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A Primary Study on Classical Particle Modeling of Electron-Wave Interference Systems

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Abstract—Quantum particles such as electrons and photons have wave-particle duality. In this paper, we regard an electron in a simple electron-wave interference system as a classical particle on which random force acts and its behavior as a stochastic process. We applied the Nelson's stochastic quantization theory to the construction of the stochastic process and confirmed by numerical simulation that the stochastic process has the same probability density function with that determined by wave functions of the Schrödinger equation describing the interference system. This primary study will be useful to model quantum effect devices so as to solve difficulty and reduce complexity in the simulation of electronic circuits built of the devices.

1. Introduction

Various kinds of quantum effect devices are being developed as successors of MOS FETs. It will be necessary to construct time domain models of the quantum effect devices for circuit simulations. Quantum particles such as electrons and photons have wave-particle duality. The Schrödinger equations describe behavior of quantum particles as wave propagation. It is often a difficult or time-consuming task to obtain samples of particle location whose probability distribution obeys a wave function obtained by solving the Schrödinger equation.

On the other hand, a conception regards a quantum particle as a classical particle on which random force acts and its behavior as a stochastic process. Theories within the conception construct a stochastic process which has the same probability density function with that determined by the wave function of the Schrödinger equation. The construction is called stochastic quantization. If a stochastic quantization method can be applied to modeling quantum effect devices, the difficulty or complexity to simulate quantum circuits can be effectively reduced.

In this paper, we construct a probabilistic lumped parameter model of an electron-wave interference system as a primary study on modeling quantum effect devices including quantum interference effect transistors [1]. The construction is based on the Nelson's stochastic quantization theory [2]. Past applications of the theory are tunneling effect analyses [3].

2. Nelson's Stochastic Quantization

A state $\boldsymbol{x}(t) \in R^N$ of a quantum system is described by the Schrödinger equation

$$i\hbar\frac{\partial\psi(\boldsymbol{x},t)}{\partial t} = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x})\right\}\psi(\boldsymbol{x},t) \tag{1}$$

Solution $\psi(\boldsymbol{x},t) : R^N \times R \to C$ of the equation is called a wave function. On the other hand, a classical probabilistic system with state $\boldsymbol{x}(t)$ is described by the Fokker-Planck equation

$$\frac{\partial\rho(\boldsymbol{x},t)}{\partial t} = \left\{-\nabla\cdot\boldsymbol{b}(\boldsymbol{x},t) + \frac{\nu}{2}\nabla^2\right\}\rho(\boldsymbol{x},t) \tag{2}$$

whose solution is a probability density function $\rho(\boldsymbol{x},t)$: $R^N \times R \to R$ of the state. A probabilistic lumped parameter system whose state distribution is governed by Eq. (2) has a potential $U(\boldsymbol{x},t)$ such that

$$-\nabla U(\boldsymbol{x},t) = \boldsymbol{b}(\boldsymbol{x},t) \tag{3}$$

and described by the Langevin equation,

$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{b}(\boldsymbol{x},t) + \sqrt{\frac{\nu}{2}}\boldsymbol{\Gamma}(t), \quad \boldsymbol{\Gamma}(t) = (\Gamma_1(t),\cdots,\Gamma_N(t)) \tag{4}$$

where $\Gamma_i(t)$, $i = 1,\cdots,N$, is a white Gaussian noise with the following correlation property:

$$\Gamma_i(t)\Gamma_j(t') = \begin{cases} \delta(t-t') & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{5}$$

Nelson's stochastic quantization theory [2] asserts that if

$$\begin{aligned} \boldsymbol{u}(\boldsymbol{x},t) + i\,\boldsymbol{v}(\boldsymbol{x},t) &= \nu\nabla\ln\psi, \\ \boldsymbol{u}(\boldsymbol{x},t) &= \boldsymbol{b}(\boldsymbol{x},t) + \boldsymbol{b}^*(\boldsymbol{x},t), \\ \boldsymbol{v}(\boldsymbol{x},t) &= \boldsymbol{b}(\boldsymbol{x},t) - \boldsymbol{b}^*(\boldsymbol{x},t) \end{aligned} \tag{6}$$

then,

$$\rho(\boldsymbol{x},t) = |\psi(\boldsymbol{x},t)|^2 \tag{7}$$

Mean backward velocity $\boldsymbol{b}^*(\boldsymbol{x},t)$ in Eq. (6) is a term contained in the following backward Fokker-Planck equation:

$$-\frac{\partial\rho(\boldsymbol{x},t)}{\partial t} = \left\{\nabla\cdot\boldsymbol{b}^*(\boldsymbol{x},t) + \frac{\nu}{2}\nabla^2\right\}\rho(\boldsymbol{x},t) \tag{8}$$

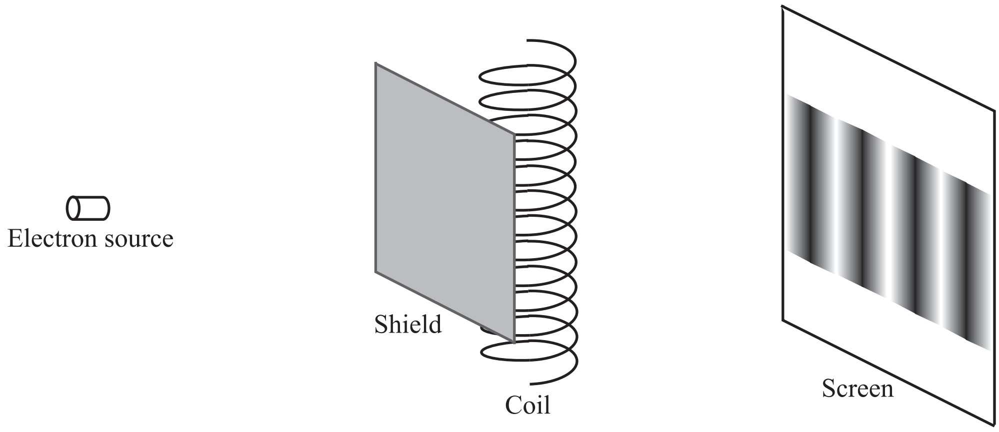

Figure 1: An Aharonov-Bohm thought-experimental system.

The assertion means that a classical probabilistic lumped parameter system (4) corresponding to a quantum system (1) can be constructed by giving the classical system a gradient of potential and magnitude of random noise satisfying Eq. (6).

Many methods were developed to get sample random numbers whose probability distribution follows a specified function. One of them is the inverse transform sampling method [4]. Let $\boldsymbol{f} = (f_1, f_2, \cdots, f_{N+1})$ be a vector function which transforms random vectors $\boldsymbol{r} = (r_1, r_2, \cdots, r_{N+1})$ with uniform probability distribution to the samples of $(\boldsymbol{x}, t) = (x_1, x_2, \cdots, x_N, t)$ whose probability density function is given by Eq. (7), that is

$$\begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_N \\ t \end{bmatrix} = \begin{bmatrix} f_1(r_1, r_2, \cdots, r_{N+1}) \\ f_2(r_1, r_2, \cdots, r_{N+1}) \\ \cdots \\ f_N(r_1, r_2, \cdots, r_{N+1}) \\ f_{N+1}(r_1, r_2, \cdots, r_{N+1}) \end{bmatrix} \tag{9}$$

Then, $\boldsymbol{f}$ must satisfy

$$\rho(\boldsymbol{x}, t) = \frac{\partial f_1^{-1}}{\partial x_1} \cdot \frac{\partial f_2^{-1}}{\partial x_2} \cdot \cdots \cdot \frac{\partial f_{N+1}^{-1}}{\partial t} \tag{10}$$

Generally, it is a difficult problem to find such transformation. The rejection sampling method [5] is another method of getting sample random numbers which obey a specified probability distribution. The method does not require transformation function $\boldsymbol{f}$. However, its execution time increases exponentially with N. On the other hand, Nelson's stochastic quantization does not require $\boldsymbol{f}$ and its execution time is in the order of N^2.

3. An Electron-Wave Interference Phenomenon

A micro-scale double-slit causes interference between quantum waves. Another quantum wave-interference system was proposed by Aharonov and Bohm [6]. Fabrication technology for micro-electronics including nano-carbon electronics makes it possible to construct Aharonov-Bohm (AB) systems. They are expected to be developed to novel electronic devices. Constructing AB systems was important not only for micro-electronics engineering but also for experimental physics in that the system could detect vector potential [7].

Figure 1 shows a thought-experimental AB system containing an infinitely long coil. Vector potential $\boldsymbol{A}(\boldsymbol{x})$, $\boldsymbol{x} = (x_1, x_2, x_3) \in R^3$, outside the coil satisfies

$$\boldsymbol{B} = \mathrm{rot}(\boldsymbol{A}(\boldsymbol{x})) \tag{11}$$

where $\boldsymbol{B}$ stands for the flux inside the coil. An electron getting out of an electron source passes by either left or right side of the coil and reaches to the screen. Let the wave function of the electron be denoted by $\psi(\boldsymbol{x}, t)$. Another wave function $\phi(\boldsymbol{x}, t)$ related to $\psi(\boldsymbol{x}, t)$ as

$$\psi(\boldsymbol{x}, t) = \exp(i\,\theta(\boldsymbol{x}))\phi(\boldsymbol{x}, t), \quad \nabla\theta(\boldsymbol{x}) = -\frac{e}{\hbar}\boldsymbol{A}(x) \tag{12}$$

satisfies

$$i\hbar\frac{\partial\phi(\boldsymbol{x}, t)}{\partial t} = \left\{-\frac{\hbar}{2m}\nabla^2 + V(x)\right\}\phi(\boldsymbol{x}, t) \tag{13}$$

Equations (12) and (13) imply that the vector potential affects the phase of the wave function. Thus, the interference pattern on the screen changes depending indirectly on flux $\boldsymbol{B}$.

4. Stochastic Process Modeling of a Simple Interference System

Figure 2 shows a double-slit system in which vector potential act on electrons. An electron passing through left or right slit moves on vector potential $\boldsymbol{A}_l(\boldsymbol{x})$ or $\boldsymbol{A}_r(\boldsymbol{x})$ and reaches to the screen. We denote the phase shift of the wave function of the electron caused by $\boldsymbol{A}_{l/r}(\boldsymbol{x})$ by $\Delta\theta_{l/r}$.

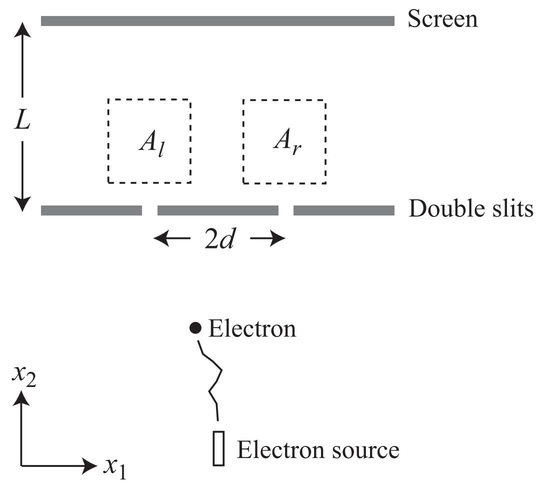

Figure 2: A simple electron-wave interference system.

We will construct a classical probabilistic particle model of electrons moving in the double-slit system and compute probability distribution of location $\boldsymbol{x}$ at which the electron attains on the screen by integrating numerically the Langevin equation describing the classical model.

The numerical experiment is carried out on the following conditions: Distance L from the slits to the screen is $L = 5$. Distance d between the two slits is $d = 1$. Average x_2-directional component of the speed of an electron is $L/5$ at the slits. The wave function of an electron is given in x_1-direction by the following Gaussian distribution with variance $a = 0.2$ around the two slit at time $t = 0$:

$$\psi_l(x_1, 0) = \frac{1}{\pi^{1/4}\sqrt{a}} \exp\left(-\frac{1}{2}\frac{(x_1 + d)^2}{a^2}\right) \quad (14)$$

$$\psi_r(x_1, 0) = \frac{1}{\pi^{1/4}\sqrt{a}} \exp\left(-\frac{1}{2}\frac{(x_1 - d)^2}{a^2}\right) \quad (15)$$

Solving the Schrödinger equation with initial distributions (14) and (15) of wave functions, we obtain evolution of wave functions $\psi_l(x_1, t)$ and $\psi_r(x_1, t)$ of an electron passing through the slits. According to Eq. (6), the superposition

$$\psi(x_1, t) = \psi_l(x_1, t) + \psi_r(x_1, t) \quad (16)$$

provides gradient $\boldsymbol{b}(x_1, t)$ of potential $U(x_1, t)$ and magnitude ν of random force in the Langevin equation (4).

Figure 3 shows x_1-directional probability distributions obtained by numerically integrating the Langevin equation when $(\Delta\theta_l, \Delta\theta_r) = (0, 0)$ and $(-\pi/2, \pi/2)$. Mass of electrons and the Planck's constant are normalized as $m = 1$ and $\hbar = 1$ in the computation. Along with the distribution, the figure shows a probability density function obtained from the superposition (16).

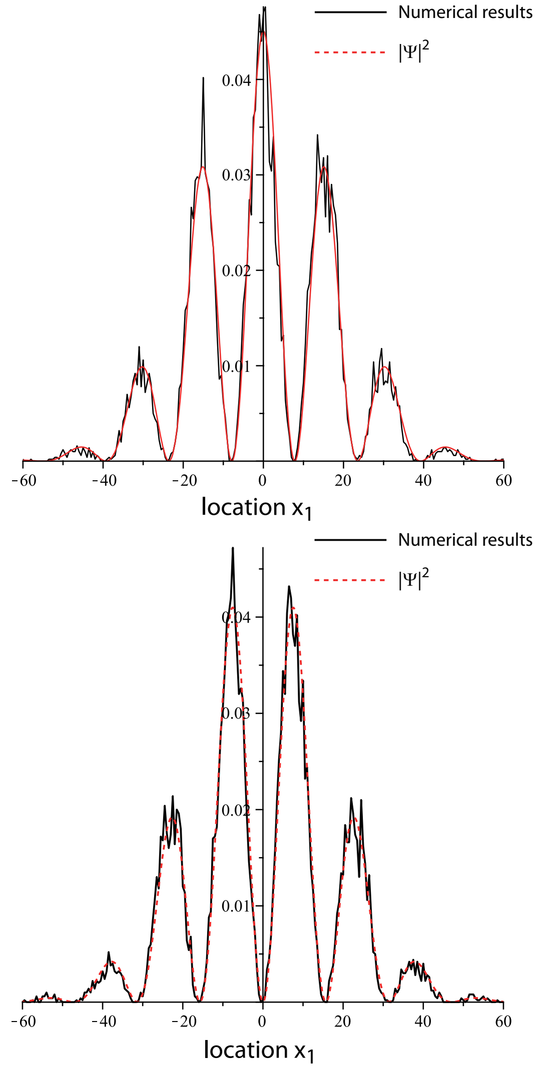

Figure 3: Probability distribution of the locations at which electrons attains when $(\Delta\theta_l, \Delta\theta_r) = (0, 0)$ (Upper) and $(-\pi/2, \pi/2)$ (Lower).

5. Conclusions

We applied the Nelson's stochastic quantization theory to an electron-wave interference phenomenon which is usually described by a partial differential equation, the Schrödinger equation. The theory derived a probabilistic ordinary differential equation, the Langevin equation, and provided sample paths of electrons. Then, we found correspondence between the distribution of the probability of positions at which electrons attain through the paths with probability distribution obtained from the Schrödinger equation. We saw experimentally that the difference between the two distributions decreased with the number of sample paths. Theoretical analysis of the differences is one of our future works.

Our other future works include suitability assessment of several different stochastic quantization methods for time domain simulation of electronic circuits built of quantum effect devices.

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