SQUIRM: Scalable QUantum Integration of Redfield Master equations

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Abstract

The Redfield master equation can produce a microscopic description of a many-body open quantum system and its accompanying environment, this is particularly important in the simulation of real-world complex networks.
An example of this is the Fenna-Matthews Olson (FMO) protein complex, a nanoscale system that is integral to the transport of energy in photosynthetic systems and can be expected to have a strong coupling with the surrounding vibrational environment.
However, a significant obstacle to applying this framework is the computational cost of calculating the Liouvillian, with which system dynamics and the steady state can be derived.
Motivated by this, we demonstrate a new method to generate the dynamics of the Redfield quantum master equation in which calculations scale with the dimension of the Hamiltonian rather than the much larger Liouvillian.
This advantage is achieved by integrating the contributions from the spectral density, phase factor, and memory kernel to construct a family of terms from which the complete dynamics can be derived.
This approach can be applied in both the laboratory and polaron frames to describe complex system-environment interactions.
Furthermore, this method is enhanced by a new variational approach, an intermediate between the laboratory and polaron frame calculations, which uses site-local optimisation to produce a general description of a system coupled to its environment.
By bringing these elements together, we demonstrate a powerful framework to meaningfully simulate very large numbers of systems, opening the door for previously unexplored complex quantum networks to be investigated with relatively few approximations and more meaningful physics.

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