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Title: Modeling and Simulations of Exciton dynamics in Light-harvesting complexes

Abstract:
Light absorption and exciton energy transport can be highly efficient in natural light-harvesting complexes. It is assumed that non-trivial interactions with the vibrational environment may give rise to these efficiencies. So far testing sophisticated models was difficult since computational methods were not powerful enough.
We present a variational matrix product states (VMPS) implementation which combines several state of the art techniques to accurately compute ground state properties and dynamics of many-body Hamiltonians. In particular we will use it to simulate a model Hamiltonian describing polaron dynamics in the light-harvesting complex LH2 of purple bacteria.
To accurately simulate the exciton-phonon interaction, we map the environmental spectral density onto a 1D-chain model using orthogonal polynomials. This method provides an exact mapping without discretization artifacts.
Time evolution is implemented in a Dirac-Frenkel style time-dependent variational principle (TDVP) instead of the commonly used Lie-Trotter decomposition of the time evolution operator. This allows optimal time evolution even for long-range 1D-Hamiltonians.
Computations in the weak and strong coupling regime of the ohmic and sub-ohmic spin-boson model agreeing with contemporary numerical results are presented to prove the capabilities of the implementation.