The different guises of hierarchical equations of motion

Meng Xu, Jürgen Thomas Stockburger, Malte Krug, and Joachim Ankerhold

Universität Ulm, Institute for Complex Quantum Systems, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Hierarchical equations of motion (HEOM) are one of the most robust and versatile approaches to the dynamics of open quantum systems, using auxiliary density operators with time-local equations of motion and typically relying on a multi-exponential decomposition of the reservoir correlation function. While HEOM methods were originally introduced as a technical method to wrest time-local dynamics from non-local path integrals, we now understand that they have – even in the deep quantum limmit – intricate links to Fokker-Planck dynamics as well as other extended-state open system methods such as the quasimode approach. Viewing the extended-state space in a unified, abstract way provides a rich structure of transformations which can significantly improve the stability and efficiency of real-world HEOM simulations.

Previous, physically motivated versions of the multi-exponential decomposition led to a proliferation of terms in the low-temperature regime, resulting in exponential computational cost. We point out a strategy which overcomes this obstacle and provides highly accurate results even for zero temperature and long times [1]. As a test case, the asymptotic algebraic decay of a sub-ohmic spin-boson autocorrelation function is numerically recovered.

[1] Meng Xu and Yaming Yan and Qiang Shi and J. Ankerhold and J. T. Stockburger, *Taming quantum noise for efficient low temperature simulations of open quantum systems*, arXiv:2202.04059