11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

Time-Dependent Carrier Transport in Quantum-Dot Array Using NEGF

Yuhui He, Danqiong Hou, Xiaoyan Liu, Gang Du, Jinfeng Kang, Jie Chen* and Ruqi Han
Institute of Microelectronics, Peking University, Beijing, 100871, China
* National Institute of Nanotechnology and Univeristy of Alberta, Canada
e-mail: xyliu@ime.pku.edu.cn

INTRODUCTION

Understanding time-dependent electron transport in mesoscopic systems is a very interesting research topic, which has drawn a great deal of research interest. [1-3] Here, we present a novel method to handle time-dependent transport in low-dimensional systems by jointly solving the nonequilibrium Green's functions (NEGF) in the time-domain and the real-space in a recursive fashion. In this way, we obtain electrical current densities in response to time-variant voltage signals.

METHODOLOGY

Our time-domain recursively solving NEGF approach is based on the time-domain decomposition (TDD) technique [4]. This approach does not need to use the wideband limit approximation for electrodes. Thus electrodes with an arbitrary-shaped density of state (DOS) can be handled. According to the electron lifetime inside the devices, we cutoff the negative infinity limit in the integral equations of the NEGF. In the simulations, we utilize a dynamically allocated data-structure, which enables us to compute current densities in response to input signals of any time duration. Another challenge when we calculate the time-dependent transport characteristics is to handle an arbitrary-length conductor between the electrodes in low-dimensional systems. We handle this problem by combining the real-space recursively solving NEGF approach with the time-domain recursive approach. With this recursive algorithm, we can get numerical solutions by using $\mathbf{O}(\log_2 N)$ computation steps for a system with N principle layers in the central conductor.

DISCUSSION

We apply this method to explore the transient and AC transport properties of a 1D quantum-dot array system, which can be used to emulate switches and interconnections made of low-dimensional materials. The electrical current densities in response to various pulses and sinusoid waveforms are simulated. The delay and distortion information is obtained, and how the hopping energy and the length of a quantum-dot array affect the transport behavior is further discussed.

The electron lifetime is extracted from the decay of equilibrium Green's functions $G_N^r(\tau)$ [Fig. 1]. It gets larger when the number of dots increases, due to the fact that it is inversely proportional to the probability of the electron escaping into the electrodes. Fig. 2 and Fig. 3 show the injection current densities (flow from the electrode where input signals are applied to the central conductor) and response current densities (flow from the central conductor to the other electrode) driven by the pulse waveform and sinusoid voltage signals, as the functions of time and the number of the quantum dots on the array. The injection current densities are almost the same for various dot numbers. The delay of response current densities is proportional to the array-length, which can be explained by the ballistic transport theory. In Fig. 3, the amplitude of the response current density of the 10-dot array is largest among the three response current densities. It is worth noticing that abrupt negative peaks exist at the beginning of the calculated injection current density curves. The amplitude of this transient overshoot is significantly attenuated as the electrons pass through the barrier between the conductor and electrode, so the response current densities at the right electrode are much smoother compared to the injection current densities. The influence of the hopping energy between neighboring quantum dots on the current densities is shown in Fig. 4. Larger hopping energy can suppress the peaks of the injection and response current densities at the barrier between the electrodes and conductor.

CONCLUSION

A novel method to handle time-dependent transport in low-dimensional systems has been proposed and applied to one-dimensional quatum-dot arrays. Interesting results are presented and discussed.

ACKNOWLEDGEMENT: The authors would like to thank Dr. Chun Fan and Aidong Sun for their help in our numerical calculations. All simulations were performed on IBM RS/6000 SP3 at the CCSE at Peking University. This work was supported by the NBRF of China (Grant 2000036502) and the US NSF (Grant CCF 0304284).

REFERENCES: [1] A.-P. Jauho, N. S. Wingreen and Y. Meir, *Time-dependent transport in interacting and noninteracting resonant-tunneling systems*, Phys. Rev. B **50,** 5528 (1994). [2] Supriyo Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge Univ. Press (1995). [3] Baigeng Wang, Jian Wang, and Hong Guo, *Current Partition: A Nonequilibrium Green's Function Approach*, Phys. Rev. Lett. **82**, 398 (1999). [4] Yu Zhu, Joseph Maciejko, Tao Ji, Hong Guo, and Jian Wang, *Time-dependent quantum transport: Direct analysis in the time domain*, Phys. Rev. B **71**, 075317 (2005).

ISBN 3-901578-16-1

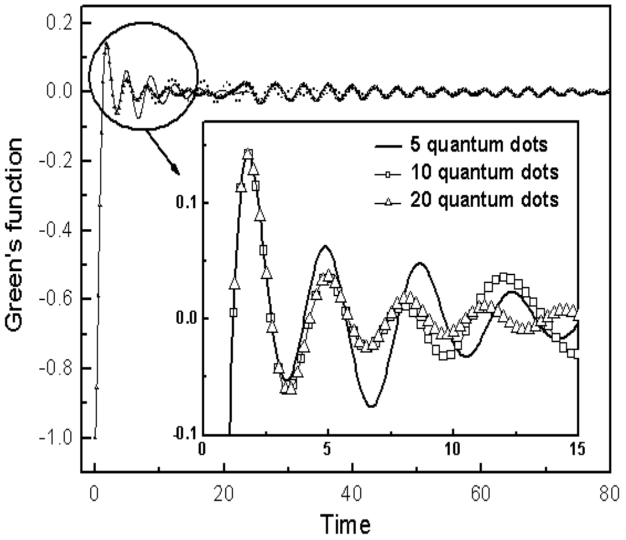
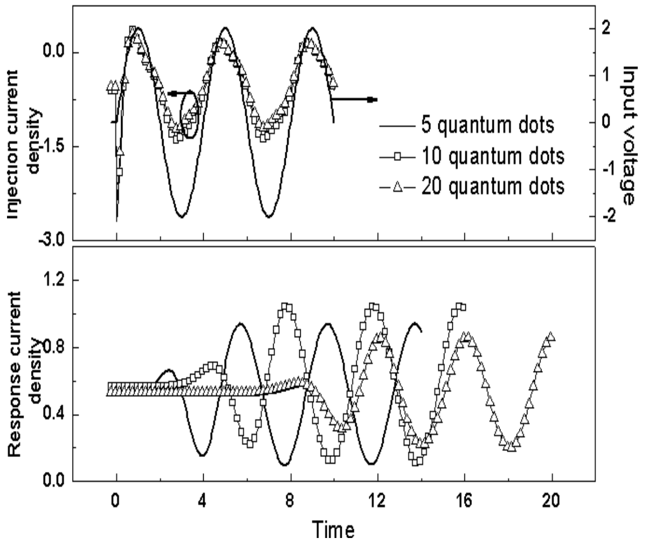
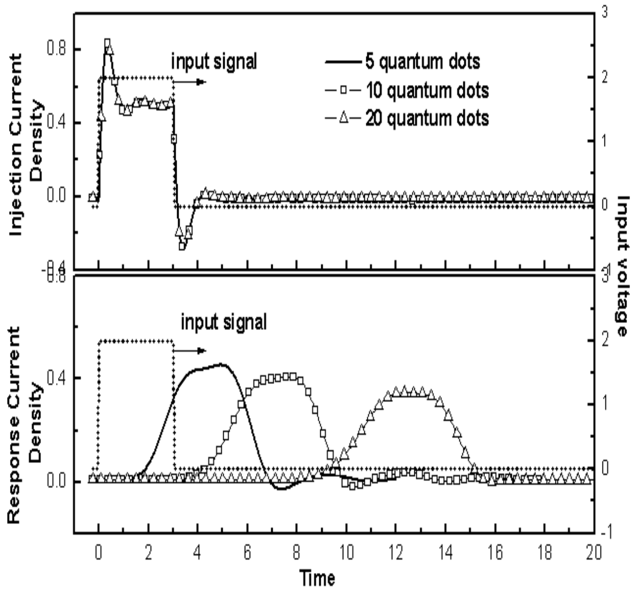


Fig. 1. Extraction of the electron lifetime from the decays of equilibrium Green's functions $G_N^r(\tau)$. Here, the numbers of dots on the quantum-dot arrays are 5, 10 and 20, respectively. The hopping energy between the neighboring dots is set to be one.



(b)

Fig. 3. Injection and response current densities driven by the sinusoid voltage signal V=2sin(πt), for 1D 5-, 10- and 20- quantum-dot arrays, respectively. The hopping energy between the neighboring dots is set to be one. A bias voltage of -2V is applied to the system.



(a)

Fig. 2. Injection and response current densities driven by the pulse waveform, for 1D 5-, 10- and 20-quantum-dot arrays, respectively. The hopping energy between the neighboring dots is set to be one.

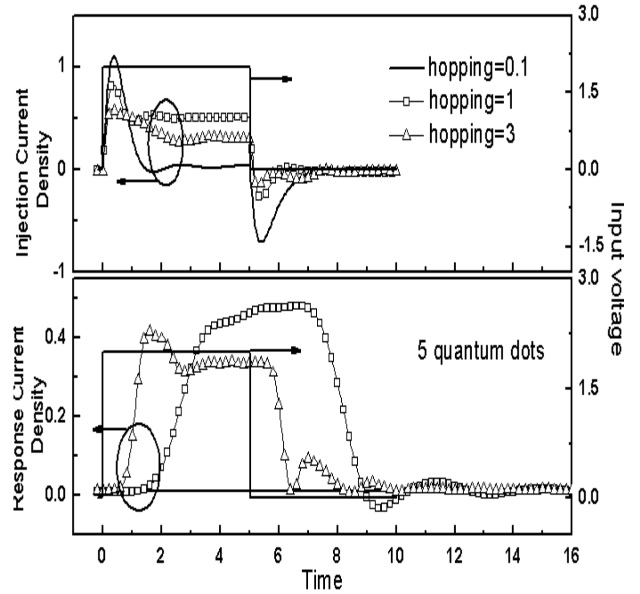


Fig. 4. Input pulse waveform and the corresponding injection and response current densities for a 1D 5-dot array. The hopping energies are 0.1, 1 and 3, respectively.