Nonequilibrium Transport and Thermoelectricity in Open Quantum Systems

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Understanding energy and charge transport in nanoscale systems requires theoretical tools capable of describing quantum coherence, interactions, and nonequilibrium environments on equal footing. A common simplification in open quantum systems is the wide-band limit, where reservoirs are assumed to have energy-independent spectral properties. While this approximation enables compact descriptions of transport, it obscures spectral information and limits the predictive power of thermodynamic modeling.

We present a framework for nonequilibrium quantum transport that overcomes this limitation while remaining computationally efficient. Within nonequilibrium Green's function theory, we develop a formulation of open-system dynamics that scales linearly in simulation time and treats structured environments with finite bandwidth [1]. The approach enables accurate time-resolved simulations of interacting quantum junctions beyond the wide-band approximation while retaining direct access to physical observables such as charge, energy, and heat currents.

The formalism further reveals new ways to probe spectral properties through transport measurements. In multi-terminal setups, the interplay between different leads allows nonequilibrium current responses to encode information about the underlying many-body spectrum, providing a route to reconstruct spectral features directly from transport observables [2].

Finally, we demonstrate how these developments enable the study and optimization of thermoelectric energy conversion in molecular junctions driven far from equilibrium. Combining accurate open-system dynamics with energy-resolved transport analysis identifies regimes where nonequilibrium effects, spectral structure, and interactions cooperate to enhance thermoelectric performance [3].

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