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Nonequilibrium elastic quantum transport using plane waves[1]
ARAN GARCIA-LEKUE, Donostia International Physics Center (DIPC), Donostia, Spain, LIN-WANG WANG, Lawrence Berkeley National Laboratory (LBNL), Berkeley, USA — In this work, we present an *ab initio* nonequilibrium electronic structure method for modeling the elastic electron transport through a nanostructure coupled to semi-infinite external electrodes and with an applied bias voltage. Our method is based on the scheme presented in Ref. [1], where the coherent quantum transport is calculated by means of the *exact* scattering states of the system obtained using plane waves and for zero applied bias voltage. In the case of a finite bias voltage, the electronic system is in a nonequilibrium situation, and the problem needs to be solved self-consistently. Here, we present an approach to obtain the self-consistent charge density and potential of the system, which are then employed in the calculation of the nonequilibrium transmission coefficient and conductance. As an illustration, results for a model system made up of a di-thiol-benzene (DBT) molecule connected by two Cu wires are provided. [1] A. Garcia-Lekue and L.W. Wang, Phys. Rev. B. **74**, 245404 (2006).

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