Towards efficient simulations of quantum transport with open–system tensor networks

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Understanding non–equilibrium quantum thermodynamics is one of the utmost tasks in designing modern nanoelectronics and quantum thermal machines. In pursuit of this, a number of recent advances pave the way toward rigorous, controlled numerical simulations of quantum transport through a low–dimensional working medium in contact with fermionic reservoirs at fixed temperatures and chemical potentials.
One notable and high–fidelity numerical approach combines tensor networks and an open system methodology, where relaxation maintains a chemical potential or a temperature drop between the finite representation of the contacts [1, 2]. External relaxation of the implicit leads results in several characteristic features. Green's function formalism [3-5] provides a clear interpretation of those features for non–interacting models. Their adequate understanding is necessary to identify the regime where the true, natural (Landauer or Meir–Wingreen) steady–state conductance is recovered in the simulation.

In the presentation, I will discuss the interpretation of the quantum transport properties in connection to the relaxation parameter within the extended reservoir approach [5]. I will comment on our findings on the efficiency of used to discretize the reservoirs [6]. Finally, I will present relevant ingredients necessary for efficient open–tensor–network simulations of quantum transport [1]. We employ the latter to demonstrate that the characteristic features observed for non–interacting models are persistent also in the case of many–body interactions in the working medium [5], building towards a universal methodology for many–body quantum transport simulations.

References:

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