

A Numerical Model of a Frequency Discriminator for Terahertz Sensing and Communication Using Photoelectric Detectors

Shota Hayakawa, Hisato Fujisaka, and Takeshi Kamio

Faculty of Information Sciences, Hiroshima City University
3-4-1 Ozuka-higashi, Asaminami-ku, Hiroshima 731-3194, Japan
Email: hayakawa@sp.info.hiroshima-cu.ac.jp

Abstract—A quantum system with a stub-structured potential is considered to be usable as a frequency discriminator of terahertz wave receiver system. In this quantum system, the electron wave is reflected or transmitted near the connection area of the stub depending on the momentum of the electron wave. In this study, by numerical analysis of the propagation of the electron wave using the difference method, we analyzed the change of reflection and transmission characteristics with respect to the momentum of the electron wave. In addition, we calculated the sample trajectories of electrons by stochastic quantization on which circuit simulator model of terahertz wave receiver system is based. By the analysis, we have confirmed that the quantum system with a stub-structured potential functions as a frequency discriminator.

1. Introduction

In recent years, terahertz wave communication has attracted attention [1]. The terahertz wave communication has an advantage that the terahertz band is not assigned for sensing and wireless communications yet and provides faster communication than current communication bands. A terahertz wave receiver system is considered to be built of a detection part [2], a frequency discrimination part [3], and a decoding part [4]. A device converting received terahertz waves into single-electrons by the photoelectric effect has been developed [2]. By using this device for the detection part, it is considered that a terahertz wave receiver system featuring miniaturization and low power communication can be realized. The detection part outputs electrons with momentum proportional to the frequency of the received terahertz wave. If the electrons are separated depending on their momentum, frequency discrimination of terahertz waves can be realized. Recently, it was simulated that coupled electron wave guides function as a quantum wave filter and can discriminate the frequency [3].

A semiconductor device with a stub-structured potential can act as a transistor exploiting electron wave interference [5]. When electron waves propagate on this semiconductor, the electron waves are expected to be reflected or transmitted near the connection area of the stub depending on the momentum of the electron wave. In this study, we numerically analyze the reflection and transmission characteristics

of the quantum system with a stub-structured potential and investigate whether it has the frequency-discriminating function [7]. By discretizing the space, we obtain eigenvectors and the eigenvalues as the wave eigenfunctions and the eigenenergies. We reduce the amount of calculation by treating the time-dependent parts of the electron waves as a continuous function with eigenvalues as parameters. In order to simulate the terahertz wave receiver system incorporated the frequency discriminator by using the existing circuit simulator, the propagation of the wave must be represented by a sample electron trajectories [3]. We calculated the sample trajectories based on Nelson's stochastic quantization [6].

2. The Schrödinger equation

The Schrödinger equation describes the motion of quantum particles. When (x, y) and t are independent variables of spatial coordinates and time respectively, the two-dimensional Schrödinger equation of the quantum particle whose mass is m is given by

$$i\hbar \frac{\partial \psi(x, y, t)}{\partial t} = H\psi(x, y, t) \quad (1)$$

$$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V(x, y) \quad (2)$$

where \hbar is the Planck constant and $V(x, y)$ is the potential. The solution $\psi(x, y, t)$ of Eq.(1) is called the wave function. The square of the absolute value of $\psi(x, y, t)$ represents the existence probability of the quantum particle.

3. Nelson's stochastic quantization

Nelson's stochastic quantization represents quantum particles by classical probabilistic particles (Brownian particles) moving according to the probability density given by $|\psi|^2$ [6]. Therefore, the motion of the quantum particles can be described by the Langevin equation. By this method, we can compute sample trajectories of the quantum particles, which is difficult to compute from the wave function of the Schrödinger equation. Langevin equations for computing trajectories in the (x, y) -plane are expressed as follows:

$$\frac{dx}{dt} = b_x(x, y, t) + \sqrt{\frac{\hbar}{2m}} \Gamma_x(t) \quad (3)$$

$$\frac{dy}{dt} = b_y(x, y, t) + \sqrt{\frac{\hbar}{2m}} \Gamma_y(t) \quad (4)$$

If the right hand sides of equations (3) and (4) are defined in the following way, the probability distribution of the particles is equal to $|\psi|^2$. The drift terms $b_x(x, y, t)$, $b_y(x, y, t)$ are the frictional force that the particle receives. They are given by

$$b_x(x, y, t) = \Re \left(\frac{\hbar}{m} \frac{\partial}{\partial x} \ln \psi \right) + \Im \left(\frac{\hbar}{m} \frac{\partial}{\partial x} \ln \psi \right) \quad (5)$$

$$b_y(x, y, t) = \Re \left(\frac{\hbar}{m} \frac{\partial}{\partial y} \ln \psi \right) + \Im \left(\frac{\hbar}{m} \frac{\partial}{\partial y} \ln \psi \right) \quad (6)$$

where \Re and \Im represent the real and imaginary parts respectively. $\Gamma_x(t)$, $\Gamma_y(t)$ are random forces that the particle receives. $\Gamma_x(t)$, $\Gamma_y(t)$ are independent white noises satisfying

$$\langle \Gamma_x(t) \Gamma_x(t_0) \rangle = \delta(t - t_0) \quad (7)$$

$$\langle \Gamma_y(t) \Gamma_y(t_0) \rangle = \delta(t - t_0) \quad (8)$$

$$\langle \Gamma_x(t) \Gamma_y(t_0) \rangle = 0 \quad (9)$$

4. Stub-structured potential

In this study, we analyze a quantum system with a stub-structured potential $V(x, y)$ shown in Figure 1. The shaded area indicates the high potential area. L_1, L_2, L_3 are the lengths that determine the shape of the potential. When electron comes in from a point marked with "a", propagation of the electron wave in the order of "abc" is called transmission and propagation in the order of "aba" is called reflection. Since this quantum system has a stub, part of the electron wave is expected to be reflected or transmitted near the connection area of the stub by the electronic wave interference. By changing the momentum of electrons and the shape of the potential, the transmission rate may be changed. Then this quantum system is considered to function as a frequency discriminator.

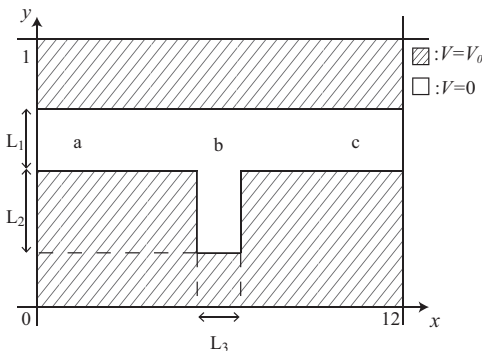


Figure 1: Stub-structured potential

5. Method of numerical analysis

5.1. Derivation of the wave function by difference method

In the stub-structured potential in Figure 1, the potential height is not constant in both directions. Since it is difficult to analytically solve the Schrödinger equation of the system with such a potential structure, we use the difference method to derive the wave function. We separate the wave function into terms of position and time.

$$\psi(x, y, t) = \psi(x, y) \exp(-i \frac{E}{\hbar} t) \quad (10)$$

Then, the Schroedinger equation (1) can be written as a time-independent Schrodinger equation.

$$E\psi(x, y) = H\psi(x, y) \quad (11)$$

We discretize the potential region in Figure 1 with respect to space. The spatially discretized wave function have values only on discrete points. By approximating the partial derivatives of Hamiltonian H by difference between values at the discrete points, equation (11) can be expressed using a vector, a matrix, and its eigenvalue as

$$E_n \Psi_n = H \Psi_n \quad (12)$$

where H is the matrix representation of the Hamiltonian H , Ψ_n and E_n are eigenvector and eigenvalue of H , respectively. The eigenvector Ψ_n whose elements are complex values on the discrete points corresponds to the wave function ψ .

5.2. Derivation of the time-evolving wave function

By using eigenvalues E_n and eigenvectors Ψ_n , the time-evolving wave function Ψ is given by

$$\Psi = \sum_n c_n \Psi_n \exp(-i \frac{E_n}{\hbar} t) \quad (13)$$

where n is a quantum number. Given the initial distribution Ψ^0 of Ψ as

$$\Psi^0(x, y) = \frac{1}{\sqrt{2\pi\sigma_x^2\sigma_y^2}} \exp\left(-\frac{(x-x_0)^2}{4\sigma_x^2} - \frac{(y-y_0)^2}{4\sigma_y^2} + ik_{x0} + ik_{y0}\right) \quad (14)$$

c_n of equation (13) is given by

$$c_n = \Psi_n \cdot \Psi^0 \quad (15)$$

In equation (14) (x_0, y_0) are initial average position, k_{x0} , k_{y0} are initial average wave numbers, σ_x^2 , σ_y^2 are variances of the position.

6. Numerical experiment

In this study, planck constant is $\hbar = 1$, mass of electron is $m = 1$ for simplifying the calculation. We set the parameters in Figure 1 as $L_1 = 0.3$, $L_2 = \pi/12$, $L_3 = 0.9$, and $V_0 = 10000$. The potential was divided into 600 in the range of $0 \leq x \leq L_x$, and into 50 in the range of $0 \leq y \leq L_y$. Then we calculated E_n and Ψ_n . The initial wave distribution was Gaussian wave packet (14) with the parameters of $x_0 = 3$, $y_0 = 0.65$, $k_{y0} = 0$, $\sigma_x = 0.5$, $\sigma_y = 0.002$. We calculated the time-evolving wave function by the method described in section 5.

Figure 2 shows the transmission rates plotted against the initial average momentum of an electron when $L_2 = \pi/12$. Figure 3 also shows the transmission rates when $L_2 = \pi/4$. Transmission rate T is the integral of the existence probability obtained from the normalized wave function with respect to the region on the right side of the stub, that is,

$$T = \sum_{\frac{L_x+L_3}{2} \leq x} \sum_y \Psi^* \Psi \Delta x \Delta y \quad (16)$$

at $t = (9 - x_0)/k_{x0}$, where Δx , Δy are the lattice constant.

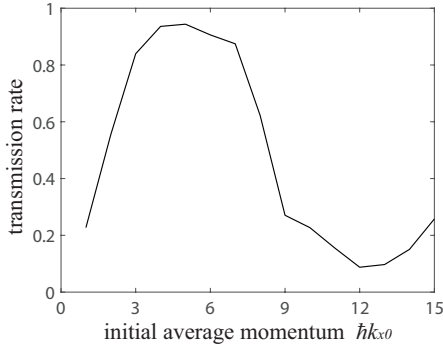


Figure 2: The transmission rates against the initial average momentum of an electron ($L_2 = \pi/12$)

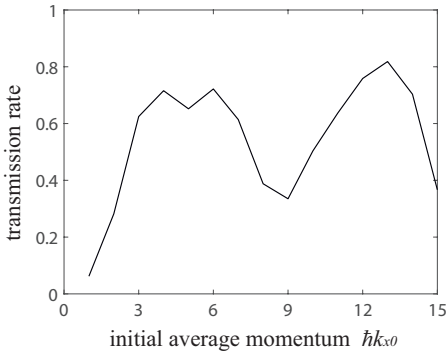


Figure 3: The transmission rates against the initial average momentum of an electron ($L_2 = \pi/4$)

As shown in figures 2 and 3, the transmission rate greatly changed with momentum. In addition, the transmis-

sion characteristics change when the length L_2 of the stub changes. It is expected that the electrons can be separated to the left and right if electrons have momenta at which the transmission rates are almost 0 and 1. Figure 4 shows the existence probability of an electron when $L_2 = \pi/12$, the initial average momentum in the x direction is $\hbar k_{x0} = 6$, and time is $t = 1$. Figure 5 shows the existence probability of an electron when the initial average momentum in the x direction is $\hbar k_{x0} = 12$, and time is $t = 0.6$.

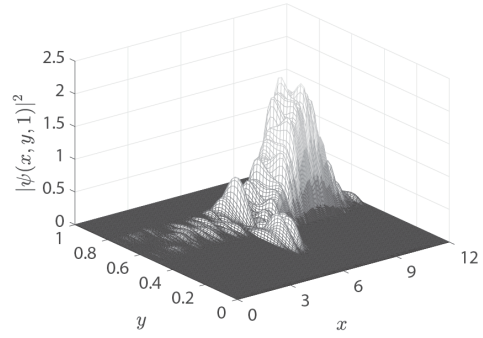


Figure 4: The existence probability of an electron ($k_{x0} = 6$, $t = 1$)

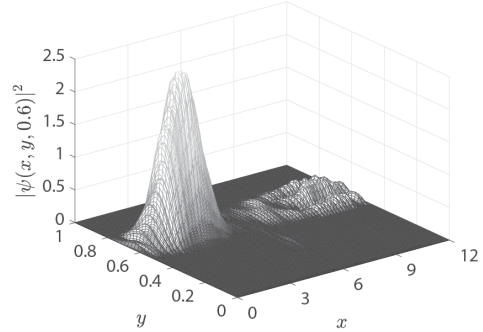


Figure 5: The existence probability of an electron ($k_{x0} = 12$, $t = 0.6$)

We calculated the sample trajectories of electrons by numerically integrating Langevin equation set (3), (4). Figures 6 and 7 show the sample trajectories of electrons (5 samples) when $\hbar k_{x0}$ is 6 and 12, respectively.

Figures 4 and 6 show that electrons move rightward while they return to the leftward in figures 5 and 7. From the above observation, it was confirmed that electrons can be separated to the left or right of the quantum system depending on the difference in momentum.

Figures 8 and 9 show the histogram of the distribution of x coordinates of the trajectories around $y = 0.65$, at $t = 1$ and 0.6 when initial x -directional average momentum is $\hbar k_{x0} = 6$ and 12 , respectively. The solid lines shown in Figures 8 and 9 are the existence probability $|\psi(x, 0.65, 1)|^2$, $|\psi(x, 0.65, 0.6)|^2$. From Figures 8 and 9, it is found that the distribution of the position of electrons obtained by computing the sample trajectories of the electrons corresponds to the curve of the existence probability $|\psi|^2$.

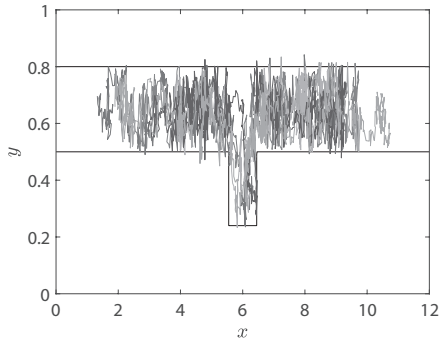


Figure 6: The sample trajectories of electrons ($k_{x0} = 6$)

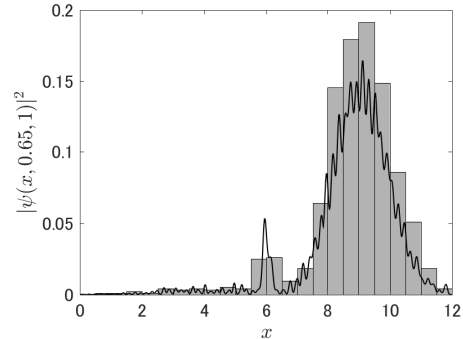


Figure 8: The distribution of the sample trajectories ($k_{x0} = 6$)

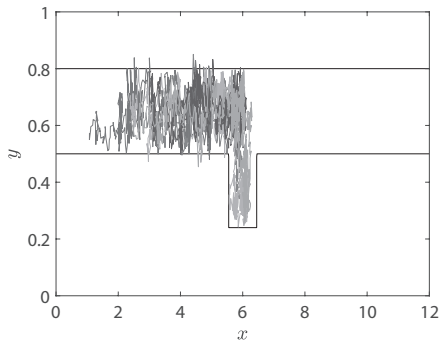


Figure 7: The sample trajectories of electrons ($k_{x0} = 12$)

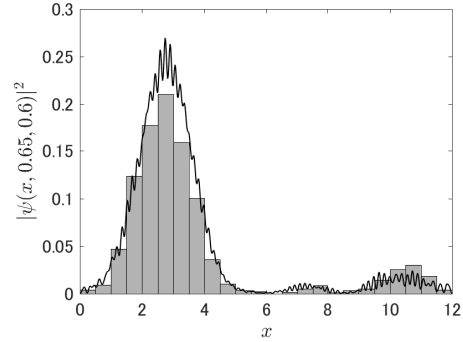


Figure 9: The distribution of the sample trajectories ($k_{x0} = 12$)

7. Conclusions

In this study, the quantum system with stub-structured potential was analyzed for the application to frequency discrimination in terahertz wave receiver system. Moreover, for modeling the quantum system in circuit simulation of the terahertz wave receiver system, we derived the Langevin Equations whose numerical solutions are sample trajectories of electrons. From these results of the analyses, we confirmed that the quantum system with the stub-structured functions as a frequency discriminator. It was also confirmed that the wave function by the numerical analysis and the sample trajectories of the electrons represent equivalent results.

Our future works include establishing approximation theory on the stub-structured quantum system by a macroscopic analog distributed parameter filter.

References

- [1] M. Tonouchi, "New Terahertz Industry," CMC Publishing, 2011 (In Japanese).
- [2] Y. Kawano, T. Uchida, and K. Ishibashi, "Terahertz Sensing with a Carbon Nanotube/Two-dimensional

Electron Gas Hybrid Transistor," *Applied Physics Letters*, Vol. 95, Issue 8, 083123-1-3, 2009.

- [3] Y. Kawabata, H. Fujisaka, and T. Kamio, "Probabilistic particle modeling of quantum wave propagation with excitation and refraction," *Proc. of IEEE Int' l Conf. on Circuits and Systems*, pp.474-477, 2014.
- [4] A. Setsuie, J. Sato, H. Fujisaka, and T. Kamio, "Single-Electron Decoder Circuits for Communication Systems Based on Quantum Mechanics," *Proc. of IEEE Workshop on Nonlinear Circuit Networks*, pp.32-35, 2016.
- [5] A. Sasaki, "Quantum Effects of Semiconductors," IEICE Publishing, 2000 (In Japanese).
- [6] E. Nelson, "Derivation of the Schrödinger Equation from Newtonian Mechanics," *Physical Review*, Vol. 150, No. 4, pp. 1079-1085, 1966.
- [7] S. Hayakawa, H. Fujisaka, and T. Kamio, "Numerical Analysis of Reflection-Transmission Characteristics of an Electron-Wave Stub Filter," *IEICE Technical Report*, NLP2017-6, pp.29-33, 2017.