Simulation of quantum transport using the hierarchical equations of motion method

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The hierarchical equations of motion (HEOM) formalism is an accurate and efficient approach to simulate the dynamics of open quantum systems [1]. Formulated as a density matrix scheme, it generalizes perturbative quantum master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of the results. In this talk, recent extensions of the HEOM method are discussed, including open quantum systems with multiple bosonic and fermionic environments [2] and a matrix product state formulation in twin space [3]. While the former is important for applications in the areas of quantum thermodynamics and quantum transport, the latter allows the simulation of significantly larger systems. Applications of the method to quantum transport in molecular junctions are presented [4], focusing on models with electronic-vibrational coupling, nonadiabatic effects, current fluctuations as well as current-induced bond rupture.

[1] Y. Tanimura, J. Chem. Phys. 153 (2020) 020901.

[2] J. Bätge, Y. Ke, C. Kaspar, M. Thoss, Phys. Rev. B 103 (2021) 235413.

[3] Y. Ke, R. Borrelli, M. Thoss, J. Chem. Phys. 156 (2022) 194102.

[4] C. Schinabeck, A. Erpenbeck, R. Härtle, M. Thoss, Phys. Rev. B 94 (2016) 201407(R); C. Schinabeck, M. Thoss, Phys. Rev. B 101 (2020) 075422; Y. Ke, A. Erpenbeck, U. Peskin, M. Thoss, J. Chem. Phys. 154 (2021) 234702; C. Kaspar, M. Thoss, Phys. Rev. B 105 (2022) 195435; Y. Ke, C. Kaspar, A. Erpenbeck, U. Peskin, M. Thoss, arXiv: 2205.04755 (2022).