Green's function methods for single molecule junctions

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We discuss theoretical Green's function methods applicable to open quantum systems out of equilibrium, in general, and single molecule junctions, in particular [1].

Two characteristic energy scales governing the physics are many-body interactions within the junctions and molecule–contacts couplings. We, therefore, identify weak interactions and weak coupling as two limits that can be conveniently treated within, respectively, the standard nonequilibrium Green's function (NEGF) method and its many-body flavors: pseudoparticle and Hubbard NEGF [2,3]. In particular, we show that the Hubbard NEGF is convenient in studies of nanoscale optoelectronics [4,5], current induced molecular dynamics [6], and nonequilibrium quantum thermodynamics [7] in junctions.

Finally, the intermediate regime, where the two energy scales are comparable, can in many cases be efficiently treated within the nonequilibrium dual approaches. We discuss recently developed auxiliary quantum master equation - dual fermion (aux-DF) [8,9] and dual-boson (aux-DB) approaches [10]. We combine ideas of exact mapping of non-Markov dynamics onto Lindblad type evolution in an auxiliary system with dual superperturbation expansions. This combination capitalizes on strong sides of both techniques which leads to formulation of relatively numerically inexpensive universal impurity solvers of high accuracy. Viability of the aux-DF and aux-DB approaches is illustrated within generic junction models, where the schemes are benchmarked against numerically exact results.

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