

Stochastic Quantization of a One-Dimensional Multi-Particle System for the Circuit Simulator Model of Photoelectric Terahertz Wave Detectors

Ibuki Nakamura[†], Keita Matsuura[†], Hisato Fujisaka[†], Masaru Fukushima[†], and Takeshi Kamio[†]

[†]Faculty of Information Science, Hiroshima City University, 731-3194 Japan

Email: keita@sp.info.hiroshima-cu.ac.jp

Abstract—A device which detects terahertz (THz) electromagnetic waves with smaller in photon energy than visible lights and outputs a single photoelectron has been developed. Employing the devices as THz detectors might provide high sensitivity to sensing and communication systems. The authors has proposed a receiver consisting of three blocks. They are the detector, a frequency discriminator separating the photoelectrons depending on their momentum, a single-electron-transistor-based decoder estimating transmitted data from the streams of the separated photoelectrons. The circuit simulator models of the blocks are necessary to aid the design of the receiver. As a basis of the model of the detector, a one-dimensional multi-particle quantum system is modeled after a classical probabilistic system composed of the Brownian particles in this paper. We confirmed by the numerical experiments of the established model that the Brownian particles moves probabilistically according to the existence probability derived from the wave function of the original quantum system.

1. Introduction

A kind of photo transistor which detects terahertz (THz) electromagnetic waves and outputs a single-photoelectron has been developed [1]. An island in the transistor is a carbon nano tube (CNT). The CNT makes it possible to detect THz photons with smaller in energy than visible light photons and output a single-photoelectron. Employing the single-electron photo transistors (SEPTs) as the THz detectors might provide high sensitivity to sensing and communication systems. In the simulation of the THz sensing and communication systems with a conventional circuit simulator, the SEPTs should be modeled as probabilistic elements in which photoelectrons behave like the Brownian particles [2]. In the island of a CNT of small diameter, electron-wave function is uniformly distributed in a circumferential direction. Then, the island is considered as a one-dimensional potential system. The electrons in the island increase and decrease one by one as the SEPT detects THz photons. Then, several excess electrons or holes exist in the island.

In this paper, we attempt to model multiple electrons moving in the one-dimensional potential system by classical Brownian like particles.

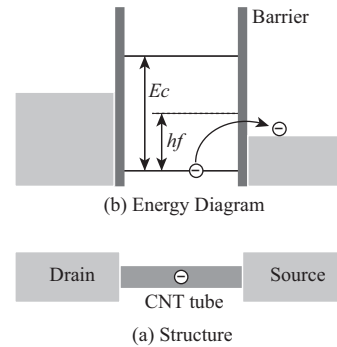


Figure 1: Structure of SEPT.

2. Single-Electron THz Detectors

Figure 1(a) shows the structure of an SEPT [1]. The space between metal drain and source terminals are bridged with a CNT. Since barriers are formed in the interfaces between the metal terminals and the CNT, the CNT becomes an island. The energy level of the excess electrons in the island is quantized as shown in Figure 1(b). Let the gap E_c between the N -th and the $(N + 1)$ -th energy levels be larger than the energy $\hbar\omega$ of THz photons and $\hbar\omega$ be larger than the energy difference between the N -th level and the level of the source terminal. Excited by THz waves, an electron in the island tunnels the barrier and move to the terminal. In this way, the SEPT outputs a photoelectron.

As mentioned in Section 1, the island is considered as a one-dimensional potential system. The following section will introduce a theory for computing the motion of the classical probabilistic particles which are the models of the electrons in the CNT island.

3. Stochastic Quantization for Multi-Particle Quantum Systems

We extend stochastic quantization of one-particle quantum systems [3] to multi-particle systems [4]. For generalization, we discuss the expansion in three-dimension.

Forward and backward Langevin Equations for N classical Brownian particles in the three-dimensional space are described by

$$-534 - dX = X(t + dt) - X(t) = \mathbf{B}_F(X(t), t)dt + d\Gamma_F(t) \quad (1)$$

$$d\mathbf{X} = \mathbf{X}(t) - \mathbf{X}(t - dt) = \mathbf{B}_B(\mathbf{X}(t), t)dt + d\mathbf{\Gamma}_B(t) \quad (2)$$

where locations \mathbf{X} of the N particles, the advection terms $\mathbf{B}_{F/B}$, and the fluctuating forces are denoted by

$$\mathbf{X}(t) = (\mathbf{x}_1(t), \dots, \mathbf{x}_N(t))^T, \quad (3)$$

$$\mathbf{B}_{F/B}(\mathbf{X}(t), t) = (\mathbf{b}_{F/B,1}(\mathbf{X}(t), t), \dots, \mathbf{b}_{F/B,N}(\mathbf{X}(t), t))^T, \quad (4)$$

$$d\mathbf{\Gamma}_{F/B}(t) = (d\gamma_{F/B,1}(t), \dots, d\gamma_{F/B,N}(t))^T \quad (5)$$

Their elements, i.e., location of particle i , its advection term, and the random force acting on it are denoted by

$$\mathbf{x}_i(t) = (x_i(t), y_i(t), z_i(t)), \quad (6)$$

$$\mathbf{b}_{F/B,i}(\mathbf{X}(t), t) = \quad (7)$$

$$(\mathbf{b}_{F/B,i,x}(\mathbf{X}(t), t), \mathbf{b}_{F/B,i,y}(\mathbf{X}(t), t), \mathbf{b}_{F/B,i,z}(\mathbf{X}(t), t)),$$

$$d\gamma_{F/B,i}(t) = (d\gamma_{F/B,i,x}(t), d\gamma_{F/B,i,y}(t), d\gamma_{F/B,i,z}(t)) \quad (8)$$

$$i = 1, \dots, N$$

The random forces are supposed to be the Markovian process with zero average,

$$\langle d\gamma_{F/B,i,p}(t) \rangle = 0, \quad (9)$$

$$\langle d\gamma_{F/B,i,p}(t) d\gamma_{F/B,j,q}(t + \tau) \rangle = \sigma^2 \delta_{i,j} \delta_{p,q} \delta(\tau), \quad (10)$$

$$i, j = 1 \dots N, \quad p, q : x, y, \text{ or } z$$

Let the probability density function of the locations of the N Brownian particles be denoted by $\rho(\mathbf{X}(t))$. The forward and backward Fokker Planck equations of $\rho(\mathbf{X}(t))$ are described by

$$\frac{\partial}{\partial t} \rho(\mathbf{X}(t)) = \quad (11)$$

$$\left\{ - \sum_{i=1}^N \nabla_i \cdot (\mathbf{b}_{F,i}(\mathbf{X}(t), t) + \frac{1}{2} \sum_{i=1}^N \sigma^2 \Delta_i) \right\} \rho(\mathbf{X}(t))$$

$$\frac{\partial}{\partial t} \rho(\mathbf{X}(t)) = \quad (12)$$

$$\left\{ - \sum_{i=1}^N \nabla_i \cdot (\mathbf{b}_{B,i}(\mathbf{X}(t), t) - \frac{1}{2} \sum_{i=1}^N \sigma^2 \Delta_i) \right\} \rho(\mathbf{X}(t))$$

In these equations, the following vector differential operators and Laplacian operators are introduced:

$$\nabla_i \equiv \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i} \right) \quad (13)$$

$$\Delta_i \equiv \nabla_i \cdot \nabla_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \quad (14)$$

When we consider the N Brownian particles as quantum mechanical particles of mass m in a potential $V(\mathbf{X}(t))$, the Schroedinger equation whose wave function $\psi(\mathbf{X}(t), t)$ and $\rho(\mathbf{X}(t))$ are related by

$$\rho(\mathbf{X}(t)) = |\psi(\mathbf{X}(t), t)|^2 \quad (15)$$

is described by

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{X}(t), t) = \left\{ -\frac{\hbar^2}{2m} \sum_{j=1}^N \Delta_j + V(\mathbf{X}(t)) \right\} \psi(\mathbf{X}(t), t) \quad (16)$$

and

$$\sigma^2 = \frac{\hbar}{2m} \quad (17)$$

We determine the advection terms $\mathbf{B}_{F/B}$ so that Eq. (15) is satisfied. Let the wave function be given by the exponential function of the sum of the action $W(\mathbf{X}(t))$ and a function $f(t)$ of time,

$$\psi(\mathbf{X}(t), t) = \exp(W(\mathbf{X}(t))) \exp(f(t)) \quad (18)$$

Let the action $W(\mathbf{X}(t))$ be described by

$$W(\mathbf{X}(t), t) = R(\mathbf{X}(t), t) + iS(\mathbf{X}(t), t), \quad i^2 = -1 \quad (19)$$

The real and the imaginary parts R, S must satisfy the following equations:

$$\sigma^2 \nabla_i R(\mathbf{X}(t), t) = \frac{1}{2} (\mathbf{b}_{F,i}(\mathbf{X}(t), t) + \mathbf{b}_{B,i}(\mathbf{X}(t), t)) \quad (20)$$

$$\sigma^2 \nabla_i S(\mathbf{X}(t), t) = \frac{1}{2} (\mathbf{b}_{F,i}(\mathbf{X}(t), t) - \mathbf{b}_{B,i}(\mathbf{X}(t), t)) \quad (21)$$

Since $f(t)$ is a function of time, R and S may be

$$R = \Re(\log(\psi(\mathbf{X}(t), t))) \quad (22)$$

$$S = \Im(\log(\psi(\mathbf{X}(t), t))) \quad (23)$$

From Equations (20), (21), (22), and (23), we obtain the advection terms $\mathbf{B}_{F/B}$.

4. Initial State and Superposition of Eigenstates

We consider a wave function satisfying a given initial distribution.

Let eigenenergy and eigenfunction sets of a quantum system with one particle be denoted by E_n and $\phi_n(x, t)$: complex function of location x and time t , n : quantum number. Eigenenergy $E_{m,n}^o$ and eigenfunction $\psi_{m,n}^o(x_1, x_2, t)$ of a two-particle quantum system without interaction between particles are given respectively by

$$E_{m,n}^o = E_m + E_n \quad (24)$$

$$\psi_{m,n}^o(x_1, x_2, t) = \frac{1}{\sqrt{2}} (\phi_m(x_1, t) \phi_n(x_2, t) - \phi_m(x_2, t) \phi_n(x_1, t)) \quad (25)$$

When particles interact with one another, eigenenergies $E_{m,n}$ and eigenfunctions $\psi_{m,n}(x_1, x_2, t)$ may be approximated by the series of $E_{n,m}^o$ and $\phi_{n,m}^o$ respectively as

$$\mathbf{E} \approx \mathbf{C} \cdot \mathbf{E}^o \quad (26)$$

$$\mathbf{E} \equiv [E_{m_1, n_1} \quad E_{m_2, n_2} \quad \dots \quad E_{M, M}]^T$$

$$\mathbf{E}^o \equiv [E_{m_1, n_1}^o \quad E_{m_2, n_2}^o \quad \dots \quad E_{M, M}^o]^T$$

$$\boldsymbol{\psi} \approx \mathbf{C} \cdot \boldsymbol{\psi}^o \quad (27)$$

$$\boldsymbol{\psi} \equiv [\psi_{m_1, n_1} \quad \psi_{m_2, n_2} \quad \dots \quad \psi_{M, M}]^T$$

$$\boldsymbol{\psi}^o \equiv [\psi_{m_1, n_1}^o \quad \psi_{m_2, n_2}^o \quad \dots \quad \psi_{M, M}^o]^T$$

C : $M \times M$ matrix with diagonal elements being 1

Let initial distributions of wave functions of two single-particle systems A and B be given respectively by

$$\phi_{\mathbf{A}}(x, 0) = \sum_m a_m \phi_m(x, 0) \quad (28)$$

$$\phi_{\mathbf{B}}(x, 0) = \sum_n b_n \phi_n(x, 0) \quad (29)$$

$a_m, b_n \in C$

Then, the initial wave function of a system with two particles given initial distributions $\phi_{\mathbf{A},\mathbf{B}}(x, 0)$ is described by

$$\psi(x_1, x_2, 0) = \sum_m \sum_n a_m b_n \psi_{m,n}^o(x_1, x_2, 0) \quad (30)$$

The above equation can be rewritten as

$$\psi(x_1, x_2, 0) = \mathbf{d} \cdot \boldsymbol{\psi}^o(x_1, x_2, 0) \quad (31)$$

$$\mathbf{d} = [a_{m_1} b_{n_1} \quad a_{m_2} b_{n_2} \quad \cdots \quad a_M b_M]$$

By using above equation and Eq. (27), initial wave function of multi-particle system with interaction is described by

$$\psi(x_1, x_2, 0) = \mathbf{d} \cdot \mathbf{C}^{-1} \cdot \boldsymbol{\psi}(x_1, x_2, 0) \quad (32)$$

Then, its time evolving wave function is given by

$$\psi(x_1, x_2, 0) = \mathbf{d} \cdot \mathbf{C}^{-1} \cdot \boldsymbol{\psi}(x_1, x_2, 0) \cdot \mathbf{e}(t) \quad (33)$$

$$\mathbf{e}(t) \equiv \left[\exp(-i \frac{E_{m_1, n_1}}{\hbar} t) \quad \exp(-i \frac{E_{m_2, n_2}}{\hbar} t) \quad \cdots \quad \exp(-i \frac{E_{M, M}}{\hbar} t) \right] \quad (34)$$

5. Sample Trajectories

We attempt to compute trajectories of two electrons in a one-dimensional two-particle system (in a CNT of limited length).

In [4], trajectories of electrons were computed when two-particle quantum system is in an eigenstate. In this paper, trajectories are computed when two-particle quantum system is in a mixture state. Then, state interaction is caused and the wave function becomes time-independent. As a result, two electrons move globally in a one-dimensional space between two barriers.

The potential $V(x_1, x_2)$ of the quantum system (16) is given by

$$V(x_1, x_2) = V(x_1) + V(x_2) + \frac{\lambda}{|x_1 - x_2|} \quad (35)$$

The barrier in Fig. 1 is regarded here as infinitely high. Then,

$$V(x) = \begin{cases} 0, & 0 < x < \pi \\ \infty, & \text{otherwise} \end{cases} \quad (36)$$

In computing the wave function and trajectories of two electrons, parameters are normalized as $m = 1$ and $\hbar = 1$. The system is considered as in a mixture state of nine

eigenstates. Given an initial state, a wave function is obtained according to Section 4. By using the wave function, trajectories of the two particles can be computed according to Section 3.

Figure 2 shows the magnitude of the wave function at various time in [1.0, 2.0] on the left column. The figure shows also locations of the two electrons on the center column when the quantum noise or the random force $\boldsymbol{\Gamma}$ in Eqs. (1) and (2) is zero and on the right column the locations when $\boldsymbol{\Gamma}$ is given as in Eqs. (9), (10), and (17), along with contour lines of the magnitude of the wave function. We see in the figure that two electrons locate where the magnitude is relatively high, namely the points at which existence probability of the particles is high, when $\boldsymbol{\Gamma} = \mathbf{0}$ and the locations fluctuate when $\boldsymbol{\Gamma} \neq \mathbf{0}$. Figures 3(a) and (b) present the trajectories in a time interval of [0, 3] when $\boldsymbol{\Gamma} = \mathbf{0}$ and $\boldsymbol{\Gamma} \neq \mathbf{0}$, respectively. We computed many sample trajectories. From the samples including Fig. 3(b), we confirmed that the average path of the trajectories for $\boldsymbol{\Gamma} \neq \mathbf{0}$ coincides almost with the trajectory for $\boldsymbol{\Gamma} = \mathbf{0}$.

6. Conclusions

The circuit simulator models of the blocks are necessary to aid the design of the receiver. As a basis of the model of the detector, a one-dimensional multi-particle quantum system has been modeled after a classical probabilistic system composed of the Brownian particles in this paper.

We confirmed by the numerical experiments of the established model that the Brownian particles moves probabilistically according to the existence probability derived from the wave function of the original quantum system.

Acknowledgment

This work was supported by JSPS KAKENHI Grant No. 15K06075.

References

- [1] 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.
- [2] 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.
- [3] E. Nelson, "Derivation of the Schrödinger Equation from Newtonian Mechanics," *Physical Review*, Vol. 150, No. 4, pp.1079-1085, 1966.
- [4] T. Murakami, H. Fujisaka, T. Kamio, "Stochastic Quantization for Quantum Systems of Multiple Particles," *IEEE Workshop on Nonlinear Circuit Networks*, pp.55-58, 2015.

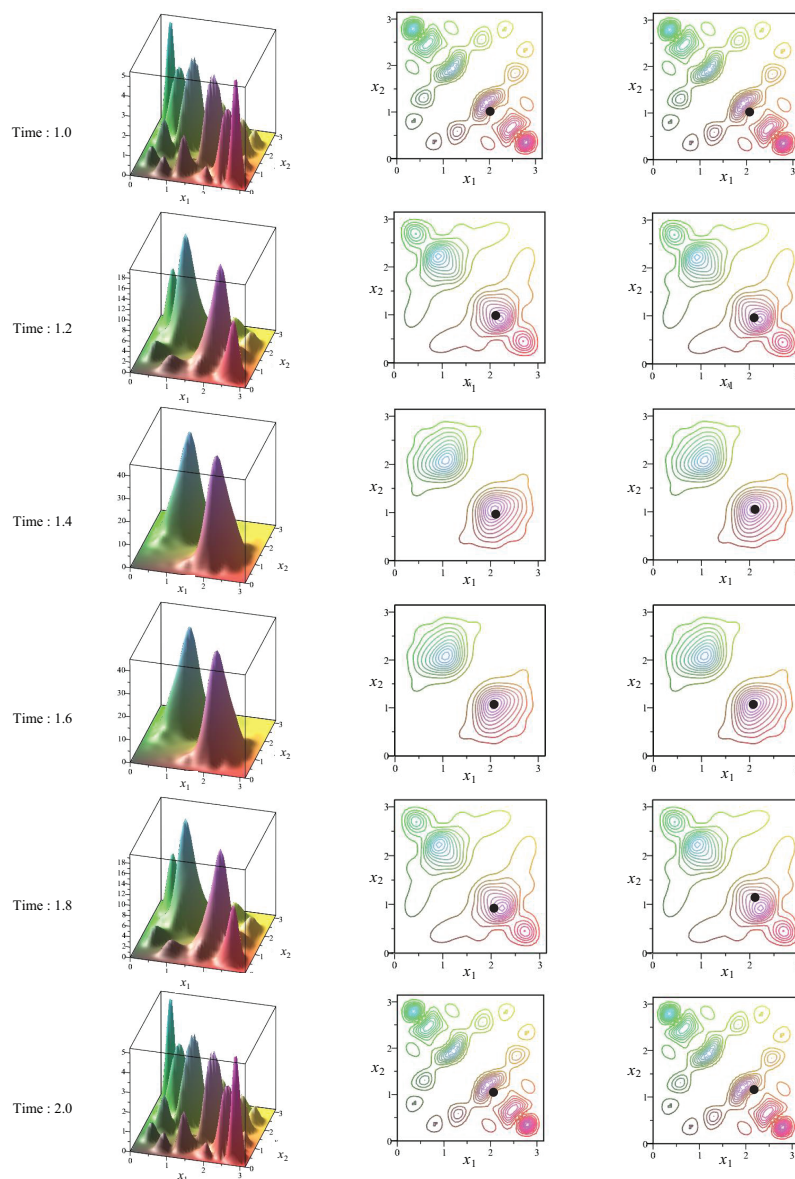


Figure 2: Wave function and locations electrons.

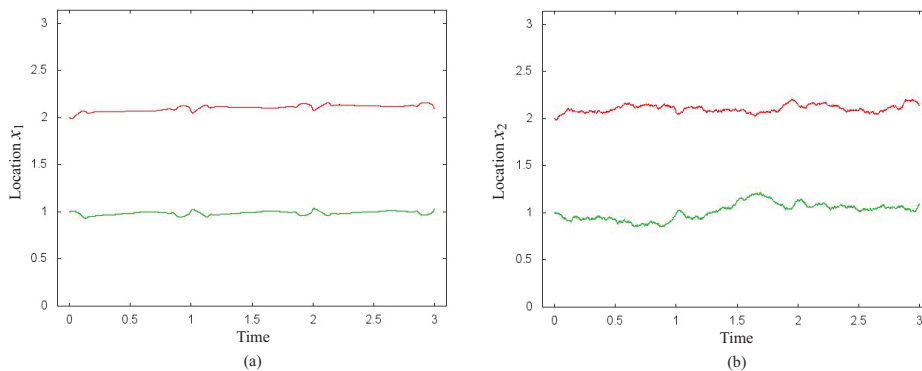


Figure 3: Sample trajectories of the two electrons.