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Open quantum systems play an important role in quantum optics and condensed-matter physics and to study phenomena like transport properties, the interplay between Hamiltonian and decoherent dynamics, as well as the formation of topological order induced by dissipation. In this context we introduce a versatile numerically tool that allows for the simulation of one-dimensional open quantum systems while ensuring positivity of the operators in every step of the algorithm. At the heart of the construction are matrix product density operators (MPDO) capturing purifications of mixed states, for which we suggest a stable and efficient scheme of manipulation preserving the form of the tensors and keeping both bond and Kraus dimensions fixed.

Systems

We want to study open quantum systems for example one-dimensional spin chains with N spins. Evolution is given by a Lindblad operator

$$\mathcal{C}(\rho) = -i \sum_{j} [h_i, \rho] + \sum_{j} \left(L_j \rho L_j^{\dagger} - \frac{1}{2} \{ L_j^{\dagger} L_j, \rho \} \right)$$

with 2-local Hamiltonian terms h_i and on-site generators L_i .

Locally purified MPO

MPO description of a state¹

 $g = M_1 - M_2 - M_3 - M_4 - M_5$

Locally purified MPO description

 $H_1 = H_2 = H_3 = H_4 = H_5$

Numerical method

Trotterize $e^{\tau \mathcal{L}}$ into layers T_i of mutually commuting strictly local channels³

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 $\rho_{t+\tau} = e^{\tau \mathcal{L}}[\rho_t] = T_L \circ \cdots \circ T_1[\rho_t] + \mathcal{O}(\operatorname{poly}(\tau))$

Apply effective evolution to local tensors of locally purified initial state ρ_0 : Ensures positivity of ρ_t for all times. Use DMRG-type algorithm in order to compress ρ_t back to trackable bond- and Kraus-dimension after each Trotter step.

Compression scheme

Use SVDs to compress the bond- and Kraus-dimension independently:

Bond-dimension







Mixed-state ansatz-class with two independent refinement parameters:

- Bond-dimension D: Controls correlations
- Kraus-dimension K: Controls mixedness
- Physical dimension d

Action of local channel can be implemented on the level of local tensors.



Why worry about positivity?

We can not efficiently test it for a given state $|^2$

Theorem

Even for physical dimension d = 2 to decide whether a given MPO is positive semidefinite is NP-hard in the system size. For large enough bond-dimension this even leads to an undecidable problem.

Application I: Array of two Photon-Josephson-junctions

Model:

- Two cavities, each coupled to a qubit
- Cavities coupled via photons
- System described by Jaynes-Cummings-Hubbard model
- Decoherence models particle loss in each sub-system



Figure: Simulation with initially three photons in right, zero photons in left cavity and qubits in groundstate. $(D = 40, K = 20, \tau = 0.01, \text{ second order Trotter})$

Application II: Transport in driven XXY-chain

Model:

- Driven XXZ-chain
- Decoherence given by Lindblad generators $L_1 = \sigma_+$, $L_2 = \sigma_-$, which



Hence, we keep positivity during the simulation in order to ensure that the result is again a quantum state.

References

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- couple to first or last spin, respectively.
- Local magnetization in good agreement with exact steady-state⁴



Figure: Local magnetization of steadystate of driven XXZ-chain. ($D = 60, K = 60, \tau = 0.1, 1000$ time steps, second order Trotter)

Outlook

Analyse different models for example Lai-Sutherland-chain

Method does not require translation invariance. Suited to consider disorder

Explore many-body localization in spin-chains

Extend to nearest neighbour Lindblad generators

Test preprocessing schemes of Lindblad before evolution