Stochastic Formalism and Simulation of Quantum Dissipative Dynamics

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Our starting point is a stochastic decomposition scheme to study dissipative dynamics of an open system. In this scheme, any two-body interactions between constituents of the quantum system can be decoupled with a common white noise that acts on the two individual subsystems.

(I) Using the decomposition scheme, we obtain a stochastic–differential equation, which reduces to generalized hierarchical equations of motion (GHEOM) and thus represents a unified treatment of boson, fermion, and spin baths.[1] Applications of GHEOM to spin baths confirm the scaling relation that maps spin baths to boson baths and characterizes anharmonic effects often associated with low-frequency or strong coupling spin modes. [2]

(II) The decomposition scheme also leads to the stochastic path integral approach, which directly simulates quantum dissipation with complex noise. The approach is applied successfully to obtain the equilibrium density matrix, multichomophoric spectra, and Forster energy transfer rate. [3] For real time propagation, we demonstrate the advantages of combining stochastic path integrals, deterministic quantum master equations [4], and possibly the transfer tensor method [5].

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[4] A hybrid stochastic hierarchy equations of motion approach to treat the low temperature dynamics of non-Markovian open quantum systems. J. M. Moix and J. Cao, J. Chem. Phys. 139, 134106 (2013)
[5] Non-Markovian dynamical maps: Numerical processing of open quantum trajectories. J. Cerrillo and J. Cao, Phys. Rev. Lett. 112, 110401 (2014)