Wave and Particle Models of Coupled Quantum Wave Guides

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Abstract—In this paper, a quantum wave filter constructed by coupling three quantum wave guides through thin barriers is analyzed. The filter is a quantum system with triple potentials in x-direction. Regarding an electron in the filter both as quantum wave and as a probabilistic particle, we describe the behavior of the electron by the Schrödinger and the Langevin equations. Solving the two equations, we found that the filter possessed bandpass characteristics and that the wave and particle nature of the electron were equivalent. We also found that an electron's kinetic energy at which bandpass curve takes peak value depended on the width of the center well and the height of the barriers between the wells.

1. Introduction

As mentioned in [1], very sensitive sensing and very low power communication will be achieved with quantum dot terahertz detectors and single-electron tunneling (SET) electron-stream processors. The sensory systems and the communication systems will require circuits functioning like front-end circuits in conventional radar and wireless communication systems. The front-end circuits may contain electric parts like filters. Frequency of electromagnetic waves is proportional to the kinetic energy of photoelectrons emitted from a device detecting the electromagnetic waves. Circuits letting photoelectrons whose kinetic energy is in a specific band pass through and eliminating photoelectrons whose kinetic energy is out of the band function as filters. They are used to remove photoelectrons excited by noise. They also may be applied to wavelength division multiple access communication systems.

Electrons have wave-particle duality. Most front-end filters acting on the photoelectrons will exploit the wave nature like conventional distributed parameter high frequency circuits. On the other hand, SET circuits processing the photoelectron streams regard the electrons as particles with probabilistic behavior. In circuit simulation, conversion from the spatially spread waves to sample particles will be high in computational complexity if the quantum front-end circuits are many-body or high dimensional quantum systems. This problem will be solved if the photoelectrons in the circuits can be described as particles. In addition, the description helps to build lumped parameter device models suitable for conventional circuit simulators [2].

By exploiting wave nature of electrons, many types of filters modeled after distributed parameter analog filters seem to be constructed [3, 4]. In [4], a quantum system with double-well potential in one direction, which is built by coupling two quantum wave guides, is proposed. It corresponds to a distributed parameter filter [5, 6] consisting of coupled lines. The problem of the quantum filter is that the isolation between waves exiting from the two guides is low. To solve the problem, we construct a quantum system with triple-well potential in one direction, which is built by coupling three quantum wave guides, in this paper. We attempt to describe behavior of electrons in the quantum system both as evolution of wave functions obtained by solving the Schrödinger equation and as probabilistic motion of particles which Nelson's stochastic quantization theory [1, 7] provides. We then investigate their equivalency.

In this paper, physical units are defined as mentioned in [1].

2. Transfer Matrix Method

In this section, we investigate a one-dimensional quantum system whose potential is expressed by

$$V(x) = V_s \text{ for } \sum_{i=0}^{s-1} L_i \le x < \sum_{i=0}^{s} L_i, s \in 1, 2, \cdots, N \quad (1)$$

In the s-th interval where $V(x) = V_s$, wave function of the following Schrödinger equation,

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

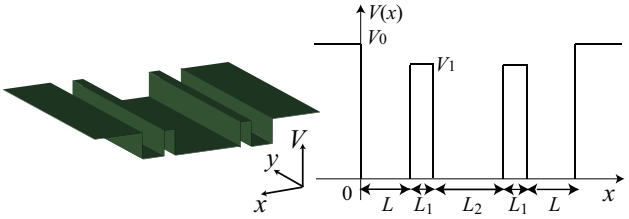
is expressed by

$$\begin{aligned} \psi(x,t) &= \phi_s(x)T(t), \quad (3) \\ \phi_s(x) &= A_s \exp(-ik_s x) + B_s \exp(ik_s x), \\ T(t) &= \exp(-i\frac{E}{\hbar}t) \end{aligned}$$

where k_s is a wave number given by

$$k_s = \frac{\sqrt{2m(E - V_s)}}{\hbar} \quad (4)$$

and E is energy of the electron. The coefficients A_s and B_s are determined by boundary conditions that wave function $\psi(x,t)$ and its spatial derivatives are continuous at the



(a) on (x, y)-plane (b) on x-axis

Figure 1: Triple-well potential.

boundaries of the intervals, that is

$$\phi_s(\frac{L}{2}s) = \phi_{s+1}(\frac{L}{2}s), \tag{5}$$

$$\frac{\partial\phi_s}{\partial x}(\frac{L}{2}s) = \frac{\partial\phi_{s+1}}{\partial x}(\frac{L}{2}s) \tag{6}$$

Substituting $\phi_s(x)$ in Eq. (3) into Eqs. (5) and (6), we obtain the following relation between the coefficients:

$$\begin{bmatrix} A_{s+1} \\ B_{s+1} \end{bmatrix} = \boldsymbol{M}_s \begin{bmatrix} A_s \\ B_s \end{bmatrix} \tag{7}$$

where $\boldsymbol{M_s}$ is a 2×2 matrix. From Eq. (7), we have

$$\begin{bmatrix} A_N \\ B_N \end{bmatrix} = \boldsymbol{M} \begin{bmatrix} A_1 \\ B_1 \end{bmatrix}, \quad \boldsymbol{M} = \prod_{i=0}^{N-1} \boldsymbol{M}_{N-i} \tag{8}$$

When amplitude of backward wave in interval with $s = N$ is zero, $A_N = 0$, transmission rate of an electron from interval 1 to interval N is defined by $r_T = (B_N/B_1)^2$ and expressed by using elements M_{ij} of matrix $\boldsymbol{M}$ as

$$r_T = \left| -M_{21}\frac{M_{12}}{M_{11}} + M_{22} \right|^2 \tag{9}$$

This procedure to compute transmission coefficient r_T is referred to as the transfer matrix method (TMM) [8, 9]. Since A_s and B_s can be computed in the TMM procedure, we obtain wave functions in all the intervals.

3. Wave Functions Describing the Electron

In this section, we investigate wave nature of an electron in quantum triple-well system. The potential of the quantum system has triple-well structure in x-direction but it is constant in y-direction as shown in Fig. 1. The potential is expressed by

$$V(x,y) = \begin{cases} V_0 & \text{for } x < 0 \\ 0 & \text{for } 0 \le x < L \\ V_1 & \text{for } L \le x < L + L_1 \\ 0 & \text{for } L + L_1 \le x < L + L_1 + L_2 \\ V_1 & \text{for } L + L_1 + L_2 \le x < L + 2L_1 + L_2 \\ 0 & \text{for } L + 2L_1 + L_2 \le x < 2L + 2L_1 + L_2 \\ V_0 & \text{for } 2L + 2L_1 + L_2 \le x \end{cases} \tag{10}$$

A Schrödinger equation describing the behavior of the electron in the potential is given by

$$i\hbar\frac{\partial\psi(x,y,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x,y)\right)\psi(x,y,t) \tag{11}$$

We express the wave function $\psi(x, y, t)$ by

$$\psi(x,y,t) = \psi(x,t)\psi(y,t) \tag{12}$$

The wave function has discrete eigen-energy $E_{x,n}$, $n = 0$, 1, 2, $\cdots$, in x-direction. Thus, $\psi(x, t)$ is given by linear combination of eigenfunctions $\psi_n(x, t)$, that is,

$$\psi(x,t) = \sum_{n=0}^{\infty} c_n\psi_n(x,t), \tag{13}$$

$$\psi_n(x,t) = \psi_n(x)\exp\left(-i\frac{E_n}{\hbar}t\right), \quad n = 0, 1, 2, \cdots$$

Time independent eigenfunctions $\psi_n(x)$ are computed by the TMM method. Coefficients c_n in Eq. (13) are determined by the following equations when initial distribution of electron location is the Gaussian distribution with expectation x_0 and variance σ_x^2.

$$c_n = \int_{-\infty}^{\infty} \phi_0(x)\psi_n^*(x)dx,$$

$$\phi_0(x) = \frac{1}{(2\pi\sigma_x^2)^{1/4}}\exp\left(-\frac{(x-x_0)^2}{4\sigma_x}\right)$$

Potential $V(x, y)$ is constant in y-direction. Thus, the wave function has continuous eigen-energy E_y in y-direction. The y-directional eigenfunction $\psi_E(y, t)$ with energy E_y, a function of y-directional momentum p_y, is expressed by

$$\psi_E(y,t) = \phi(y)\exp\left(-i\frac{E_y(p_y)}{\hbar}t\right), \tag{14}$$

$$\phi(y) = \exp\left(i\frac{p_y}{\hbar}y\right), \quad E_y(p_y) = \frac{p_y^2}{2m}$$

The y-directional wave function $\psi(y, t)$ in Eq. (12) is determined by the following equations when the electron locates at y_0 in y-directional expectation and has momentum p_y whose distribution is expressed by wave function $\phi_0(p_y)$:

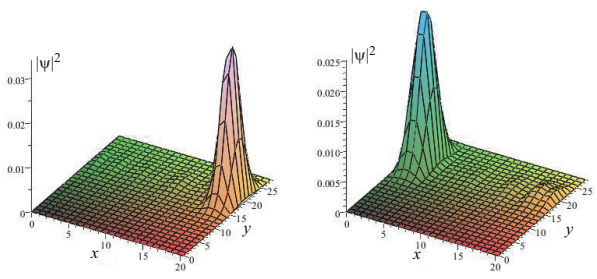
$$\psi(y,t) = \int_{-\infty}^{\infty} \phi_0(p_y)\psi_E(y,t)dp_y, \tag{15}$$

$$\phi_0(p_y) = \frac{1}{(2\pi\sigma_{p,y}^2)^{1/4}}\exp\left(-i\frac{p_y}{\hbar}y_0 - \frac{(p_y - p_{0,y})^2}{4\sigma_{p,y}^2}\right)$$

where $p_{0,y}$ and $\sigma_{p,y}^2$ are expectation and the variance of the Gaussian momentum distribution $|\phi_0(p_y)|^2$.

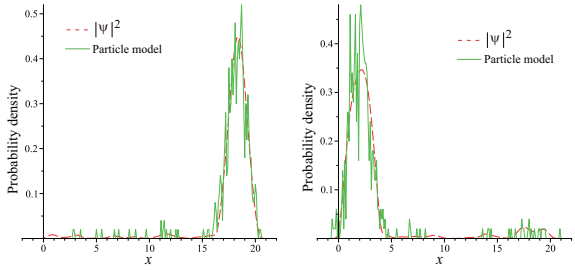
4. Probabilistic Particle Model of the Electron

As the wave function is determined, Nelson's stochastic quantization derives a nonlinear Langevin equation whose solution has the same probability distribution as that determined by the wave function [1, 7].



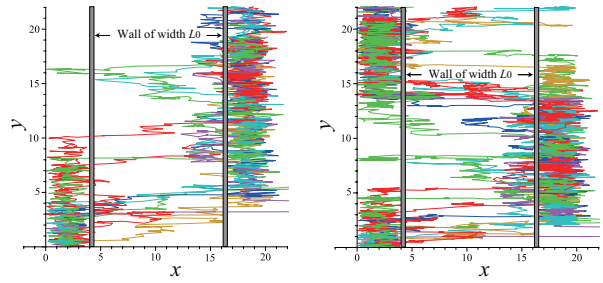
(a) $p_{0,y}$=8, t=330 (b) $p_{0,y}$=4, t=660

Figure 2: Wave functions in the quantum triple-well system.



(a) $p_{0,y}$=8, t=330 (b) $p_{0,y}$=4, t=660

Figure 4: Marginal probability distribution in terms of x-coordinate of an electron in the quantum triple-well system.



(a) $p_{0,y}$=8 (b) $p_{0,y}$=4

Figure 3: Sample trajectories of an electron in the quantum triple-well system.

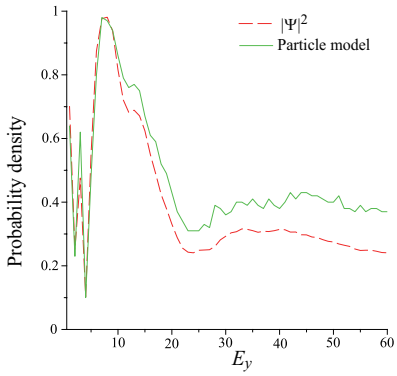


Figure 5: Kinetic energy E_y of an electron versus probability that the electron exits from a well on L+2L_1+L_2 ≤ x < 2L+2L_1+L_2.

5. Numerical Experiments

In the following numerical examples, the parameters of the potential are set to $V_0 = V_1 = 10.0$, $L = 4.0$, $L_1 = 0.2$, and $L_2 = 12.0$.

Figures 2 and 3 show the wave function and the sample solutions of the Langevin equation when $(x_0, y_0) = (2.0, 0)$, $\sigma_x^2 = 5.0$, $p_{0,y} = 8$ and 4, and $\sigma_{p,y}^2 = 0.5$.

Marginal probability distribution in terms of x-coordinate of an electron is computed both from the wave function $\psi(x,t)$ and from the sample solutions of the Langevin equation. The two distributions obtained by the different two methods are almost equal as shown in Fig. 4.

From probability distribution of electron location, we estimate probabilities that electrons leave from the right well. A probability that an electron leaves the triple-well system from a well on L+2L_1+L_2 ≤ x < 2L+2L_1+L_2 is plotted against its y-directional kinetic energy $E_y = p_y^2/2m$ in Fig. 5 when the electron enters at the left well on $0 \le x < L$, which is obtained by integrating numerically the probability on L+2L_1+L_2 ≤ x < 2L+2L_1+L_2 at $y = 20$. If the electron is an photoelectron, its kinetic energy is proportional to the frequency of electromagnetic excitation wave. Thus, the triple-well quantum system with an output at one of two side wells functions as a filter letting photoelectrons pass through or eliminating photoelectrons depending on the frequency.

We investigate the dependency of the filter characteristics on the potential parameters by analyzing wave functions of the Schrödinger equation. In Fig. 6, the y-directional electron kinetic energy $E_{y,peak}$ at which probability that electrons leave from the right well is maximum is plotted against the width L_2 of the center well. The figure shows that energy $E_{y,peak}$ changes periodically depending on L_2. This is because the quantum electron wave becomes standing wave in x-direction in the wells. We plotted $E_{y,peak}$ against the height V_1 of barriers between the wells in Fig. 7. As V_1 increases, $E_{y,peak}$ decreases. This is because high barriers decreases average x-directional velocity of electrons.

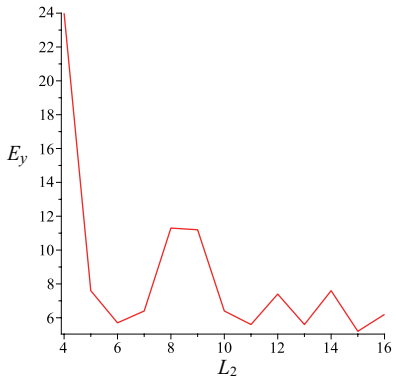


Figure 6: Width L_2 of the center well versus y-directional electron kinetic energy $E_{y,peak}$ at which probability that electrons leave from the right well is maximum.

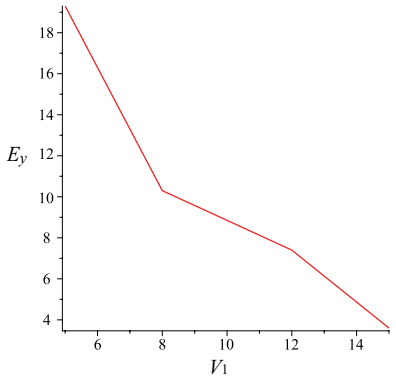


Figure 7: Height V_1 of barriers between the wells versus y-directional electron kinetic energy $E_{y,peak}$ at which probability that electrons leave from the right well is maximum.

6. Conclusions

The problem of a quantum wave filter constructed by coupling two quantum wave guides through thin barriers is that the isolation between waves exiting from the two guides is low. In this paper, in order to solve the problem, a quantum system with triple wells in x-direction has been analyzed. We found that the filter possessed bandpass characteristics. The characteristics obtained by solving the Schrödinger equation and from the Nelson's stochastic quantization were almost equal. We also found that an electron's kinetic energy at which bandpass curve takes peak value depended on the width of the center well and the height of the barriers between the wells. This results are useful in the design of this kind of quantum wave filter.

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