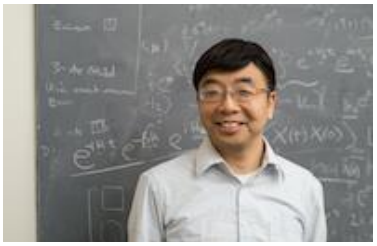
NITheP Colloquium

Monday, 14 September 2020, 16h00

Prof Jianshu Cao
Massachusetts Institute of Technology.



Stochastic Formalism and Simulation of Quantum Dissipative Dynamics

Abstract: 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.

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]

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].

[1] A unified stochastic formalism of quantum dissipation: I. Generalized Hierarchical equation, Hsien and Cao, JCP 148, p014103 (2018)
[2] A unified stochastic formalism of quantum dissipation: II. Beyond linear response of spin baths. Hsien and Cao, JCP 148, p014104 (2018)
[3] Equilibrium-reduced density matrix formulation: Influence of noise, disorder, and temperature on localization in excitonic systems. J. Moix, Y. Zhao, and J. Cao, Phys. Rev. B 85, 115412 (2012)
[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)

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Bio: Jianshu Cao is a professor of chemistry at MIT. He received a Ph. D. in physics from Columbia University in 1993. After postdoctoral research at the University of Pennsylvania and then at UCSD, he joined the MIT faculty in 1998. He is primarily known for his work on condensed-phase quantum dynamics and single-molecule kinetics. His current research program consists of two components: (i) the development of theoretical and computational methods to model quantum dynamics in light-harvesting systems, organic semiconductors, and quantum devices, and (ii) the analysis of non-equilibrium chemical networks and its implications in biophysical processes.Over the last five years (2015-2019), the Cao group has published a total of 50 papers, including publications in Nature Communications, Nano Letters, PRL, JPC Letters, CHEM, and Chemical Sciences. Jianshu Cao has taught 'non-equilibrium statistical mechanics' for years at MIT, and his lecture notes on the subject are published on MIT Open-Course-Ware (OCW). He is actively involved in the scientific community, presenting talks n public lectures, organizing conferences, serving on editorial and review panels, and participating in student/scholar exchange programs.

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