This is one of reasons why we employ the infinite potential model of surrounding barrier.

The Schrödinger equation for this model may be written as

$$\mathcal{H}\varphi(x,y,z) = E_{tot}\varphi(x,y,z) \tag{1}$$

with

$$\mathcal{H} = -\frac{\hbar^2}{2m}\Big(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\Big) + V, \tag{2}$$

where V is the potential energy, including the externally applied electric field. We plot the potential profile of V in Fig.2 and refer to three different regions as region-1, -2 and -3, respectively.

Since the potential is infinite at outer boundaries of our system, eigenfunctions of $\mathcal{H}$ can be written in the following form :

$$\varphi(x, y, z) = \psi(x)\phi(y)e^{ik_z z} \tag{3}$$

Substituting 3 into 1 and noting that V depends only on x, we get

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E_x\psi(x), \tag{4}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(y)}{dy^2} = E_y\phi(y), \tag{5}$$

and

$$E_x + E_y + \frac{\hbar^2}{2m}k_z^2 = E_{tot}. \tag{6}$$

Hereafter, we denote E_x simply by E and discuss mainly eq.4 in the coordinate x.

If there is no electric field, it is easy to solve the eigenvalue equation analytically. Taking an exponential function in the region-2 (the barrier region) and sinusoidal functions in the region-1 and the region-3 (the wire regions), and imposing usual boundary conditions for eigenfunctions [8]. We obtain the equation determining the energy levels

$$\frac{\tan{(KA)} + \tan{(KB)}}{(U_0 - K^2)\tan{(KA)}\tan{(KB)} + K^2} = -\frac{\tanh D\sqrt{U_0 - K^2}}{K\sqrt{U_0 - K^2}}, \tag{7}$$

for the case $K^2 < U_0$ and

$$R\sin KA(R\sin KB\sin RD - K\cos KB\cos RD) \tag{8}$$

$$-K\cos KA(K\cos KB\sin RD + R\sin KB\cos RD) = 0 \tag{9}$$

with

$$R = \sqrt{K^2 - U_0} \tag{10}$$

for the case of $K^2 > U_0$. In the expressions, all variables are normalized by appropriate constants ; $A = a/L_0$ (width of region-1), $D = d/L_0$ (width of barrier region), $B = b/L_0$ (width of region-3), $\hbar^2/2mL_0^2 = \mu$ (energy unit), $U_0 = V_0/\mu$ (barrier height), $K = L_0 k$ (wave vector), where L_0 is taken as $10\mathring{A}$ for conveniency in the present paper.

In the presence of the electric field, however, we resort to the numerical method : Analytical solutions are still avairable but not convenient to handle. In this paper, the finite element method [17] is employed to solve the equation 4.

2.2   Time Dependent Solution Starting from Localized State of An Electron in One of Wires

We now study the time development of electronic states localized in either of wires at the beggining. The solution of the time dependent Schrödinger equation

$$i\hbar\frac{\partial\psi(t, x)}{\partial t} = \mathcal{H}\psi(t, x) \tag{11}$$

may be given as

$$\psi(t,x) = \sum_{n}^{\infty} c_n \psi_n(x) e^{-i\frac{E_n}{\hbar}t} \tag{12}$$

where $\{ \psi_n(x) \}$ is a complete orthonormal set of eigenfunctions of our system and in this paper we take

$$\psi(0,x) = \sqrt{\frac{2}{A}} \sin \frac{\pi}{A} x \qquad (0 \leq x \leq A) \tag{13}$$

as the initial condition which describes the state of one electron localized in one of two wires. The coefficient c_n's are thus determined by

$$c_n = \int_0^A \psi(0,x)\psi_n^*(x)dx \tag{14}$$

The probability that an electron exists in the other wire at time t is calculated as

$$F(t) = \int_{A+D}^{L} | \psi(t,x) |^2 dx \tag{15}$$

where $L = A + D + B$.

All these procedure are performed numerically in the presence of externally applied electric field using the finite element method.

3   Eigenfunctions and Electron Transfer With and Without External Electric Field

Let us first present the energy levels and their eigenfunctions in two cases of structures, (a) two wires having an equal width, $a = 40\mathring{A}, d = 8\mathring{A}, b = 40\mathring{A}, V_0 = 0.2667$ eV, and (b) two wires having a different width, $a = 40\mathring{A}, d = 8\mathring{A}, b = 30\mathring{A}, V_0 = 0.2667$ eV. The results are shown in Table.1 and in Fig.3. Note that the probability amplitude profile is quite different for these two cases.

As mentioned in the introduction, the structural difference between two wires appears in the eigenstate wave function as the difference of amplitudes in each wire. For example, when one wire has a larger width than the other as in the case (b), the groud state has a dominant amplitude in the lager wire and the first excited state has a dominant amplitude in the smaller wire. The case of equivalent wires gives the symmetric states for the ground state and antisymmetric states for the first excited state, as shown clearly in the figure.

The initial state of an electron localized in one of wires is expanded in the series as $\psi(0,x) = \sum_{n}^{\infty} c_n \psi_n(x)$ using the eigenfunctions belonging to the eigenvalues listed in the table. In the following example, we have computed this series expansion to the eighth order, but values of initial four c_n ($n = 1 \sim 4$) are listed in the table2. The probability amplitude profile of the approximate initial wave function is shown in Fig.4.

The probability $F(t)$ generally shows oscillatory modulations and takes the maximum at some t. Let us call the maximum value as "the transfer efficiency". Values of $F(t)$ are calculated and shown in Fig.5 in two structural cases of wires. It is clearly observed that an electron is almost completely transfered in the symmetric case but the efficiency is about two orders of magnitude less in the nonsymmetric case. The dependence of the transfer efficiency on the barrier height in the latter case is shown in Fig.6 which indicates that the transfer much decreases for higher barriers.

We now consider the effects of externally applied electric field. Let us first note that the ground state of the different width case has a dominat amplitude in the larger wire and the transfer efficiency is very small without an electric field. As shown in Fig.7 the profile of wave function strongly changes depending on the applied field and the amplitude of the narrower wire side greatly increases with the field.

From the perturbational point of view based on the independent wire approximation, this is interpreted as follows. By applying an electric field, the energy levels of each wire approach and, at some strength of field, become nearly degenerate, realizing the same situation as the equal width case. Eventually, the ocsillatory moduration of probability becomes nearly similar to the equal width case and results in the large transfer from one wire to the other.

When the field becomes too strong, however, the equivalent wire situation clearly breaks down (see Fig.8). Thus the electric field which gives the maximum of the transfer efficiency is expected to have some optimum value. One can confirm this from the result of actual calculation of tranfer efficiency as the function of field strength as shown in Fig.10. This situation is, in principle, similar to the resonant tunnelling phenomena [18].

An estimation of time τ necessary for an electron to transfer from one wire to the other in the present case gives 0.840 ps for the structure parameters, $a = 40\mathring{A}, d = 8\mathring{A}, b = 30\mathring{A}, V_0 = 0.2667eV, E_G = 1.64 \times 10^6(V/m)$. If we assume that electrons moves in the form of wave packets along the direction of wires, such wave packet moves

$$l_c = v_F\tau = 1.57 \times 10^8 \times 0.84 \times 10^{-12}(cm) = 1.3188 \times 10^4(\mathring{A}) \tag{16}$$

to the linear direction of wire, where the Fermi velocity is taken to be $v_F = 1.57 \times 10^8(cm/s)$ for a typical value [12]. Therefore, if the output wave guide is connected or the length of wire is chosen to be l_c, the electron can transfer to the other wire under the control of externally applied electric field.

4 Concluding Remarks

1. Under the assumption that the phase coherency of wave function is kept in a given mesoscopic structure, the ocsillatory modulation of probability amplitude (quantum beat) between

parallel two wires coupling via a thin potential barrier is analized with and without the existence of an externally applied field.

2. Time necessary for an electron to transfer from one wire to the other is estimated as the order of one picosecond for the typical mesoscopic strucutres.

3. The transfer efficiency strongly depends on the structure parameters and an externally applied electric field. Therefore, it suggests us that the phenomena can be applied to the electron directional coupler controlable by external electric field, if a proper structure is chosen.

There are several problems which are not considered in the present analysis, for example another characteristic effects in such mesoscopic system (UCF, localization effect along the wire etc. [19]) which will become important when one makes an experiment actually to observe "quantum beat" of carrier electrons, although the quantum beat occurring in the decay process of exciton states selectively excited in a coupled quantum well system having slightly different well width is already observed experimentally as appeared in a few reports.

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eV	(a)	(b)
E_1	1.8661×10^{-2}	1.9416×10^{-2}
E_2	2.0361×10^{-2}	3.2728×10^{-2}
E_3	7.3890×10^{-2}	7.7379×10^{-2}
E_4	8.1349×10^{-2}	1.2821×10^{-1}
E_5	1.6342×10^{-1}	1.7409×10^{-1}
....	.....	.....

Table 1: Eigenvalues of initial five energy levels. (a) symmetric width case, (b) nonsymmetric width case

	(a)	(b)
c_1	0.691083	0.979283
c_2	−0.700961	−0.106381
c_3	−0.128388	−0.143585
c_4	0.074810	−0.028903
....	.....	.....

Table 2: Coefficients of first four eigenfunctions in the series expansion $\sum_n^\infty c_n \psi_n(x)$ of the initial localized state $\psi(x, 0)$. (a) corresponds to symmetric width case, and (b), nonsymmetric width. Note that the ground state is enough to describe the localized state in the latter case but first two states have to be superposed with equal weight for the former case.

wave packets of
electrons

wire   A

wire   B

L

= a + d + b

Electric Field

Fig.1(a)

d

a   b
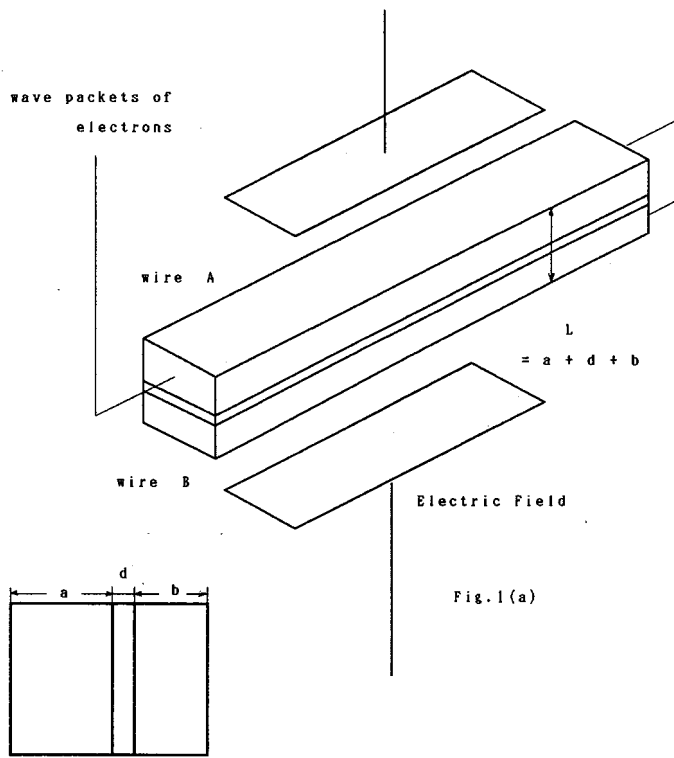
Figure 1: Schematic description of our model system (two parallel quantum wires). Except insides of wires and barrier region, the potential is assumed to be infinite. The shape of cross section is shown simultaneously.
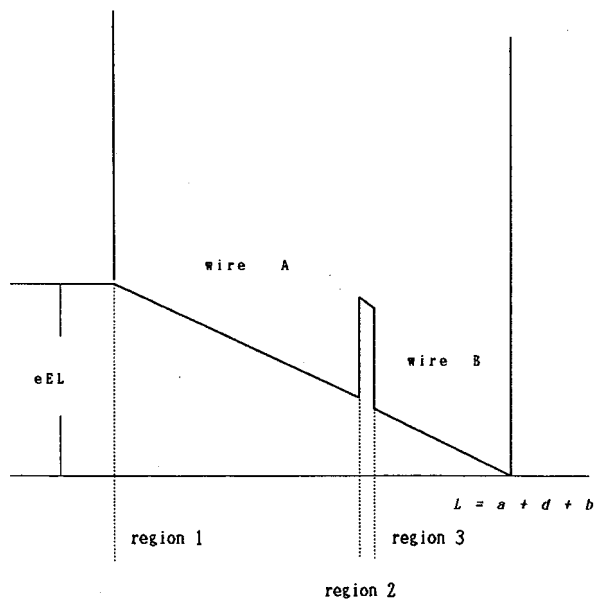

wire   A

wire   B

eEL

$L = a + d + b$

region 1

region 3

region 2

Figure 2: A typical potential profile along the perpendicular direction to the barrier wall under an external electric field E, where $L = a + d + b$.
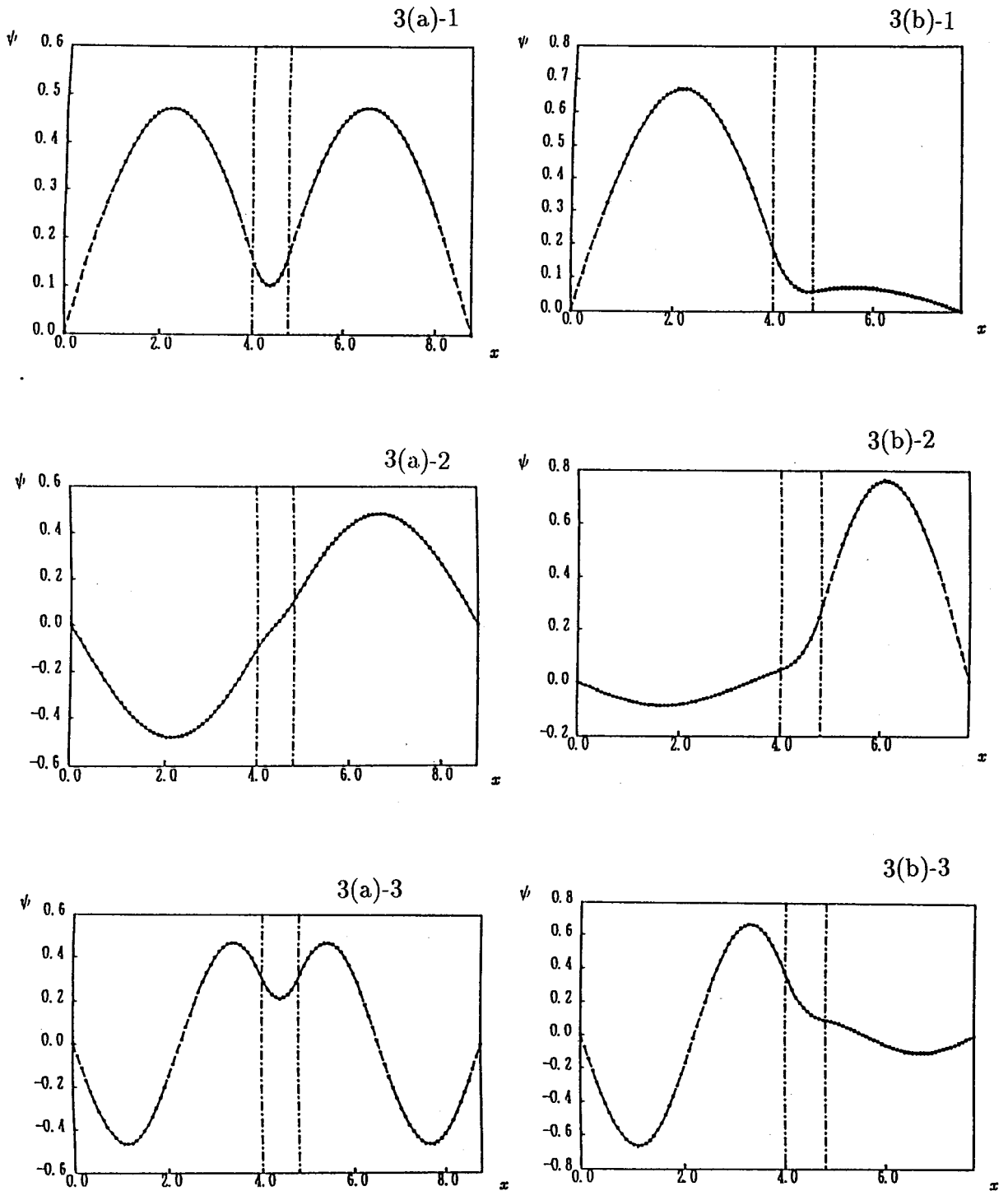
Figure 3: The profile of eigenfunctions for initial three levels. (a) symmetric width (b) nonsymmetric width. Note that in the former case we have the same amplitude in both wires but in the latter the amplitude is dominant in one of wires.
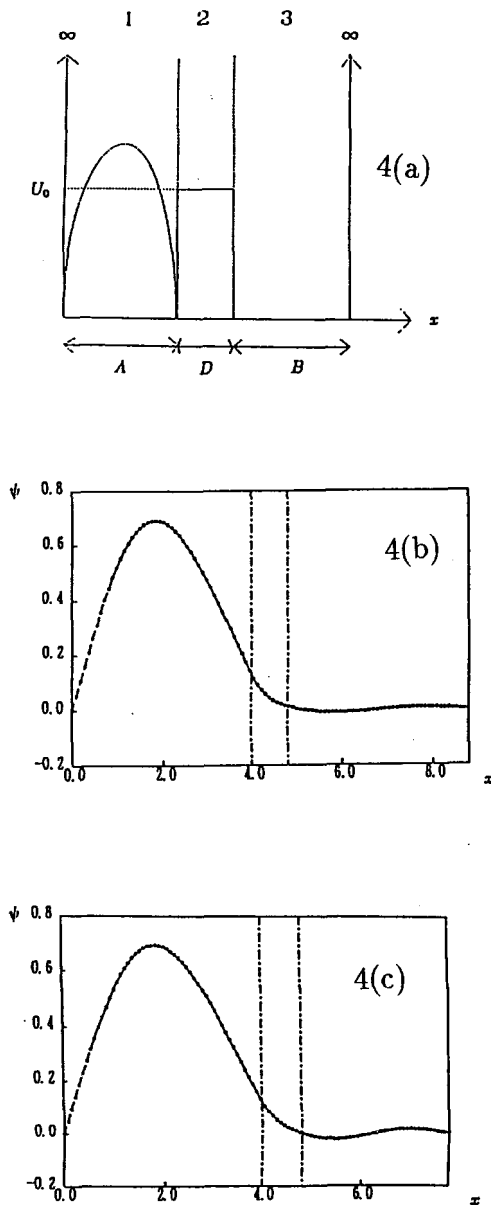
Figure 4: (a) Schematic description of an electron localized in one of wires. (b) The localized state approximated by lowest eigenfunctions in the symmetric width case. (c) The same approximative state in the nonsymmetric width case.
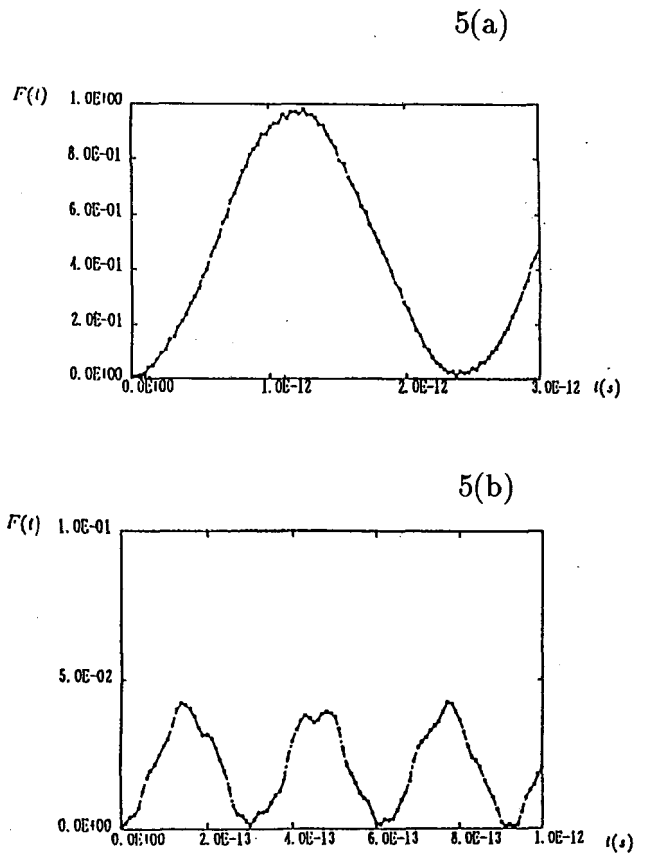
Figure 5: (a) The probability that an electron exists in the other wire at time t in the symmetric width case. Note that the fine structure in the time dependence is due to the slight mixing of higher energy states. (b) The same probability in the nonsymmetric width case. Note the scale of the ordinate axis and that the maxima are almost two order of magnitude less than (a).
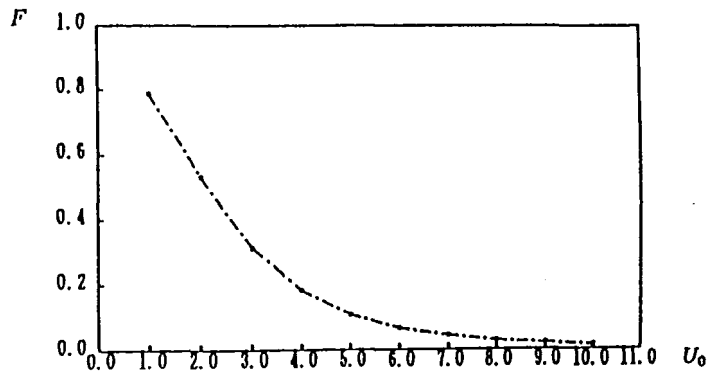
Figure 6: Values of maxima (transfer efficiency) in Fig.5 as a function of the potential barrier height.
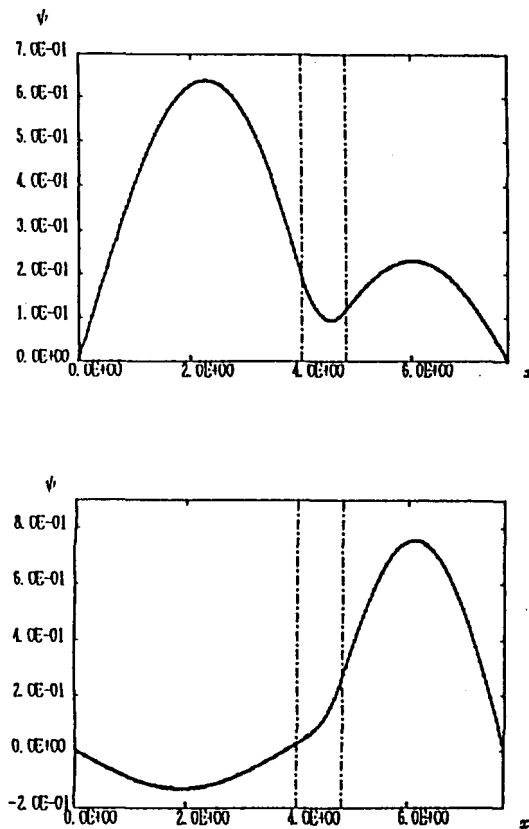

Figure 7: Wave function profiles of initial two levels in nonsymmetric width case with externally applied electric field. Note that, in the ground state, the amplitude in the other wire increases by electric field effect.
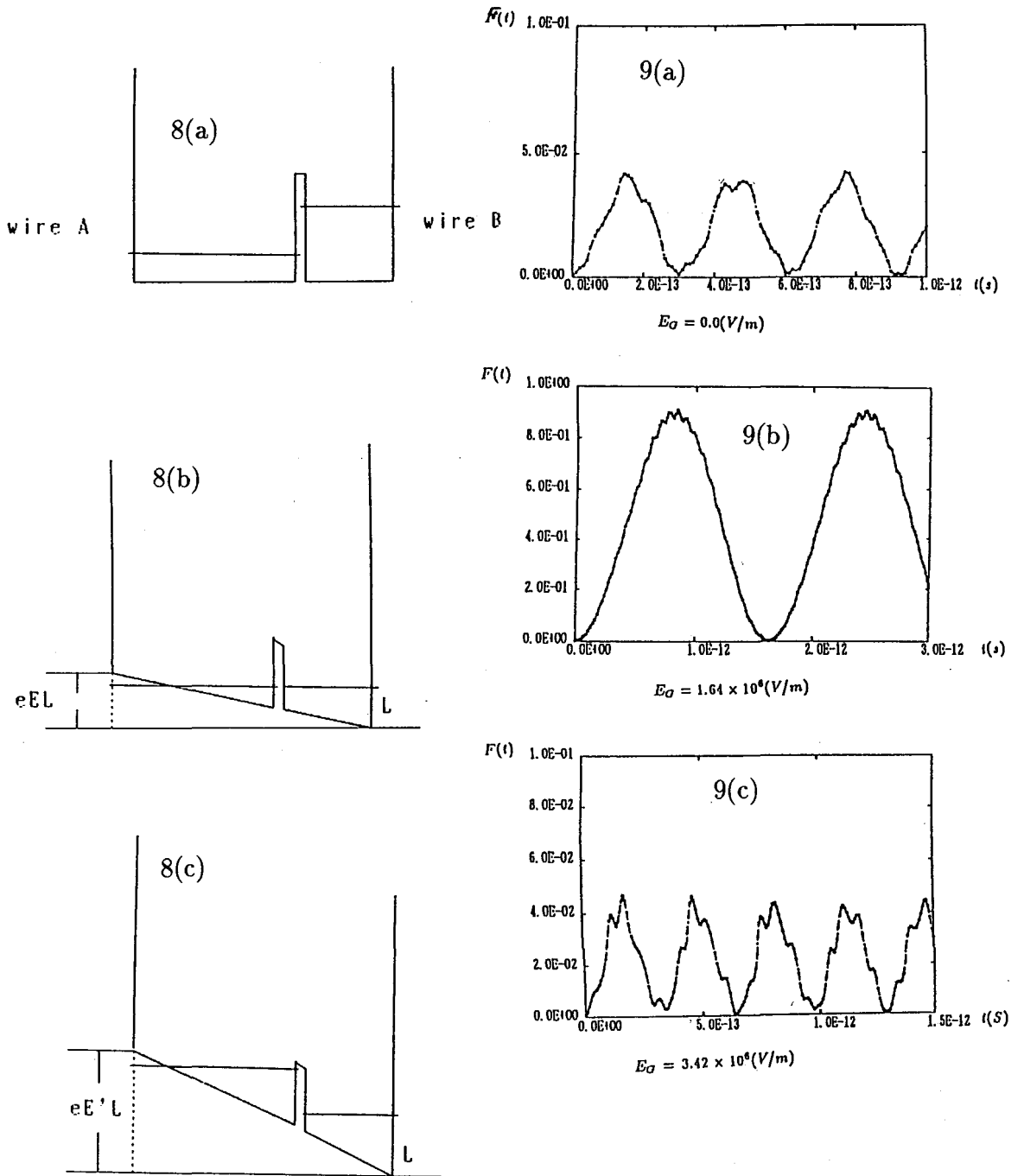
Figure 8: Schematic description of potential profiles for three electric field strenghs.

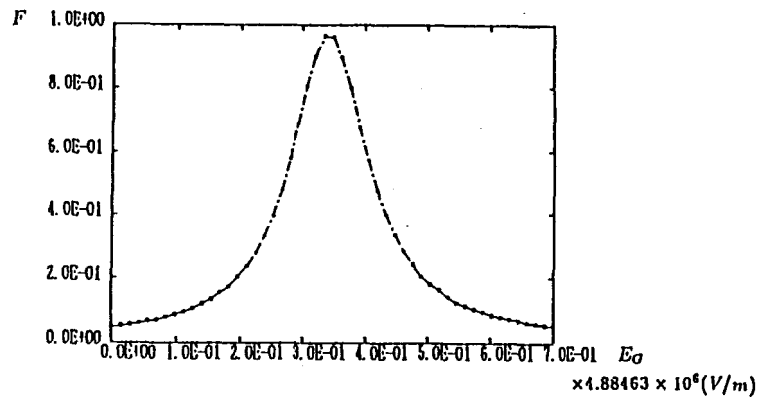Figure 9: Probability $F(t)$ that an electron exists in the other wire at time t for three cases of Fig.8.

Figure 10: Transfer effeciency as a function of applied electric field. At the optimum elelctric field, the same situation as the resonant tunneling is realized, in principle.