Thermoelectric energy conversion in molecular junctions out of equilibrium

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Understanding time-resolved quantum transport is essential for advancing modern quantum technologies [1], particularly in nano- and molecular junctions under time-dependent perturbations [2]. Traditional steady-state approaches are not designed to capture the transient dynamics required to control electronic behavior on ultrafast timescales. Here, I present a non-equilibrium Green's function formalism based on the recently developed iterated generalized Kadanoff-Baym ansatz (iGKBA) [3] to study thermoelectric quantum transport beyond the wide-band limit approximation (WBLA). Charge and energy currents are computed using the Meir-Wingreen formula, and the transition from Lorentzian line-width functions to the WBLA is analyzed, revealing unphysical divergences in the latter. The results underscore the significance of finite-bandwidth effects and demonstrate the efficiency of the iGKBA in modeling time-resolved thermoelectric transport, with benchmark comparisons against the full Kadanoff-Baym theory [4]. The framework is further applied to compute time-resolved thermopower and thermoelectric energy conversion efficiency in molecular junctions.

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