Path Integral Monte Carlo Simulations of Nanowires and Quantum Point Contacts

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We are studying the conductivity of semiconductor nanostructures with a fixed-node path integral Monte Carlo technique. The fixed-node technique uses a variational principle to map fermionic problems into effective bosonic problems, which are then evaluated with standard quantum Monte Carlo techniques. While fixed-node is an approximation, it has the useful properties of being variational and being able to recover the exact answer when the exact nodes or phases of the density matrix are known. In these finite-temperature simulations we use the free-particle density matrix as a fixed-node constraint to efficiently simulate dozens of interacting electrons. We have calculated charge densities, pair correlation functions, and the current-current Matsubura Green's functions for quantum wires and quantum point contacts. The Kubo formula yields the DC conductivity, from which we can solve the conductance. We can calculate the voltage drops across the devices, and see that the conductivity can have significant non-local contributions when device features are comparable to average electron-electron separations, such as in tunnel junctions. See `http://phy.asu.edu/shumway` for simulation codes, preprints, and more information. Work supported by NSF Grant. No. DMR 02-39819.