Quantum dynamics and thermodynamics using the hierarchical equations of motion method

Michael Thoss

University of Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany

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 developments of the HEOM method are discussed, including the combination with tensor network approaches [2] and extensions that allow the efficient treatment of structured spectral densities [3]. Applications of the HEOM method are discussed to nonadiabatic quantum dynamics of molecules at metal surfaces [4]. Furthermore, the principle of minimal dissipation is employed to investigate thermodynamic properties such as work, heat, and entropy production in open quantum systems [5]. As a specific example, a quantum Otto cycle in the Anderson impurity model is studied.

[1] Y. Tanimura, J. Chem. Phys. 153, 020901 (2020); J. Bätge, Y. Ke, C. Kaspar, M. Thoss, Phys. Rev. B 103, 235413 (2021).

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

[3] H. Tikahashi, S. Rudge, C. Kaspar, M. Thoss, R. Borrelli, J. Chem. Phys. 160, 204105 (2024).

[4] R. J. Preston, Y. Ke, S. L. Rudge, N. Hertl, R. Borrelli, R. J. Maurer, M. Thoss, J. Chem. Theory Comput. 21, 1054 (2025).

[5] S. Gatto, A. Colla, H.-P. Breuer, M. Thoss, Phys. Rev. A 110, 032210 (2024); arXiv:2601.21546 (2026).