Electron Transport in Nano-Structures: Computer Simulation

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Abstract: The Coulomb Blockade (CB) observed in nano-structures such as metallic or semiconductor quantum dots (QD) attracts a great interest from both the fundamental physics and the potentially practical applications. In this report some important behaviors of the CB have been systematically investigated for QDs and tunnel junction arrays in the presence of disorders, when the traditional analytical methods are impotent. To calculate the ground state energy and thence to study the level spacing statistics of a square disordered QD, the many particle tight-binding Hamiltonian has been solved by the exact diagonalization and by the Hartree-Fock self-consistent simulation. While the results obtained by two methods are in good agreement for the systems of 4 to 6 electrons, the Hartree-Fock simulation allows us to deal with much larger systems, up to 50 electrons. The level spacing distribution obtained in simulation evolves from the Wigner form in the noninteracting limit to a shifted Gaussian one for strong interaction cases. The effects associating with the shape and size of samples, with boundary conditions as well as external magnetic field have been analyzed in detail. The simulation results, on one side, describe well experimental data for various systems such as disordered GaAs QDs, and on the other side, suggest some new features to the problem.

For one-dimensional tunnel junction arrays the curren-voltage characteristics have been Monte-Carlo simulated using the semiclassical and full capacitance matrix description.. The threshold voltage V_{th} of the CB is evaluated as a function of the gate capacitance C_0, the array length N, the temperature, and the degree of disorder. The disordered effect is found to be essential, while the long range interaction included in the full capacitance matrix calculations, when decreasing V_{th}, weakly affects the qualitative behavior of the CB for the $V_{th}(C_0)$ and the $V_{th}(N)$ dependences.

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