Quantum Thermodynamics of Nanoscale Molecular Systems.

Michael Galperin

University of California San Diego, Dept. Chem. & Biochem., UH 3218, MC 0340, 9500 Gilman Drive, La Jolla, USA

We discuss an energy-resolved variant of quantum thermodynamics for open systems strongly coupled to their baths. The approach generalizes the Landauer-Buttiker inside-outside duality method [Phys. Rev. Lett. 120, 107701 (2018)] to interacting systems subjected to arbitrary external driving. It is consistent with the underlying dynamical quantum transport description and is capable of overcoming limitations of the only other consistent approach [New J. Phys. 12, 013013 (2010)]. We illustrate viability of the generalized inside-outside method with numerical simulations for generic junction models.

This material is based upon the work supported by the National Science Foundation under Grant No. CHE-2154323

[1] J. Zhou, A. Li, and M. Galperin, arXiv:2308.06893 (2023).

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

[3] N. Bergmann and M. Galperin, Eur. Phys. J. Spec. Top. 230 (2021) 859.