A Green's function perspective on the nonequilibrium thermodynamics of open quantum systems strongly coupled to baths

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Rapid development of experimental techniques at the nanoscale in the last decade has led to miniaturization of devices for energy storage and conversion to sizes where quantum mechanics becomes relevant. For example, thermoelectric single atom and single molecule junctions are expected to operate more effectively compared to their bulk analogs due to possible utilization of quantum effects. Proper description of performance of nanoscale devices for energy conversion requires development of corresponding nonequilibrium quantum thermodynamics. Moreover, with molecules chemisorbed on at least one of the contacts, thermodynamic theory should account for strong system-bath couplings. In recent years there is a surge of research in this field both experimentally and theoretically. Another active area of research establishes a connection between thermodynamic and information theory.

One of the guiding principles for theoretical research is consistency of the thermodynamic description with underlying system dynamics. The latter is conveniently described within nonequilibrium Green's function (NEGF) techniques. Here, we give dynamical NEGF based perspective on thermodynamics formulations suggested in the literature for open quantum systems that are strongly coupled to baths [1]. For the thermodynamic formulation consistent with underline dynamics, we derive bath and energy resolved expressions for entropy, entropy production, and information flows [2]. Resulting expressions reduce to expected forms in limiting cases of weak coupling or steady state. Formulation of the flows in terms of only system degrees freedom is convenient for simulation of thermodynamic characteristics of open nonequilibrium quantum systems. We utilize standard NEGF for derivations in noninteracting systems, Hubbard NEGF is used for interacting systems.

[1] N. Bergmann and M. Galperin, Eur. Phys. J. Spec. Top. (2021) https://doi.org/10.1140/epjs/s11734-021-00067-3

[2] N. Seshadri and M. Galperin, Phys. Rev. B103 (2021) 085415.