

An open Wilson chain approach to nonequilibrium quantum impurity problems

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Quantum dots, nanotubes, adatoms, molecular junctions, and other nanoscale structures serve as versatile platforms for realizing quantum impurity physics and exploring strong electron correlations under nonequilibrium conditions. Beyond fundamental interest, these systems play a central role in understanding thermoelectric phenomena such as thermopower and energy conversion at the nanoscale, offering prospects for efficient energy harvesting in future quantum devices. Moreover, the behavior of Kondo correlations in such systems out of equilibrium is crucial for understanding low-temperature transport and coherence in these systems. However, theoretically describing such systems under nonequilibrium conditions remains notoriously challenging. Conventional approaches, though highly successful in equilibrium, rely on finite-size discretizations of continuous reservoirs that fail to represent nonequilibrium particle and energy excitations accurately. A consistent description of nonequilibrium phenomena may therefore benefit from formulations that treat the impurity as coupled to infinite reservoirs.

In this work we introduce an open chain approach that extends the numerical renormalization group (NRG) framework to describe quantum impurity systems in steady-state nonequilibrium. In particular, we transform the two-lead problem into an effective Wilson chain which is extended by coupling high-energy reservoirs to each Wilson site. The steady state of such an open chain is obtained using the Bloch-Redfield formalism [1]. We studied the nonequilibrium spectral function and transport properties of a single impurity Anderson model coupled to two metallic leads under finite potential bias and temperature gradients. Despite its simplicity, our approach achieves good agreement with established theoretical results while requiring significantly fewer computational resources than state-of-the-art methods.

References:

- [1] J. Böker and F. B. Anders, Restoring the continuum limit in the time-dependent numerical renormalization group approach, *Phys. Rev. B* 102, 075149 (2020).
- [2] A. Manaparambil and F. B. Anders, Open Wilson chain numerical renormalization group approach to quantum transport, (Manuscript under preparation).