Quantum simulation of correlated electron transport

Haobin Wang
Department of Chemistry and Biochemistry,
New Mexico State University, Las Cruces, New Mexico 88003, USA

Abstract

The effect of vibrational and electronic correlation is investigated for electron transport processes based on an Anderson impurity model that describes a molecular junction connecting to two metal leads. Time-dependent electric current as well as its steady-state value are evaluated employing the multilayer multiconfiguration time-dependent Hartree theory in second quantized form, an efficient and numerically exact methodology to treat quantum dynamics for systems containing identical particles. It is shown that, depending on different physical regimes, inclusion of vibrations may either increase or decrease the steady-state electric current comparing with the corresponding elastic electron transport. For situations where the energy of the bridge state is located close to the Fermi energy, the simulations show the time-dependent formation of a polaron state that results in a pronounced suppression of the current corresponding to the phenomenon of phonon blockade. We show that this phenomenon cannot be explained solely by the polaron shift of the energy but requires methods that incorporate the dynamical effect of the vibrations on the transport. Other phenomena such as Coulomb blockade will also be discussed based on the simulation results.