

Efficient simulation of finite-temperature open quantum systems

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Abstract

Chain-mapping techniques in combination with the time-dependent density matrix renormalization group are a powerful tool for the simulation of open-system quantum dynamics, but suffer from an unfavorable algorithmic scaling with increasing temperature. We prove that the thermal contribution to the dynamics can be shifted from the initial state of the environmental modes to a temperature-dependent spectral density characterizing the system-environment interaction. As a consequence, as long as the initial state of the open system is pure, the global system-environment state remains pure at all times. This enables the efficient simulation of open quantum systems interacting with highly structured environments in any temperature range.

Over the last two decades, a variety of numerically exact approaches for the simulation of open quantum systems have been proposed. These methods allowed for the description of features that were not accurately described by approximate methods, such as the Markov, Bloch-Redfield or perturbative expansion techniques [1]. In particular, the Time Evolving Density operator with Orthogonal Polynomials (TEDOPA) [2] algorithm is a numerically exact and certifiable method [3] for the nonperturbative simulation of OQS that has found application for the description of a variety of open quantum systems. TEDOPA belongs to the class of chain-mapping techniques [4] which are based on a unitary mapping of the environmental modes onto a chain of harmonic oscillators with nearest-neighbor interactions. The main advantage of this mapping is the more local entanglement structure which results in an improved efficiency of density matrix renormalization group (DMRG) techniques [5]. While TEDOPA is very efficient at zero temperature, a regime that is hard to access by other methods such as hierarchical equations of motion [6] and path integral methods [7], its original formulation suffers from a unfavorable scaling when increasing the temperature of the bosonic bath. Because of this, other approaches, such as the hierarchical equation of motion are currently the method of choice in the high temperature regime.

In this seminar we present a formulation of TEDOPA for finite-temperature bosonic environments [8] that allows for its extension to arbitrary temperatures without loss of efficiency. Our approach relies on the equivalence between the reduced dynamics of an OQS interacting with a finite-temperature bosonic environment characterised by some spectral density and the dynamics of the same system interacting with a zero temperature environment and a suitably modified spectral density, and further exploits fundamental properties of the theory of orthogonal polynomials [2].

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