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Modeling Exciton Dynamics: A Finite-Dimensional Effective Environment via Pseudomodes

The transfer of energy among chromophores is a topic of particular interest in the field of physical chemistry and a key to understanding the efficiency of photosynthetic processes. The quantum dynamics underlying transfer processes often stems from an intricate balance between coherent quantum evolution and irreversible dissipative processes, calling for a meaningful partition of the problem into the system of interest and its environment. The molecular excited-state environment includes the multitude of intra-molecular vibrations, scaffold and solvent degrees of freedom, posing challenges for an effective theoretical description and explicit numerical simulation. Several studies highlighted that slow (non-Markovian) fluctuations [1] and strongly coupled vibrations significantly affect the efficiency of energy transfer [2]. Among the theoretical frameworks to handle non-Markovian dynamics, the pseudomode model [3] consists of replacing the continuum of environmental degrees of freedom with a few dissipative quantum Harmonic Oscillators (HOs), as illustrated in the Figure below. These HOs are chosen to approximate the influence of the original environment on the system dynamics.
In this work, we explore the setting of pseudomodes to simulate the non-Markovian exciton transfer in a dimer [4]. The emphasis is on the dynamics of the pseudomode itself; how it relates to the properties of the original environment and how the truncation of the ideally infinite Hilbert space of the pseudomodes affects the results. For example, we found out that in the pure dephasing dynamics between the ground and the excited state, the occupation states of pseudomodes follow a Poisson distribution. But, when studying a dimer,the pseudomode loses the Poisson behaviour. In this case, a special property arises for which truncating the HOs at two states gives better scaling than a single HO with higher dimension. This encourages the mapping of the pseudomodes onto qubits, and therefore the implementation of the method with quantum algorithms for universal quantum computation [5].

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References

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Theme

Theme 3. Theoretical and experimental methods for quantum effects in energy processes

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