QmeQ 1.0: An open-source Python package for calculations of transport through quantum dot devices - DTU Orbit (11/02/2019)

QmeQ is an open-source Python package for numerical modeling of transport through quantum dot devices with strong electron–electron interactions using various approximate master equation approaches. The package provides a framework for calculating stationary particle or energy currents driven by differences in chemical potentials or temperatures between the leads which are tunnel coupled to the quantum dots. The electronic structures of the quantum dots are described by their single-particle states and the Coulomb matrix elements between the states. When transport is treated perturbatively to lowest order in the tunneling couplings, the possible approaches are Pauli (classical), first-order Redfield, and first-order von Neumann master equations, and a particular form of the Lindblad equation. When all processes involving two-particle excitations in the leads are of interest, the second-order von Neumann approach can be applied. All these approaches are implemented in QmeQ. We here give an overview of the basic structure of the package, give examples of transport calculations, and outline the range of applicability of the different approximate approaches.

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