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Multi Electron Wave Packet Dynamics in Applied Electric Fields

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Abstract

We investigated multi-electron wave packets dynamics considering the Coulomb interaction under the applied electric field by solving the time-dependent Hartree-Fock equation. Our results show that the coulomb interaction works to prolong the lifetime of the wave packets as the time evolves in the no electric field situation as well as in the applied electric field. It is also noted that the applied electric field also prolong the wave packet lifetime, especially when the Coulomb repulsion is relatively small. It indicates that the particle pictures of the electrons tend to be dominant under the applied electric field.

1. Introduction

The device size, physical gate length as well as channel length, has aggressively scaled down in order to obtain the required high performance [1]. There would be a few numbers of electrons in such a nano scale transistor channel region. It is, thus, expected that electron correlation plays a crucial role for the electrons dynamics in the nano-scale channel and affects the device performance. For this reason, it would be required the investigation about transport in semiconductor that is taken into account the electron correlation so as to understand the fundamental physics which governs future nano device systems.

The electric field between source and drain electrodes is expected to increase drastically owing to the aggressive miniaturization of device channel length. In such a situation, it is difficult to expect coherent electron transport though the channel with high electric field. Thus, we have to establish a new approach instead of conventional electron transport approaches [2]. We treat the electrons in the semiconductor channel as wave packets, which describe a crossover feature between the particle and the wave pictures of electrons, as schematically illustrated in Fig.1. There are various studies focused on the dynamics of the single electron wave packet until now [3]. In this work, we investigate multi-electron wave packets dynamics considering the Coulomb interaction under the applied electric field. The electron in the uniform electric field will undergo periodic oscillation, known as the Bloch oscillation [4]. We adopt the electric field that the Bloch oscillation can be safely ignored in the calculation.

2. Method

In this study, we start with the one-dimensional the 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 (1) with 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,

$$\begin{aligned}\left[H_{eff}\langle x|i\rangle\right]_{x=n} &= (V_n + 2\gamma)\langle n|i\rangle - \gamma\langle n-1|i\rangle - \gamma\langle n+1|i\rangle \\ &= \sum_m\left[(V_n + 2\gamma)\delta_{n,m} - \gamma\delta_{n,m-1} - \gamma\delta_{n,m+1}\right]\langle m|i\rangle\end{aligned} \tag{2}$$

where

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

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 [5, 6],

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

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. These three terms in equation (4) are expressed as

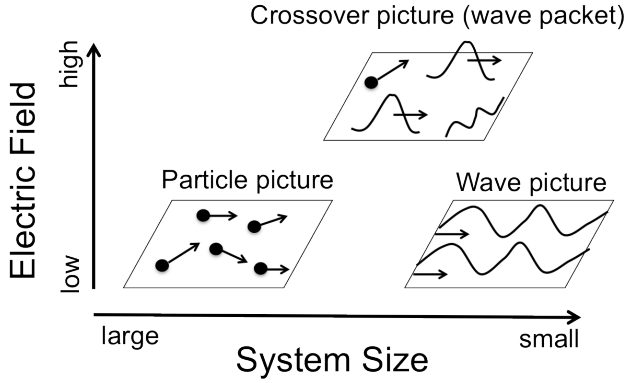

FIG 1: Schematic illustration of difference among three pictures of electrons: particle, wave and the wave packet dynamics.

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

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

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

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

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

where Δt is a small increment of time. We performed Taylor series expansions for the time evolution operator up to fourth order to calculate next time step wave function [7, 8]. In addition, we scaled time by $1/\gamma$. We study the dynamical properties of the two electron wave packets by investigating the charge density distributions of each electron.

Under these conditions, we study the dynamical properties of the two electron wave packets by investigating the charge density distributions of each electron. We set the initial wave functions as the Gaussian wave packets [9]. In order to discuss the lifetime of the wave packet, we consider the width of a wave packet by estimating standard deviation of the position operator that is represented by

$$\sigma = \sqrt{\left\langle (\Delta x)^2 \right\rangle} = \sqrt{\left\langle x^2 \right\rangle - \left\langle x \right\rangle^2} \tag{9}$$

where $\langle x \rangle$ and $\langle x^2 \rangle$ is the expectation value of the x and x^2, respectively.

3. Results and Discussion

Figure 2 schematically shows the initial state of our calculation and the potential profile adopt in our calculation that represents the applied electric field in the semiconductor channel. The potential is linearly dropped between the source and the drain, $E=-0.05x$. We performed numerical calculation of the two electron wave packets dynamics under this electric field varying the strength of the coulomb interaction. The effect of the electric field is estimated by the comparison with the no electric field case.

Figure 3 shows the width of the wave packet, which is located at right side in Fig.1, represented by the standard deviation at t=20 as a function of the magnitude of the electron-electron interaction U/γ. Our results indicate that the coulomb interaction works to prolong the lifetime of the wave packets as the time evolves in the no electric field situation as well as in the applied electric field, as shown in Fig.3. It is also noted that the applied electric field also prolong the wave packet lifetime, especially when the Coulomb repulsion is relatively small. It indicates that the particle pictures of the electrons tend to be dominant under the applied electric field. Moreover, we will also discuss the electric field dependence of the lifetime of the wave packets.

Acknowledgements

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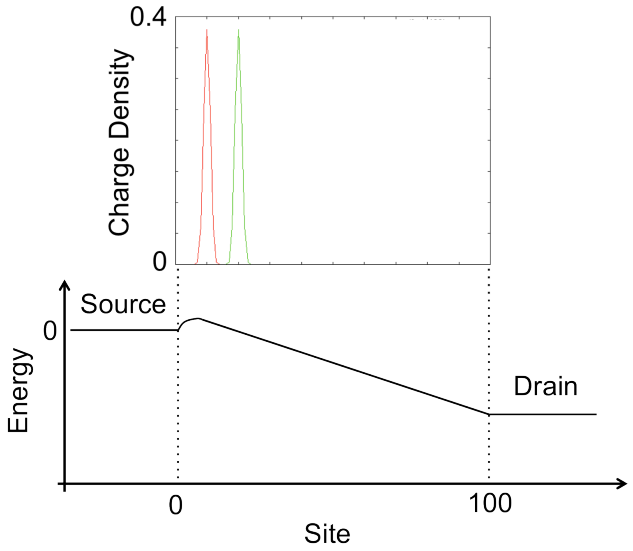

FIG. 2: Initial state of our calculation and potential profile of the channel in applied electric field.

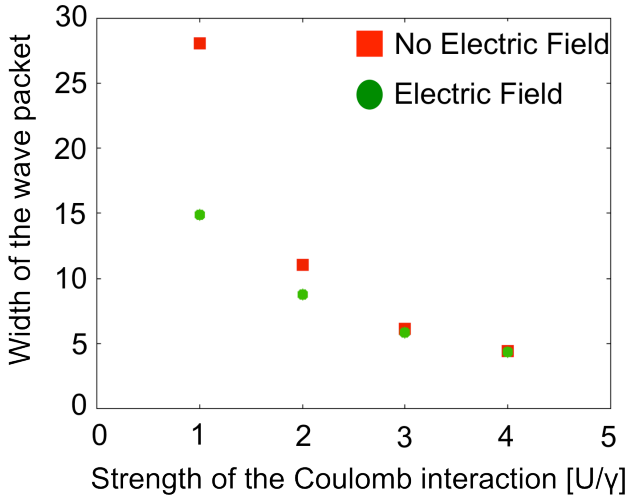

FIG. 3: The width of the wave packet located at the right side as a function of the strength of the Coulomb interaction U/γ at t=20.

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