Efficient Self-Consistent Quantum Transport Simulator for Quantum Well Devices

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Silicon quantum dot systems have attracted enormous efforts [1-2] in the past decade to explore their potential as qubits for quantum computing due to the promise of long spin coherence times and the well-established Si manufacturing processes. We have developed a Quantum Computer Aided Design (QCAD) device simulator [3] that solves for electrostatic potential, single- and multi-electron wave functions and energies, and that has been extensively used to accelerate the development of Si double quantum dot (DQD) qubit work at Sandia National Laboratories. To model additional features of interest to experimentalists, such as current flow across tunnel barriers, we needed a carrier quantum transport capability. In principle, we have to solve a self-consistent 3D quantum transport problem for DQDs, which would require excessive development time and computing resources due to the inherent complexity of 3D transport and the relatively large size of DQDs (on the order of micrometers in each direction). Alternatively, we can first perform QCAD electrostatic simulations of DQDs, identify the tunnel barrier path of interest along which current flows, and then perform 1D self-consistent quantum transport simulations to obtain the current-voltage relation. This procedure allows for very fast simulation time and provides good general guidance on device designs.

To set the context, Figure 1(a) shows an experimental Si DQD with the gate insulators and top metal gate not shown. Under certain gate bias and interface charge conditions, the device is flooded with electrons in the left and right regions but a barrier is formed between the two dots as shown in Fig. 1(b). The potential energy profile across the barrier obtained from QCAD is given in Fig. 1(c). We want to know how the barrier will change and what is the tunnel current when applying a source-drain voltage to the barrier. The applied voltage in experiment can be relatively large with respect to k_BT, e.g., 50 mV at 4 K (about 143 k_BT), to overcome effects of any possible unknown defects around the barrier region. Because of the high voltage, we are required to have a self-consistent solution of quantum transport across arbitrary 1D barriers.

Our self-consistent transport is based on the Contact Block Reduction (CBR) method [4]. It turns out that when we apply the general 3D CBR approach to 1D applications, we obtain a set of very simple equations that allow for easy implementation and very fast simulation. In particular, within the CBR method, the transmission across arbitrary single or multiple barriers becomes trivial to compute and extremely fast compared to the standard techniques for a tri-diagonal Hamiltonian [5]. For example, when computing transmission as a function of energy across the barrier in Fig. 1(c) using Matlab, CBR takes only 1 s on one CPU of a 2.6 GHz laptop, whereas matrix inverse requires more than 1000 s.

The Poisson-CBR self-consistency is achieved by adapting the predictor-corrector scheme [6] to open systems [7]. The resulting nonlinear Poisson equation is solved by a straightforward Newton method as the Jacobian matrix is tri-diagonal in 1D. Electron density is computed using the LDOS obtained by CBR. The self-consistent loop often achieves convergence within just ten iterations. Figure 2 shows simulation results at T = 10 K of a test RTD device that contains several coupled resonant states. The current-voltage curve shows interesting characteristics: the increase in part (A) is mainly because source states (left side) are in

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resonance with the states in the well, as seen by the relatively sharp transmission and current spectrum at 45 and 50 mV, while the increase in part (B) is due to single-barrier tunneling and quantum interference from the right barrier which is below the source Fermi level at 0, with the interference effect seen by the broad peaks in transmission spectrum at 55 and 60 mV.

We will present the self-consistent Poisson-CBR simulation results of tunnel barriers in DQDs and compare with transport measurements at various gate conditions. We also intend to expand the code for ballistic transport through an arbitrary number of 1D barriers and release it under an Open Source license, which will allow people to quickly obtain *self-consistent* quantum transport solution in quantum-well types of devices for design guidance.

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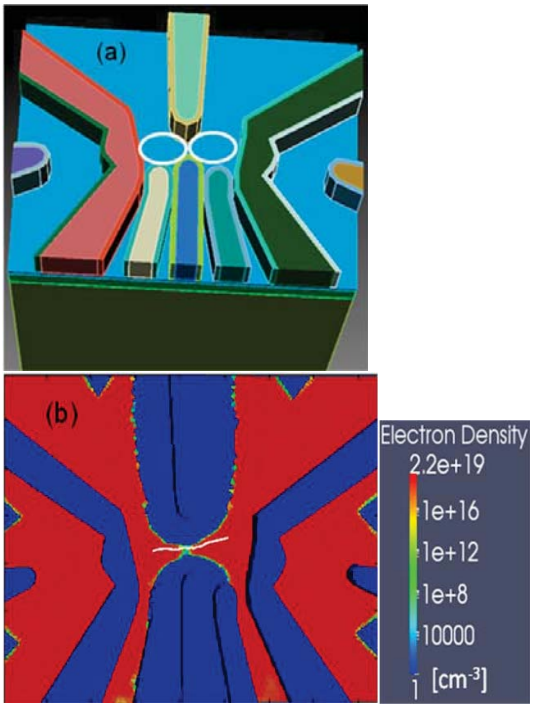

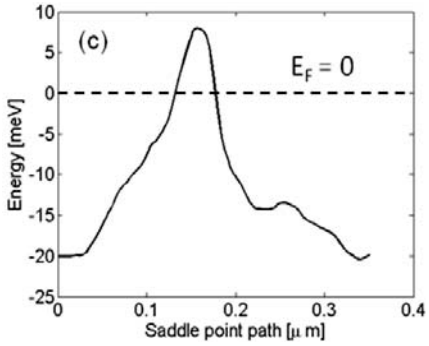

Fig.1. (a) Experimental Si DQD with depletion gates and Si substrate shown and the two white circles denote the dots. (b) Top view of electron density at the Si/SiO2 interface under certain conditions, with the left and right regions flooded with electrons but a barrier formed between the dots. Depletion gates are overlaid on the figure. The white curve across the barrier denotes the saddle-point path found by a searching algorithm in QCAD. (c) The potential energy barrier obtained in QCAD along the white curve with the left of the path as starting point.

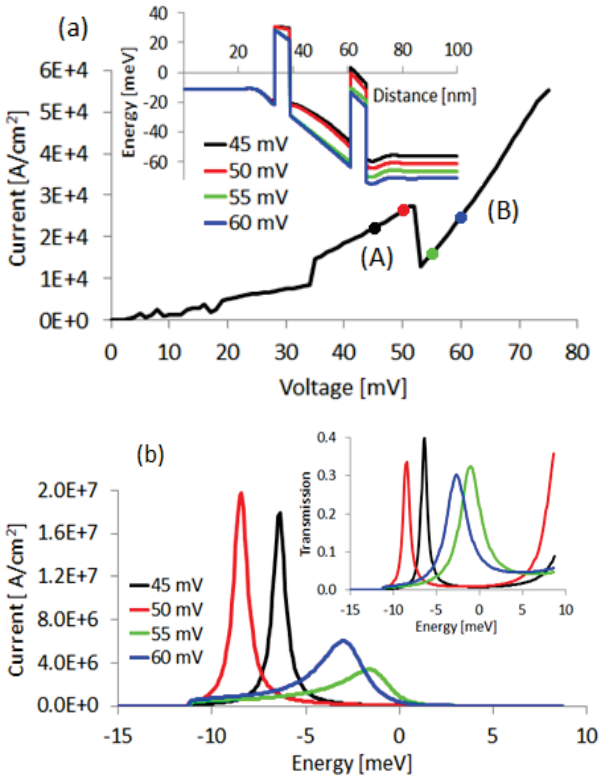

Fig.2. (a) Current-voltage relation of a test RTD at T = 10 K. The four circles denote the voltages at which the self-consistent band profiles are plotted in the inset. The small ripples in currents at low voltages are believed to be due to numerical noise. (b) Current spectrum at four voltage points, with the inset showing the corresponding transmission function.