Extended Abstracts of the 2012 International Conference on Solid State Devices and Materials, Kyoto, 2012, pp302-303

Effect of Coulomb Interaction in Electron Wave Packet Dynamics in Nanoscale Devices

T. Shiokawa[1], Y. Takada[2,6], S. Konabe[1,6], M. Muraguchi[4,6], T. Endoh[3,4,6], Y. Hatsugai[1,4,6] and K. Shiraishi[1,5,6]

[1] Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba, 305-8571, Japan
[2] Faculty of Engineering, Tokyo University of Science, Chiyoda, Tokyo 102-0073, Japan
[3] Center for Spintronics Integrated Systems, Tohoku University, Sendai, 980-8577, Japan
[4] Graduate School of Engineering, Tohoku University, Sendai, 980-8579, Japan
[5] Center for Computational Science, University of Tsukuba, Tsukuba, 305-8577, Japan
[6] CREST, Japan Science and Technology Agency
Phone: +81-29-853-5600-8233 E-mail: tshiokawa@comas.frsc.tsukuba.ac.jp

1. Introduction

Semiconductor devices are getting smaller and smaller. There is a device whose channel length is shorter than electron mean free path. In such a ballistic region, electrons are expected to behave obeying the law of quantum physics. However, once we apply normal voltage (~1V) between source and drain, in the channel emerges extremely strong electric field (~1MV/cm). Sano reported that in nanoscale channel, electrons have high kinetic energy even in the drain electrode and not be in their equilibrium state [1]. In this situation, electron waves cannot conserve their coherence and the particle nature will appear. We put attention to this quantum-classical crossover region and use wave packets, which have crossover nature between waves and particles. In the numerical calculation, we take Coulomb interaction to investigate the behavior of electrons in this parameter region.

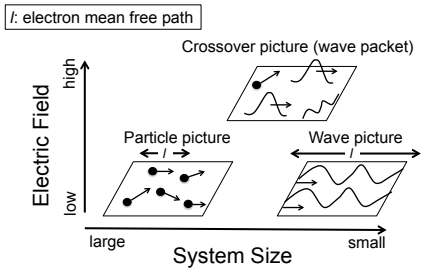

Fig. 1: Schematic illustration of difference among three pictures of electrons; particle, wave and the wave packet dynamics.

2. Method

In this study, we start with the one-dimensional effective mass Hamiltonian as

$$H_{eff} = -\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2} + V(x) \tag{1}$$

where m^* is the effective mass of the electron and . $V(x)$ is an effective external potential. We discretize this effective-mass Hamiltonian on a discrete lattice whose lattice constant is a,

$$\left(\frac{\partial^2}{\partial x^2}\langle x|i\rangle\right)_{x=n} \to \frac{1}{a^2}\left[\langle n+1|i\rangle - 2\langle n|i\rangle + \langle n-1|i\rangle\right]$$

$$\left[V(x)\langle x|i\rangle\right]_{x=n} \to V_n\langle n|i\rangle$$

This discretized Hamiltonian can be mapped onto a nearest-neighbor tight-binding Hamiltonian,

$$\left[H_{eff}\langle x|i\rangle\right]_{x=n} = (V_n + 2\gamma)\langle n|i\rangle - \gamma\langle n-1|i\rangle - \gamma\langle n+1|i\rangle$$

$$= \sum_m \left[(V_n + 2\gamma)\delta_{n,m} - \gamma\delta_{n,m-1} - \gamma\delta_{n,m+1}\right]\langle m|i\rangle \tag{2}$$

where

$$\gamma = \frac{\hbar^2}{2m^*a^2} \tag{3}$$

We employed the above-discretized tight binding Hamiltonian in this study. The number of lattice site is 100 in our calculation that is conceived to sufficient to describe the basic characteristics of the system. We also set the lattice constant a to unity.

We calculate the time evolutions of the each electron wave functions by solving the time-dependent Hartree-Fock equation in order to take into account the coulomb interaction [3],

$$i\frac{\partial}{\partial t}\left|i^{(1)}\right\rangle = H_{HF}\left|i^{(1)}\right\rangle = (T + G - F)\left|i^{(1)}\right\rangle \tag{4}$$

where, H_{HF} is the one-body Hartree-Fock Hamiltonian which is composed by the tight binding Hamiltonian T, coulomb potential G and exchange potential F. We have taken the atomic unit $\hbar = e = 1$ in the present work. The three terms in equation (4) are expressed as

$$T = -\gamma\sum_n \left(c_n^+ c_{n+1} + h.c.\right) \tag{5}$$

$$G\left|i^{(1)}\right\rangle = \sum_j \left\langle j^{(2)}\left|\frac{U}{|x_1 - x_2|}\right|i^{(1)}j^{(2)}\right\rangle \tag{6}$$

$$F\left|i^{(1)}\right\rangle = \sum_j \left\langle j^{(2)}\left|\frac{U}{|x_1 - x_2|}\right|i^{(2)}j^{(1)}\right\rangle \tag{7}$$

where γ is hopping parameter, U is the strength of the electron-electron repulsion, which qualitatively represents the magnitude of screening effects. The i and j indicate the orbitals of the electron wave functions and its suffixes (1) and (2) correspond to the position x_1 and x_2, respectively. Further, $c+$ and c represent creation and annihilation operators of electrons, respectively. In our calculation, the Hamiltonian is scaled by the hopping parameter γ.

The formal solution of the time-dependent Hartree-Fock equation is expressed as

$$\left|i(t + \Delta t)\right\rangle = \exp(-iH_{HF}\Delta t)\left|i(t)\right\rangle \tag{8}$$

where Δt is a small increment of time. We performed Taylor series expansions for the time evolution operator up to fourth order. We study the dynamical properties of the two electron wave packets by investigating the charge distributions of electron.

3. Results and Discussion

Figure 2 and Fig. 3 show the time evolution of wave packets. In this study, we used two wave packets; each peak of the packet means one electron in the figures. The left edge of the figure is considered a source electrode and the other edge is considered as drain electrode. The electric field is set as fixed potential, which goes down linearly from left side (source) to right side (drain). We also show Fourier transformed results after showing the real space results. Whole dynamics are performed in the first Brillouin zone. Figure 2 is the results when the strength of Coulomb interaction is weak (U=1). Electron wave packets go to right side of the system, by the electric field. Figure 3 is the results with strong Coulomb interaction (U=10). In this case, the electron wave packet goes

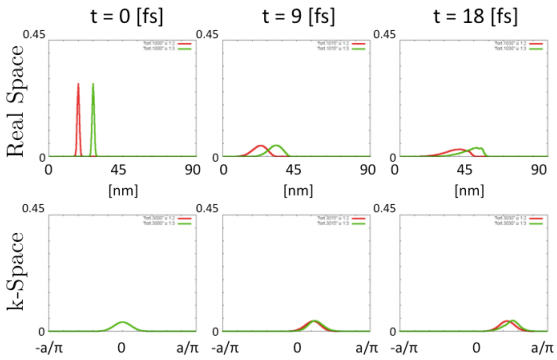

Fig. 2: Two electron wave packets dynamics with weak Coulomb interaction (U=1). Above figures are in real space dynamics and below figures are in k-space. The horizontal axis in upper figure is mapping site, in below figure that means wave number in one Brillouin zone. The vertical axis means each electron's density in both figures.

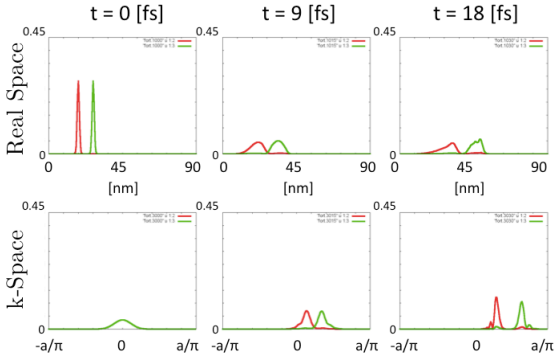

Fig. 3: Two electron wave packets dynamics with strong Coulomb interaction (U=10).

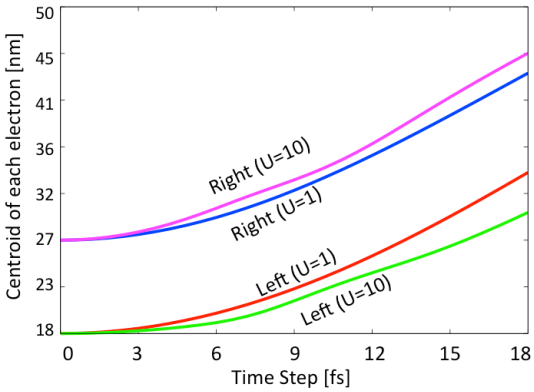

Fig. 4: Centroid of each electron. The above pair is right packet and the below pair is left packet.

right side by the electric field and feels strong Coulomb repulsion, which interacts each other.

To see more detailed nature of the behavior of wave packets, we obtained some quantities of each electron. In Fig. 4, we show the time evolution of averaged position of the electrons. With strong Coulomb interaction, the left (latter) electron is less accelerated compared with the weak Coulomb interaction case. On the other hand, the right (former) electron has moved more in strong interaction case than in the weak interaction case. This suggests that Coulomb interaction modulates the behavior of the electrons.

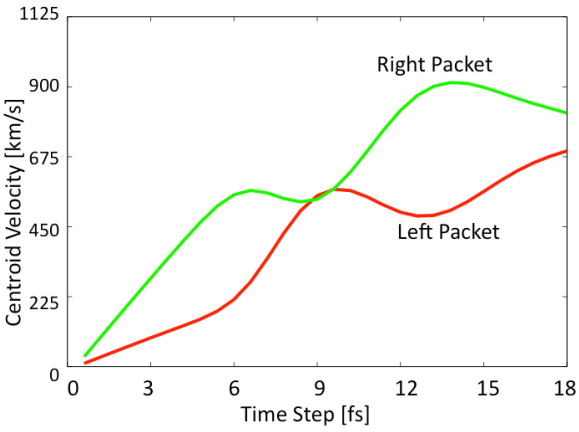

Fig. 5: Time evolution of centroid velocity when U=10.

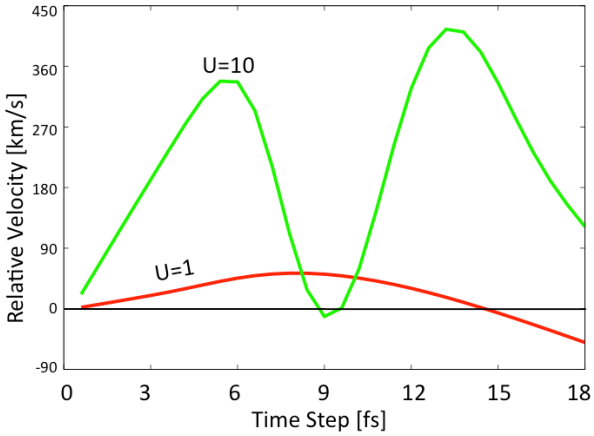

Fig. 6: Time evolution of relative velocity of each centroid of wave packets.

Figure 5 shows the centroid velocity in the case of strong Coulomb interaction. The velocity is strongly modulated by the interaction and the electric field. At the critical time, right and left packets have the same velocity. Their relative velocity (V_{Right} – V_{Left}) is shown in Fig. 6. With the strong Coulomb interaction, the velocity oscillates in early time region, although this does not appear with weak Coulomb interaction.

The velocity of the electrons in a ballistic region can be reduced by the effect of Coulomb interaction. We must pay much care for how Coulomb interaction is effective in considering system, when we consider the behavior of electrons transporting in nanoscale channel.

Acknowledgements

This work was supported by Grants-in-Aid for Scientific Research from Ministry of Education, Culture, Sports, Science and Technology, Japan.

References

[1] N. Sano, Jpn. J. Appl. Phys. 50, 010108 (2011)
[2] P. A. Dirac, Proc. Camb. Phil. Soc. 26, 376 (1930)
[3] Y. Takada, et al., Jpn. J. Appl. Phys. 51, 02BJ01 (2012)