Quantum Lattice-Gas Automata Simulation of Electronic Wave Propagation in Nanostructures

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The quantum lattice-gas automata (QLGA) have been studied to simulate the time-dependent Schrödinger equation [1-3]. It is particularly well suited to implementation on a quantum computer; the many-body quantum system can be simulated very efficiently [1]. On the other hand, its emulation on a classical computer would also have an advantage, because its unitarity might lead better behavior than standard finite-difference methods [2, 3]. In this study, we apply the QLGA method to the analysis of the one-particle quantum wave propagation in nanoscale devices. To this end, we develop a new algorithm to implement the open boundary condition into the QLGA method.

In the QLGA simulation, the space is discretized and qubits are assigned to each node of the lattice [3]. The each qubit contains the probability amplitude of whether the lattice node is occupied or not by the simulated particles. In this study, we have assigned the qubit array outside the simulation region to store the information about the particles which have flown out across the boundary. Then it becomes possible to simulate the open systems with the QLGA simulation.

In order to verify the validity of the open boundary condition, the transmission coefficients for the quantum tunneling through the square potential barrier were calculated. As shown in Fig. 1, the simulated results are in good agreement with the exact analytical solution. The QLGA simulation is easily extended to the simulation in *n*-dimensional space. As an example, we performed 2D simulation of quantum tunneling through a potential barrier with surface roughness. Figure 2 shows the time evolution of the plane wave injected toward the barrier. The electron wave is scattered by the surface roughness, and the interference patterns are observed. Note that the outgoing waves are absorbed smoothly at the boundary, which shows that the boundary condition algorithm works well.

The QLGA simulation can be applied to the more complicated systems. The other simulation results as well as the details of the simulation algorithms will be presented at the conference.

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[3] J. Yepes and B.M. Boghosian, Com. Phys. Commu. **146**, 280 (2002).

A full journal publication of this work will be published in the Journal of Computational Electronics.

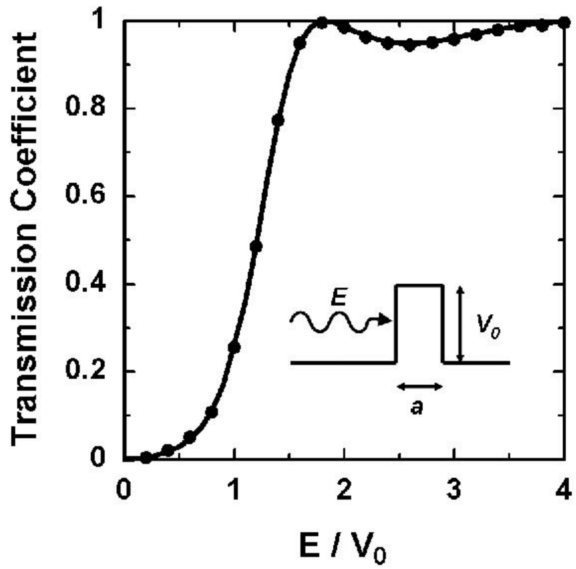

Figure 1: The transmission coefficients of quantum tunneling through a square potential barrier. E is the energy of the incident wave and V_0 the barrier height energy. The dots are the results of the QLGA simulation, while the solid line shows the exact analytical solution.

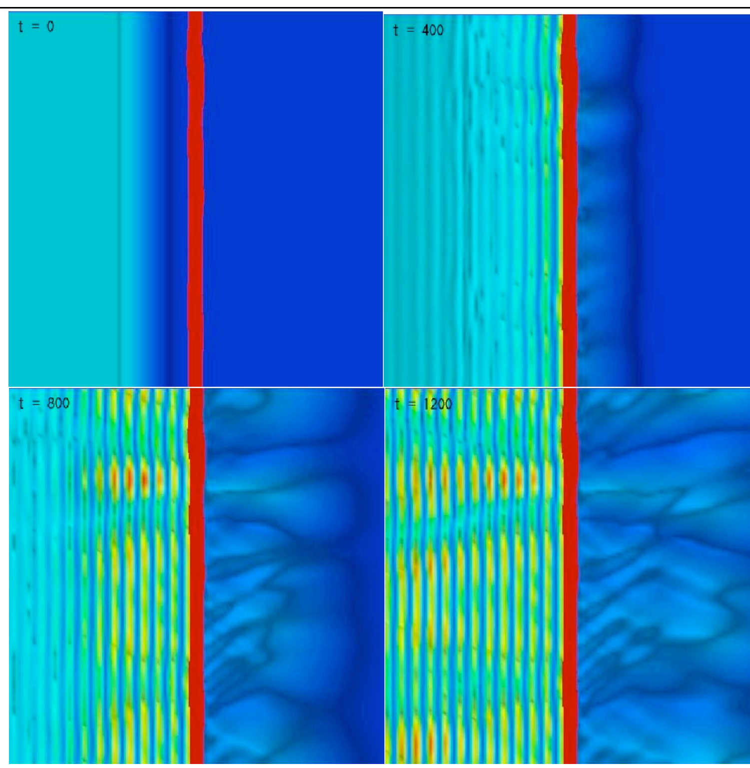

Figure 2: Quantum tunneling through the potential barrier with surface roughness. The norm of the wave function is plotted. The barrier region is colored by red.

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