

Hubbard nonequilibrium Green functions

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We introduce diagrammatic technique for Hubbard nonequilibrium Green functions. The formulation is an extension of equilibrium considerations for strongly correlated lattice models to description of current carrying molecular junctions. Within the technique intra-system interactions are taken into account exactly, while molecular coupling to contacts is used as a small parameter in perturbative expansion.

Progress in experimental techniques at nanoscale made measurements of noise in molecular junctions possible. These data are important source of information not accessible through average flux measurements. Emergence of optoelectronics, recently shown possibility of strong light-matter couplings, and developments in the field of quantum thermodynamics are making counting statistics measurements of even higher importance. Theoretical methods for noise evaluation in first principles simulations can be roughly divided into approaches applicable in the case of weak intra-system interactions, and those treating strong interactions for systems weakly coupled to baths. We argue that due to structure of its diagrammatic expansion and the fact of utilizing many-body states as a basis of its formulation recently introduced nonequilibrium Hubbard Green functions formulation is a relatively inexpensive method suitable for evaluation of noise characteristics in first principles simulations over wide range of parameters.

We demonstrate the viability of the approach with numerical simulations of current, noise, and noise spectrum for a generic junction model of quantum dot coupled to two electron reservoirs in non-, weakly and strongly interacting regimes. Results of the simulations are compared to exact data (where available) and to simulations performed within approaches best suited for each of the three parameter regimes.

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