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Multi-electron Wave Packet Transport Dynamics in Nanoscale Channel

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Abstract

We have investigated semi-classical electron transport in a bland-new viewpoint of “multi-electron wave packet”. Our numerical calculation shows that electrons tend to transport forming collective state with a realistic Coulomb interaction. This phenomenon may cause the intrinsic current fluctuation. Recent classical transport simulation pointed out that the speed limit of Si CMOS is around 100 GHz because of the current fluctuation that originates from the discreteness of electrons. Our results indicate that as scaling, this kind of current fluctuation becomes more serious due to the collective motion of multi-electron wave packets. In this paper, we propose that it is significant for the next generation of Si CMOS to be controlled the behavior of multi-electron wave packets from viewpoints of its structure or material.

1. Introduction

With increasing miniaturization of VLSI, the channel lengths of CMOS transistors are approaching the order of 10 nm. In such a ballistic region, quantum effect must be considered in the transport of electrons and electrons should be treated as waves. [1, 2] On the other hand, with nanochannel (~ 10 nm), extremely high source-drain electric field (~ 1 MV/cm) is inevitable, when typical voltage (~ 1 V) is applied. In such a situation, quantum waves cannot maintain its coherence in the whole systems, so that classical particle nature of electrons will appear. [3] In short, classical-quantum (particle-wave) crossover nature governs the electron transport in future nanodevices as schematically shown in Fig. 1. We thus treated electrons as wave packets to describe crossover characteristics between waves and particles. [4-6]

In this paper, we focus on multi-electron wave packet, which is a collective state of electrons. In an unscreened channel, long-range repulsion of electrons will be dominant to electron transport. Once a gate voltage is applied, electrons go into the channel form source electrode. (Fig. 2 (a)-(b)) When some electrons stay in a nanochannel, the electrons form Coulomb repulsion potential that makes the next electrons unable to enter the channel. (Fig. 2 (c)) After that, the channel electrons move to drain electrode and the source electrons enter the channel collectively. (Fig. 2 (d))

Moreover, logic nanodevices are approaching its limit for improving the performance only by the conventional scaling, Last year, Kamioka et al. show that the speed limit of CMOS devices is around 100 GHz because of current fluctuations that is caused by discreteness of electrons, treating electrons as particles. (Fig. 3) [7] In this study, we aim to investigate this current fluctuation taking quantum effects into account and suggest a guiding principles to suppress the fluctuations in future devices.

2. Method

In this study, we employ discretized spinless effective mass Hamiltonian with long-range Coulomb interaction. The dependence of the strength of Coulomb interaction (U) has studied. In the case of Si, U is around 0.2~0.6. To investigate the time evolution, we approximate the long-range Coulomb interaction by time-dependent Hartree-Fock approximation, which enables the consideration the Pauli principle for electrons in nanochannels. (Fig. 4) To drive current in the periodic boundary system, (in a circular ring system), we further adopt hypothetical magnetic field along z direction as shown in Fig. 5. Peierls phase factor represents hypothetical magnetic field.

3. Results and Discussion

Figure 6 shows the charge density’s time-evolution of 5 electrons under a uniform electric field of 0.2 MV/cm. With Coulomb interaction of U=1, electrons transport collectively despite of existence of Coulomb repulsion. We call this collective state “multi-electron wave packet”. It consists of five electrons in this case. To investigate the formation of multi-electron wave packets, we carry out longer time-evolution in one-dimensional ring using 20 electrons. (Figs. 7-8) Though the charge densities fluctuate during the time-evolution, electrons tend to form multi-electron wave packets with realistic Coulomb interaction of U=0.5. To study this tendency more quantitatively, we calculated time-average of correlation functions. As is seen in Fig. 8, the stronger interaction, the larger the peak positions shift, indicating that the number of multi-electron wave packets are changed depending on the strength of Coulomb interaction. To summarize above calculated results, we can propose the following concept. Electrons transport forming multi-electron wave packets, which is essential crossover picture between particles and quantum waves as schematically shown in Fig. 9. However, formation of multi-electron wave packet is suppressed under strong Coulomb interactions. It is noted that the current fluctuation will depend on the number of electrons that form each multi-electron wave packet, when electrons transport collectively forming multi-electron wave packet. Considering the speed limit of 100 GHz obtained by Kamioka’s particle simulations, CMOS devices may reach its speed limit of the order of 10 GHz in the near future, since each multi-electron wave packet contains typically 10 electrons (Figs. 10-11). Moreover, we can propose a recipe to reduce fluctuations that originates from the discreteness of multi-electron wave packets. To reduce the fluctuation, suppression of multi-electron wave packet state is important. Low-dimensional structures or small dielectric constant materials, both cause stronger Coulomb interaction, will help the suppression of formation of multi-electron wave packet state.

4. Conclusion

We have investigated electron transport in a nanoscale channel. We have shown that electrons tend to transport collectively, forming “multi-electron wave packet”. This will make worse the current fluctuations that caused by the discreteness of electrons. Moreover, we have proposed a recipe to reduce the intrinsic fluctuation that originates from “multi-electron wave packet”.

References

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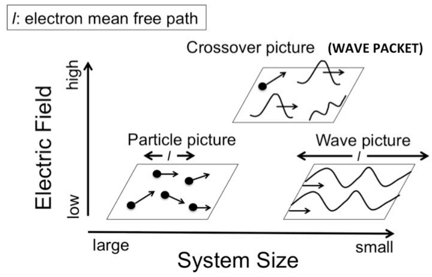


FIG. 1. Schematic illustration of electron transport depending on system size and electric field; particle, wave and wave packet.

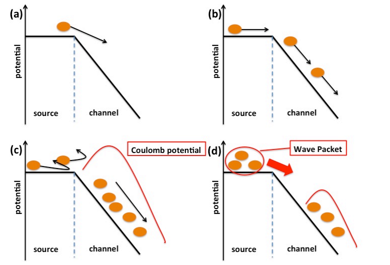


FIG. 2. (a) An electron goes into a channel. (b) Electrons go into the channel one after another. (c) Channel electrons form Coulomb potential and next electrons are repelled. (d) After that, some electrons go into the channel together forming multi-electron wave packet.

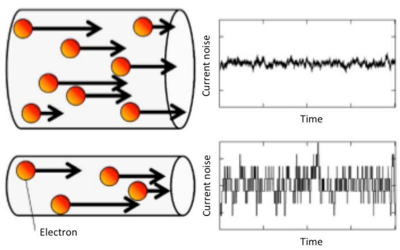
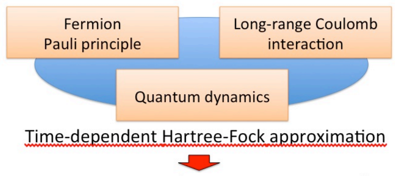


FIG. 3. (Ref. 7) Current noise caused by the discreteness of electrons. When the number of electrons is very small, the fluctuation of carried charge will not be negligible.



$$i\frac{\partial}{\partial t}\psi_r(x_i)=(T+V)\psi_r(x_i)+\left[\sum_s\int dx_j\frac{U}{|x_i-x_j|}|\psi_s(x_j)|^2\right]\psi_r(x_i)$$
$$-\sum_s\left[\int dx_j\psi_s^*(x_j)\frac{U}{|x_i-x_j|}\psi_r(x_j)\right]\psi_s(x_i)$$

FIG. 4. We want to consider Pauli principle, long-range Coulomb interaction and its quantum dynamics. For these, time-dependent Hartree-Fock approxima-tion is applied.

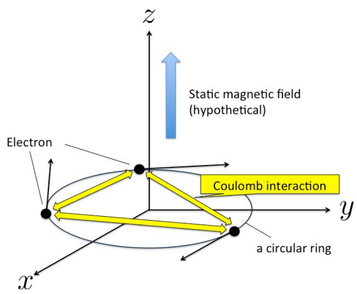


FIG. 5. Schematic illustration of our calculation system of a circular ring. To drive current, hypothetical static magnetic field is applied.

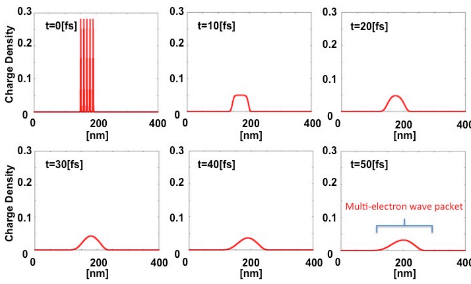


FIG. 6. Snapshots in the time-evolution of charge density with Coulomb interaction of U=1 under static electric field of 0.2 MV/cm. Electrons transport collectively forming "multi-electron wave packet" in spite of Coulomb repulsion.

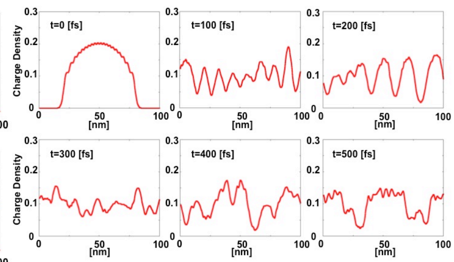


FIG. 7. Snapshots in the time-evolution of charge density with realistic Coulomb interaction of U=0.5 under static hypothetical magnetic field in one-dimensional ring. There are 20 electrons in the system but seem less than 10 wave packets.

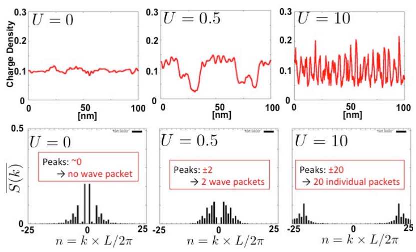


FIG. 8. Snapshots of electron distribution and correlation function $S(k)$ at t = 500 [fs] in the case of static hypothetical magnetic field. The number of multi-electron wave packet is modulated by the strength of Coulomb interaction and the correlation functions show the number of multi-electron wave packets.

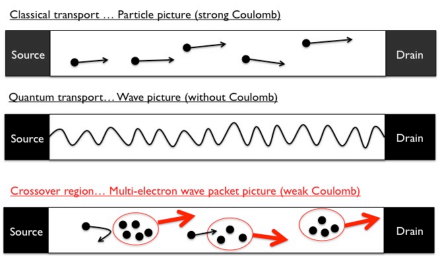


FIG. 9. This schematic figure shows that in the crossover region between particles and waves, multi-electron wave packet will be formed. In one multi-electron wave packet, some electrons are in quantum coherence state, while multi-electron wave packet itself transport as a classical particle.

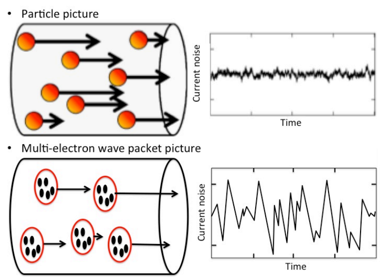


FIG. 10. In particle picture model, current noise is not serious with long channel, large number of carriers, and slow speed. But with multi-electron wave packet picture, current noise caused by discreteness of electrons will be serious for each wave packet has more charges.

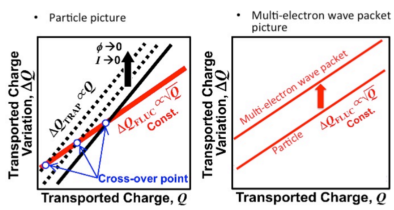


FIG. 11. With particle picture, the current fluctuations are dominant noise around 100 GHz. (Ref. 7) With multi-electron wave packet picture, however, the fluctuations will get worse as shown in the right schematic figure.