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Numerical studies of electron transfers in two-dimensional multiple quantum dots

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Abstract

Quantum dynamical properties of electron transfers through multiple quantum dots (QDs) are numerically investigated. The QDs are modeled as two-dimensional electron systems and the conductive properties are calculated from the time evolution of the electron wavefunctions. In addition, we propose a new technique dealing with the electron–electron correlation and demonstrate the dynamical simulations of the Coulomb blockade as well as the spin blockade.

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Keywords: Quantum dots; Electron transfer; Coulomb blockade; Spin blockade

1. Introduction

Recent progress of experimental techniques in nanostructures enables precise control of electron numbers in a two-dimensional system such as multiple quantum dots [1–4]. One of the interests on electronic properties in the quantum dots is to know microscopic characteristics of electron transfers under the dominating electron–electron correlations. In this paper, we present some new numerical methods for simulations of microscopic electron transfers and discuss usability for two-electron systems. We introduce our models and methods of the numerical calculations in the next two sections. Then, some results of the time evolution of the Schrödinger equation for single- and two-electron are shown and we discuss our new method for electron transfers in the last section.

2. Computation model

We model the double-dot structure as the two-dimensional system shown in Fig. 1. The diameter of each dot is 270 a.u. (≈ 14 nm) and two dots are separated by 360 a.u. (≈ 19 nm). Motions of the electrons are confined in the black area of Fig. 1(a) since the area is surrounded by the infinite hard wall. Considering a TFT-like device, the left edge and the right edge are supposed to be source and drain, respectively. We introduce a gate voltage applied in the quantum dots as a harmonic potential energy given in the dot circle area. The feature map of the potential energy along the x-axis ($y = 0$) is shown in Fig. 1(b). Because of the Coulomb repulsive force, the dot is electrostatically occupied by one electron when the depth of the potential ≤ 0.001 a.u. (gate voltage $V_g \approx 27$ mV). Since the deeper trapping potential enables the dot to keep the more electrons, we perform calculations with some different V_g for simulations of the Coulomb blockade.

In order to discuss details of electron transfers through the quantum dots, we pursue the time evolution of the one electron wavefunction with the time dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi = H\psi. \tag{1}$$

The Hamiltonian H of a single electron (mass $= m$):

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V, \tag{2}$$

contains the potential V which indicates the system structure as well as V_g, i.e. V has finite value in the region where an electron exists, otherwise $V = \infty$. We use a Gaussian wave packet as the

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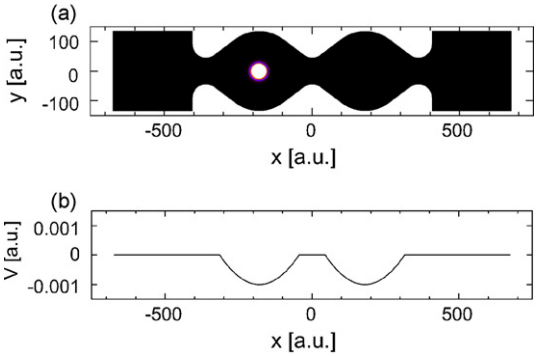

Fig. 1. Computational model system of the double quantum dots: (a) two-dimensional structure and (b) the potential feature map. Diameter of the quantum dot is 270 a.u. ($\approx$14 nm) and the two dots are separated by 360 a.u. ($\approx$19 nm). The electrons move in the black area (a) surrounded by the infinite hard wall.

initial wavefunction of the single electron:

$$\psi(x,y) = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left[-\frac{x^2+y^2}{2\sigma^2} + i(k_x x + k_y y)\right], \tag{3}$$

where σ represents the width of the Gaussian wave packet and the value of σ is 5% of the dot diameter in our calculations. $|\psi(t=0)|^2$ is indicated by the white circle in the left dot in Fig. 1(a). Note that k_x denotes the momentum of the wave packet, $p_x = \hbar k_x$ (x-axis direction) and the initial kinetic energy of the electron is set by k_x and k_y. The numerical evolution in time of the wave packet is performed by the split operator method [5] with the time step $\Delta t = 0.04134$ a.u. $= 0.001$ fs and the mesh size $\Delta x = \Delta y = 1$ a.u. $= 0.0529$ nm.

3. Two-electron system

Investigating the Coulomb- and/or the spin-blockade numerically, we propose a new technique for the time evolutions of the wavefunction in a two-electron system which is based on the Nelson's stochastic mechanics [7,8]. We here consider the electron motion whose path is in-differentiable on all over the system because of its quantum fluctuation. Then the electron motion should be treated as stochastic process, $X = \{X(t) | -\infty < t < \infty\}$ as for x-coordinate. The evolution in time of the stochastic process $X(t)$ is given by Ito-type stochastic differential equation:

$$\mathrm{d}X(t) = v_X\,\mathrm{d}t + \sqrt{\frac{\hbar}{2m}}\mathrm{d}W(t), \tag{4}$$

where $W(t)$ denotes the Wiener process represented by the normal random number $N(0, 1)$. When the drift velocity v_X is related to the wavefunction ψ as

$$v_X = \frac{\hbar}{m}\left(\mathrm{Re}\frac{\nabla_x\psi}{\psi} + \mathrm{Im}\frac{\nabla_x\psi}{\psi}\right), \tag{5}$$

the electron motion is quantized and the time evolution of the stochastic process becomes equivalent to the Schrödinger equation [7]. This means the time evolution of the electron motion is calculated quantum-dynamically from Eqs. (4) and (5) with the wavefunction ψ as the solution of Eq. (1)[9]. Note that the electron path obtained from the stochastic differential equation is just a sample path and the average of many trial paths becomes the probability density $|\psi|^2$.

With the advantage obtaining the electron path at every time step, we introduce approximately electron–electron Coulomb potentials of the two-electron system in the single electron Hamiltonians:

$$H_1(\vec{r}_1,t) = -\frac{\hbar^2}{2m}\vec{\nabla}_1^2 + \frac{e^2}{|\vec{r}_1 - \vec{R}_2(t)|} + V(\vec{r}_1) \tag{6}$$

for the electron 1 and

$$H_2(\vec{r}_2,t) = -\frac{\hbar^2}{2m}\vec{\nabla}_2^2 + \frac{e^2}{|\vec{r}_2 - \vec{R}_1(t)|} + V(\vec{r}_2) \tag{7}$$

for the electron 2. The stochastic paths of the electron 1 and 2 are denoted as $\vec{R}_1$ and $\vec{R}_2$, respectively. Then the single wavefunctions of the electrons $\psi_1(\vec{r}_1)$ and $\psi_2(\vec{r}_2)$ are calculated from the single-electron Schrödinger equations. The drift velocities $\vec{v}_1$ and $\vec{v}_2$ are related with the total wavefunction $\Psi(\vec{r}_1,\vec{r}_2)$ as follows:

$$\vec{v}_1 = \frac{\hbar}{m}\left(\mathrm{Re}\frac{\vec{\nabla}_1\Psi}{\Psi} + \mathrm{Im}\frac{\vec{\nabla}_1\Psi}{\Psi}\right) \tag{8}$$

and the same for $\vec{v}_2$. Being the antisymmetricity requirement, the total wavefunction Ψ constructed by the single electron wavefunctions is expressed by the Slater determinant, that is

$$\Psi = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) + \psi_2(\vec{r}_1)\psi_1(\vec{r}_2)) \tag{9}$$

for anti-parallel spin electrons or

$$\Psi = \frac{1}{\sqrt{2}}(\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_2(\vec{r}_1)\psi_1(\vec{r}_2)) \tag{10}$$

for parallel spin electrons.

In the above approximation, computational costs for evaluating the electron–electron interactions are reduced in comparison to usual mean field approximations which need to integrate over wavefunctions of all other electrons. Our new technique is valid for the system including many electrons (>2) because the other electrons are treated as the point charges in the single electron Hamiltonian.

4. Results and discussions

As a single electron transport property, we first calculate transmission functions [6] of the double quantum dots and a related strait-like structure. The strait has almost the same apertures as the double dots at both ends but has a straight line of 90 a.u. width in the pass. Transmission functions T_{SD} s of these systems from source to drain, or from the left edge to the right edge, are illustrated in Fig. 2. T_{SD} is directly related with the electrical conductance g via the Landauer formula, $g = (2e^2/h)T_{\mathrm{SD}}$. Although the T_{SD} of the strait shows the stepwise-change which is the characteristic response of a