Tensor Network Simulations of Open Quantum Systems

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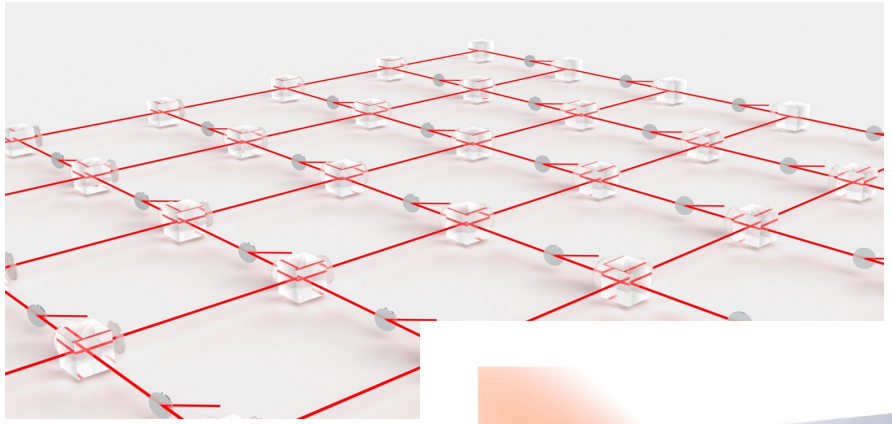
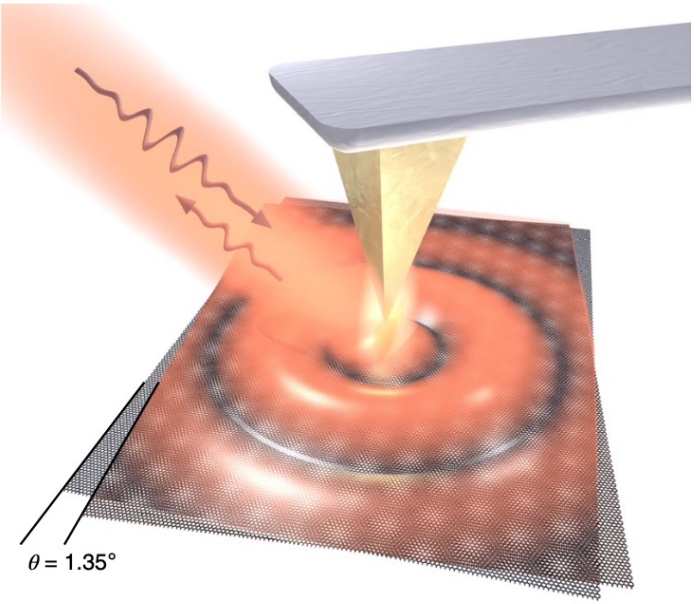
14 May 2024 • Pedagogical/Journal Club Presentation

What are open quantum systems

- Generic features
  - Dissipation and decoherence
  - Exceptional points
  - Non-equilibrium steady states
- Open Bosonic systems
  - Gain and loss in photonic crystals
  - Non-reciprocal transport in BECs
- Open Fermionic systems
  - Qubits decohering due to an environment
  - Quantum materials hybridized by a substrate



PRL **129**, 113601 (2022)



Nat. Phys. **17**, 1161 (2021)

Lindblad Master Equation

- Time-local time evolution by a memoryless bath $i\dot{\rho} = \mathcal{L}[\rho]$

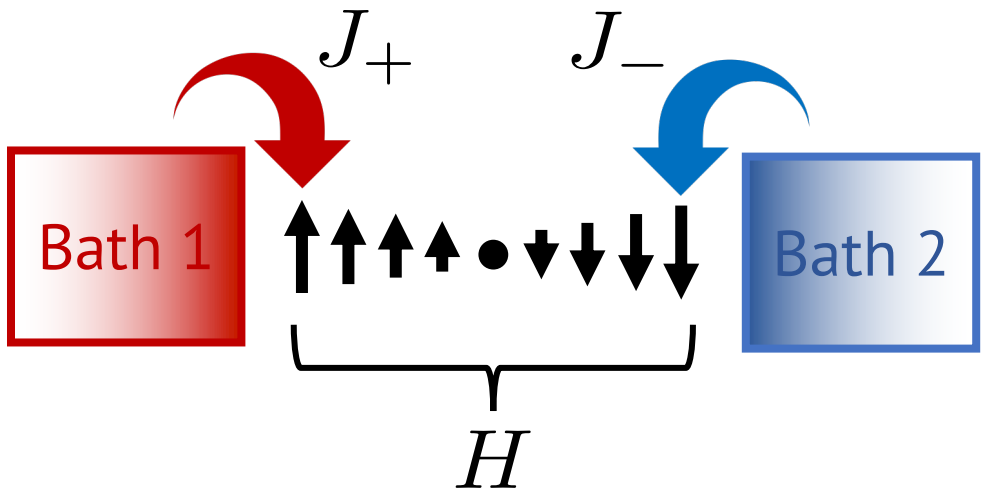
$$i\dot{\rho} = (\mathcal{L}^{\text{coh.}} + \mathcal{L}^{\text{n.h.}} + \mathcal{L}^{\text{jump}})[\rho]$$

where,

$$\mathcal{L}^{\text{coh.}}[\rho] = [H, \rho]$$

$$\mathcal{L}^{\text{n.h.}}[\rho] = -i\frac{\Gamma}{2}\sum_m \{J_m^\dagger J_m, \rho\}$$

$$\mathcal{L}^{\text{jump}}[\rho] = i\frac{\Gamma}{2}\sum_m 2J_m \rho J_m^\dagger$$



Spin chain with boundary dissipation. Jump operators linear in spins map to jump operators linear in fermions under Jordan-Wigner transformation.

Energy scales
- J: spin-spin coupling
- h: transverse field
- Γ: dissipation strength

What are tensor networks

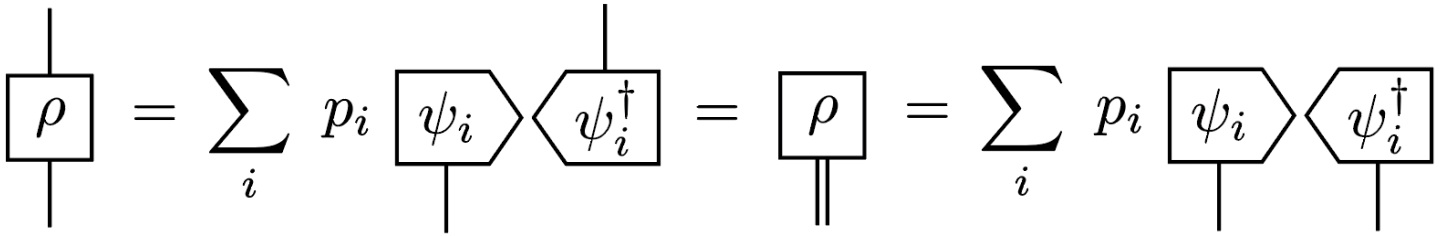
- See Physics 662
- Matrix product states

https://itensor.github.io/ITensors.jl/dev/examples/MPSandMPO.html

  - Fixed entanglement representations of quantum states
- Matrix product operators
  - A tensor with more legs than a state, but constructed similarly
- DMRG
  - Ground-state finding algorithm
- TEBD
  - Time-evolution algorithm

How to simulate open quantum systems

- Singular value decomposition still works for non-Hermitian systems
- One method is to use “vectorization” of the local Hilbert space



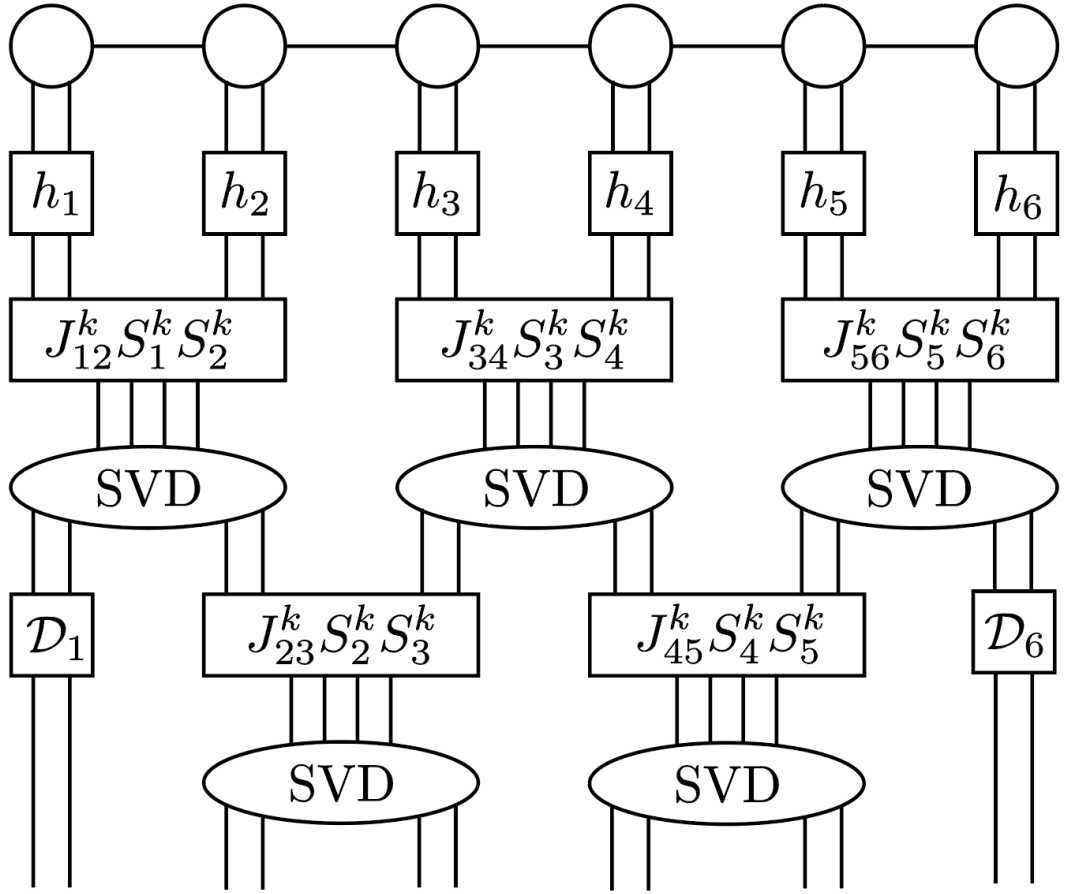
- Larger bond dimension, but still simulating the evolution of an MPS
- Evolution given by $|\rho(t)\rangle = e^{-i L_{vec} t}|\rho(0)\rangle$

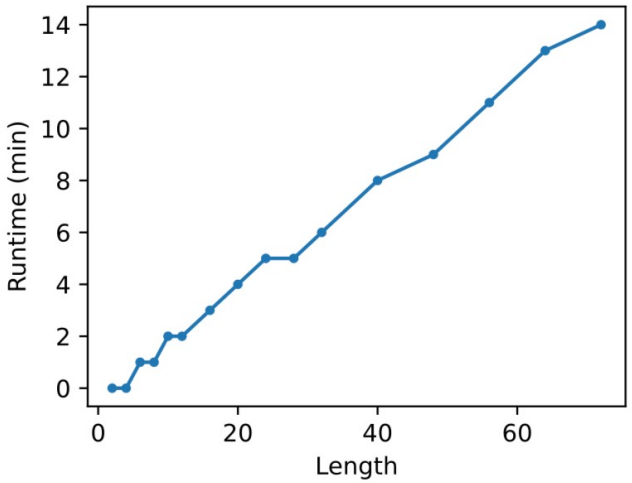
$$L_{\text{vec}} = 1 \otimes H - H^{\top} \otimes 1 - i \sum_m \frac{\gamma_m}{2} ((J_m^\dagger J_m)^{\top} \otimes 1 + 1 \otimes J_m^\dagger J_m - 2(J_m^\dagger)^{\top} \otimes J_m)$$

See PRL 93, 207204 (2004), and PRL 93, 207205 (2004)

Time-Evolving Block Decimation (TEBD)

- Trotterized time evolution followed by decomposition into tensors with fixed bond dimension χ
- Circles are an initial product state
- Rectangles are exp(-i O dt) for boxed O
- One cycle in evolution is visualized
- Here: χ~15, L~100
  - Lit: χ~100, L~100
- Inflated local dim versus closed sys.





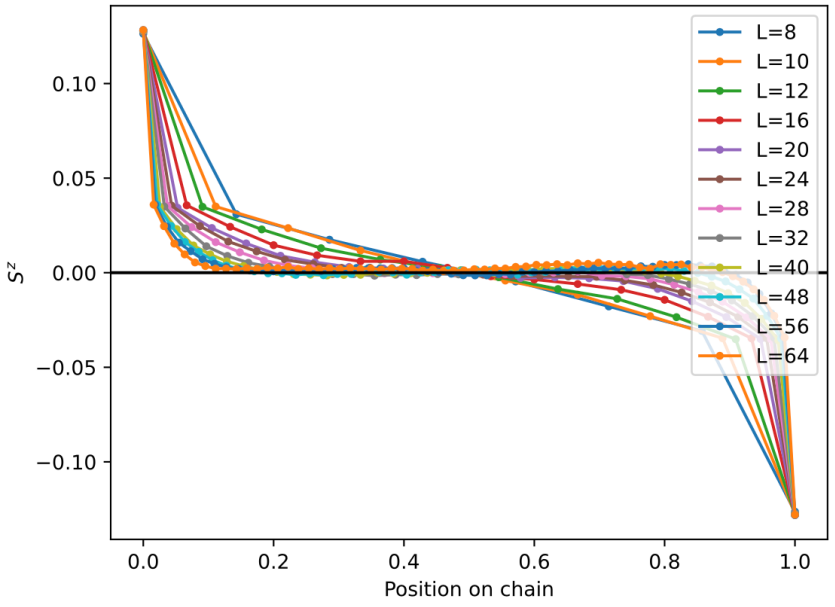
How to do this in Python

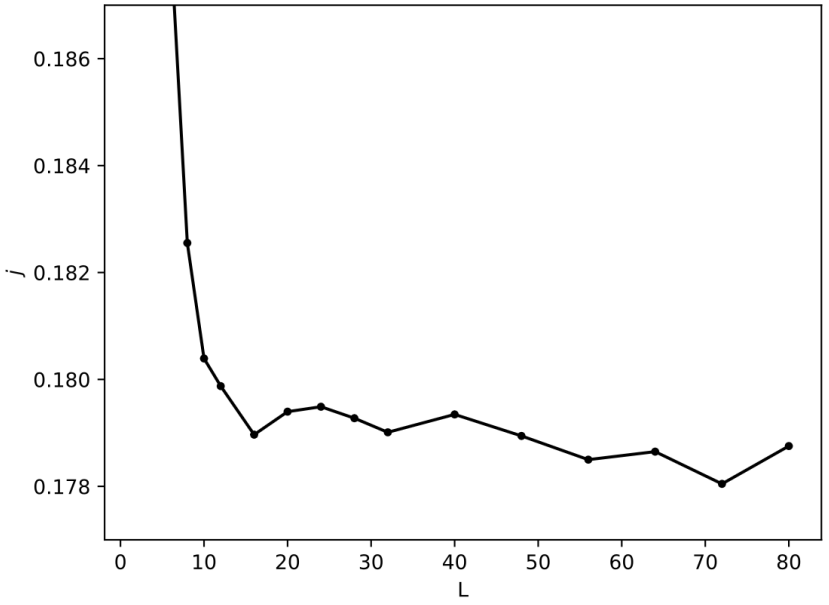
- We use TenPy which has pre-built classes for MPS, MPO, and routines such as TEBD, TDVP, and DMRG
- Steps
  - Define **`Site()`** – specify leg dimensions and operators
  - Define **`Model()`** – pretend that the vectorized Lindabladian is a non-Hermitian Hamiltonian
  - Specify parameters – both for the system and simulation
  - Run – this could take a while (or not)

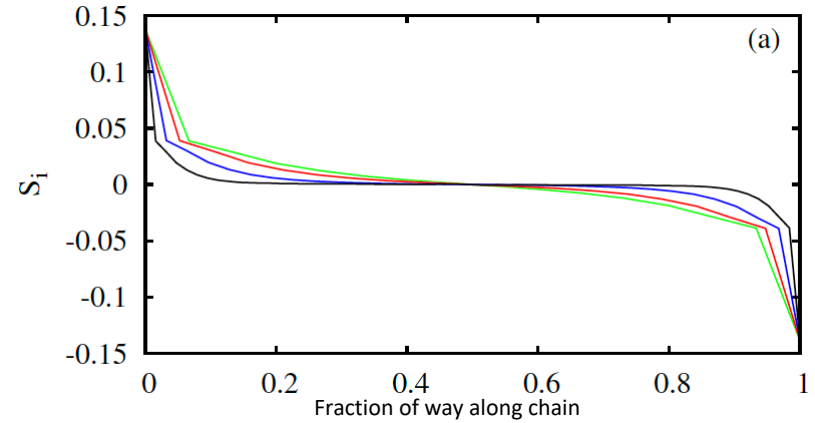
- SHOW CODE HERE!

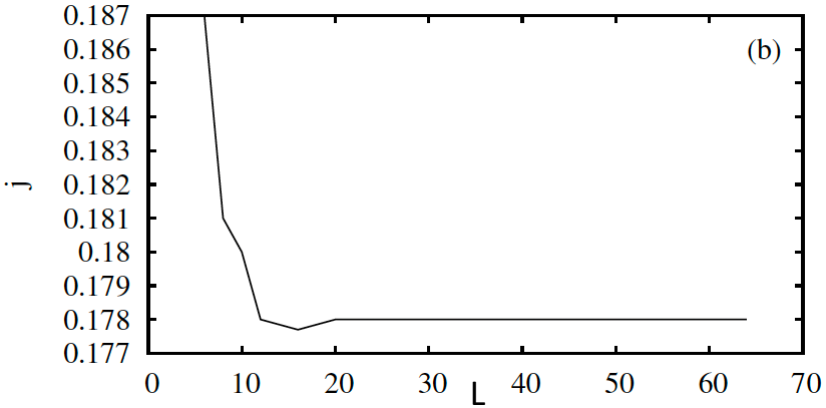
Reproducing Results: XXZ model transport

- We condiser the model $H = \sum_{i=1}^{L-1} J^x S_i^x S_{i+1}^x + J^y S_i^y S_{i+1}^y + J^z S_i^z S_{i+1}^z + \sum_{i=1}^{L} h^x S_i^x + h^y S_i^y + h^z S_i^z$
- With jumps given by $J_1^+ = \left(\frac{1-\tanh(\mu_L)}{1+\tanh(\mu_L)}\right)^{1/4} S_1^+, \quad J_1^- = \left(\frac{1+\tanh(\mu_L)}{1-\tanh(\mu_L)}\right)^{1/4} S_1^-, \quad J_L^+ = \left(\frac{1-\tanh(\mu_R)}{1+\tanh(\mu_R)}\right)^{1/4} S_L^+, \quad J_L^- = \left(\frac{1+\tanh(\mu_R)}{1-\tanh(\mu_R)}\right)^{1/4} S_L^-$
- Can calculate arbitrary correlation functions
- Here $\langle S^z_n \rangle$ and $j = \langle S^x_n S^y_{n+1} - S^y_n S^x_{n+1} \rangle$





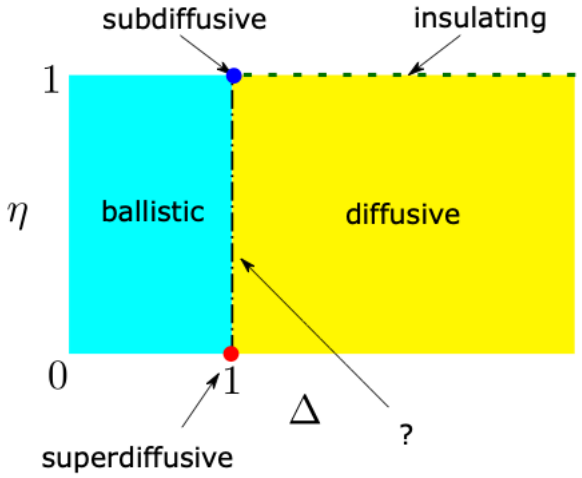




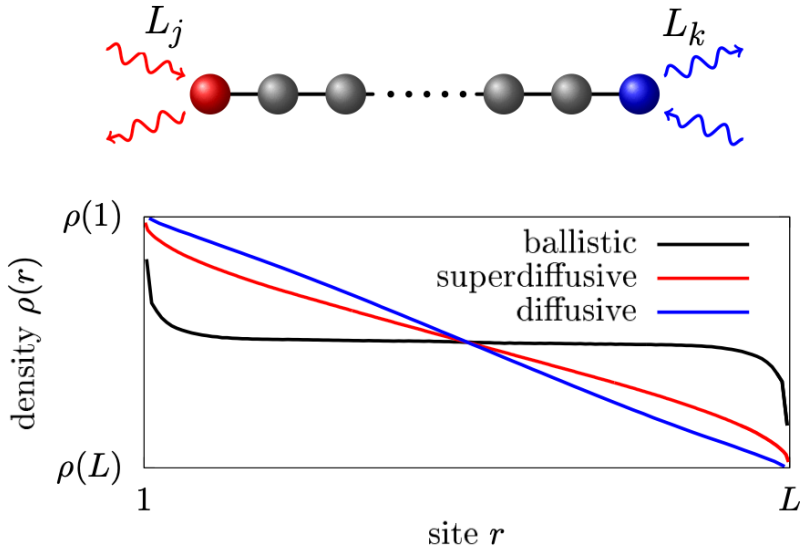
Prosen, J. Stat. Mech. (2009) P02035

XXZ model (continued)

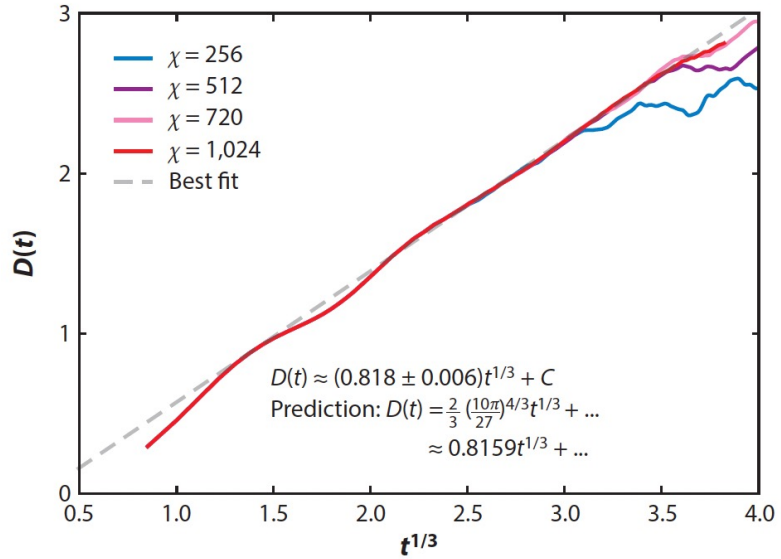
- Can see unusual scaling of the spin transport
- KPZ point of “superdiffusive” dynamics
- Understood as vanishing of Drude weight in an integrable system



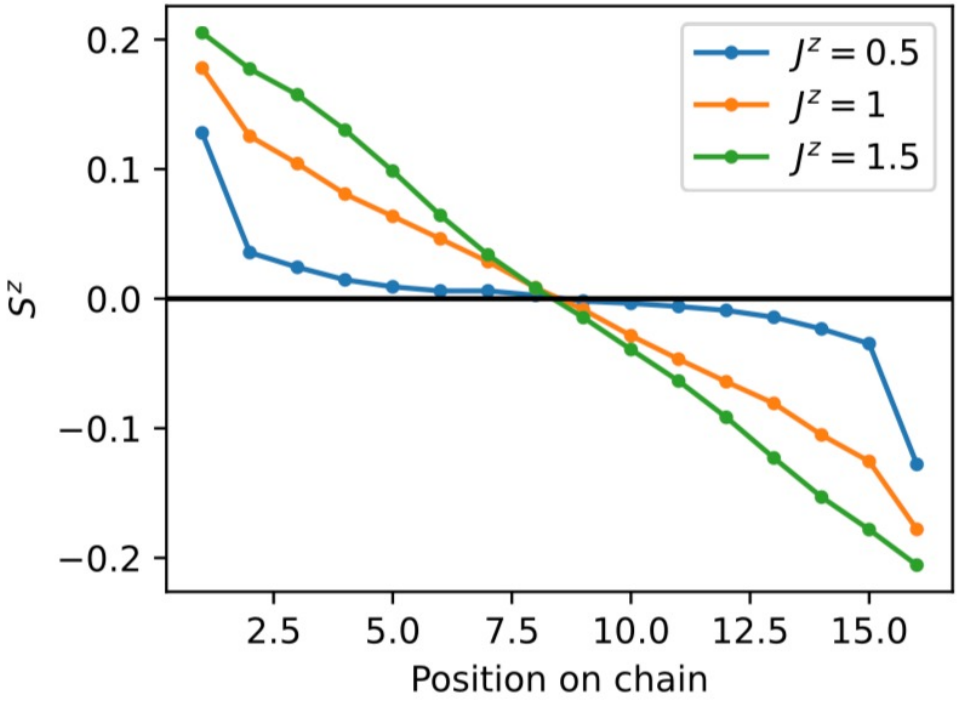
RMP 94, 045006 (2022)



Bertini, RMP 93, 25003 (2021)



Gopalakrishnan, Ann. Rev. Cond. Mat 15, 159 (2024)



Further options & optimizations

Conserved charges

- In closed systems we can simplify our analyses by working in fixed symmetry sectors—e.g. the fixed number sectors of the XXZ model
- Such simplifications should still be possible for open systems
- Additionally for some open systems (e.g. with 1-site local dissipation) there should be further symmetries to simplify, for example that

$$[1 \otimes H, H^{\top} \otimes 1] = 0$$

- See Quantum Sci. Technol. 4, 013001 (2019) for further discussion

Other Algorithms

- TEBD
- Krylov
  - Break H into a sum over Krylov subspaces and evolve each separately
- TDVP
  - Optimize over a tangent space to a class of MPSs
- Local RK (LRK)
  - Runge-Kutta evolution
- QT-N
  - Evolve over N trajectories

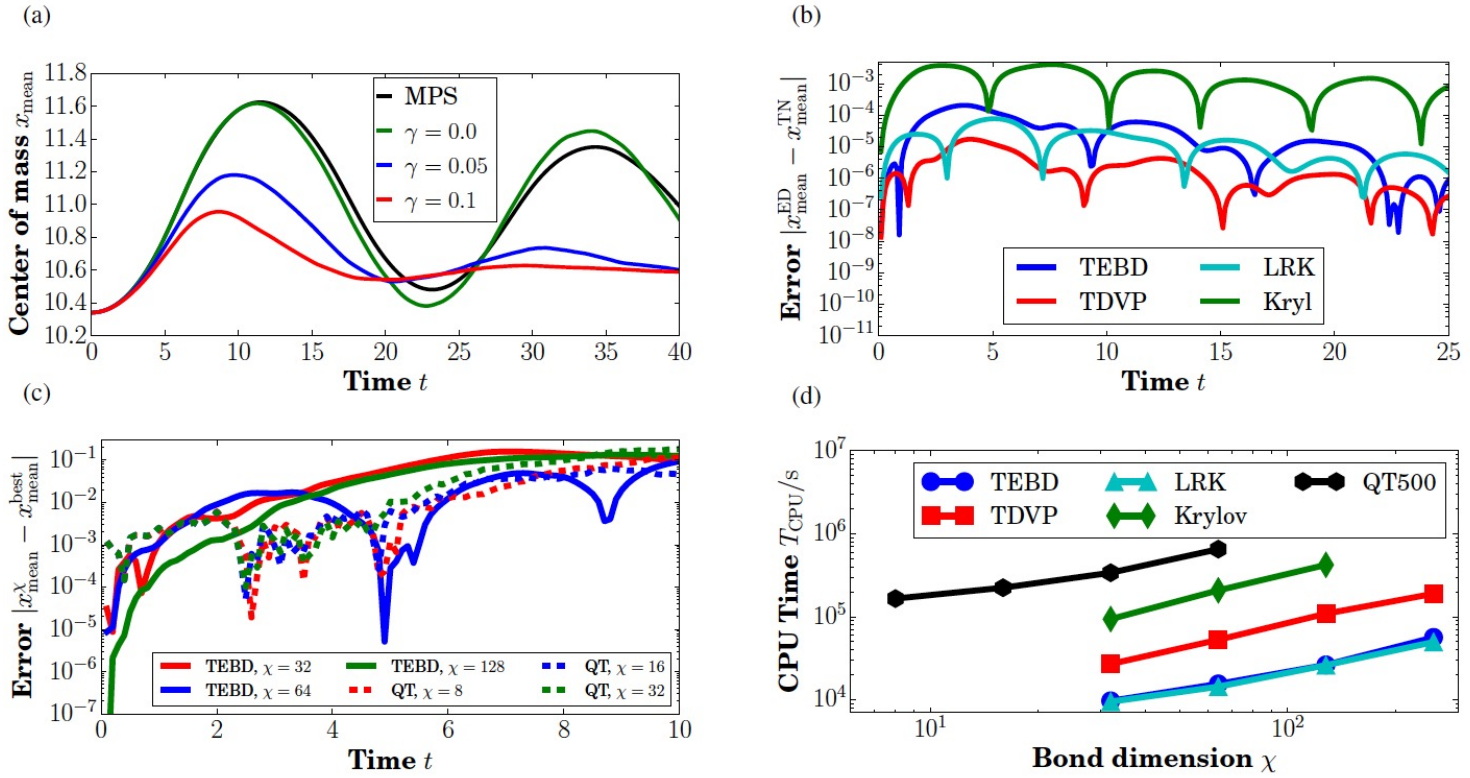


Figure 7. *Convergence of open quantum system Bose-Hubbard dynamics.* (a) The center of mass starts oscillating after we release the potential on the right well at time $t = 0$ and keep only a one-site potential in the middle to separate wells. We observe that the simulations for MPS and MPDO of a closed system mismatch after about ten time units. The coupling of the system to a dephasing damps the oscillations. (b) We compare the error of tensor network (TN) methods against exact diagonalization for a small system of $L = 5$. (c) We compare the errors of QTs with TEBD and $N_{\mathrm{QT}} = 500$ and simulations with MPDOs and TEBD to the TEBD simulations with the highest bond dimension, i.e., $\chi = 256$. Errors grow fast and show the numerical challenges associated with this problem setup. (d) We compare the computational resources for MPDO and QT algorithms. The coupling to the environment is $\gamma = 0.05$. TEBD and LRK use the least resources, then comes TDVP. The quantum trajectories with N_{QT} and TEBD are located above MPDOs with TEBD. Due to the limitation in bond dimension in this example and the possibility of parallelizing, they are an attractive option.

Quantum Sci. Technol. 4, 013001 (2019)