SIMULATING MANY-BODY OPEN QUANTUM SYSTEMS WITH MATRIX PRODUCT STATES

Introduction & outline

Open quantum systems (OQS) refers to systems interacting with an environment

Examples: → qubits with electronics
→ electrons with lattice vibrations
→ . . .

Restriction 1: we will consider only systems coupled weakly to memoryless i.e. Markovian environments, described by the Lindblad eq:

$$\dot{\hat{\rho}} = -i[\hat{H}, \hat{\rho}] + \sum_e \hat{L}_e \hat{\rho} \hat{L}_e^\dagger - \frac{1}{2}\{\hat{L}_e^\dagger \hat{L}_e, \hat{\rho}\} \quad ; \hat{L}_e : \text{jump operators}$$

(system) (environment)

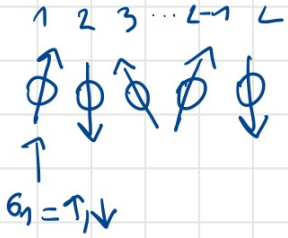
- Since analytic treatments are typically constrained to non-interacting systems and exact diagonalization to small systems, it is very useful to employ tensor network methods
- Restriction 2: we will consider only 1D tensor networks known as matrix product states (MPS)

PART 1
- MPS basics
- ground states & time evolution

→ PART 2
- dissipative time evolution
- steady states
- Lindbladian spectra

1) Introduction to MPS

- Consider a spin 1/2 chain



[1]

- The description of a general pure state $|\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots\sigma_L} c^{\sigma_1\sigma_2\ldots\sigma_L} |\sigma_1,\sigma_2,\ldots\sigma_L\rangle$

requires 2^L coefficients.

- If we consider only product states: $|\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots\sigma_L} c^{\sigma_1} \cdot c^{\sigma_2} \cdots c^{\sigma_L} |\sigma_1,\sigma_2,\ldots\sigma_L\rangle$

we need only $2 \cdot L$ coefficients. But: no entanglement!

- Generalization: $|\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots\sigma_L} M^{\sigma_1} M^{\sigma_2} \cdots M^{\sigma_L} |\sigma_1,\sigma_2,\ldots,\sigma_L\rangle$

Note: first matrix is row matrix & last matrix is column matrix, so that multiplication gives a number.

$\sim 2 \cdot L \cdot \chi^2$ coefficients

χ: matrix dimension

This is called a <u>matrix-product state</u>.

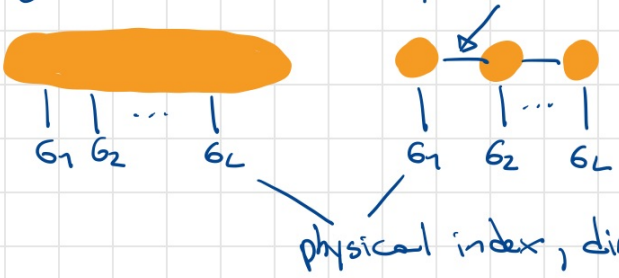
Intuition: χ → 1: product state, no entanglement

→ $\gg 1$: highly-entangled state

- In fact, <u>any</u> state $|\psi\rangle$ can be written as an MPS [1].

However, χ can grow exponentially. bond index, dim. $= \chi$

Graphically:



Example: $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$

$M_1^0 = (1\,0)$, $M_1^1 = (0\,1)$, $M_2^0 = \begin{pmatrix}1\\0\end{pmatrix}$, $M_2^1 = \begin{pmatrix}0\\1\end{pmatrix}$

$|\psi\rangle = (M_1^0|0_1\rangle + M_1^1|1_1\rangle) \otimes (M_2^0|0_2\rangle + M_2^1|1_2\rangle) = \frac{1}{\sqrt{2}}(|0_1 0_2\rangle + |1_1 1_2\rangle)$

- For L sites: $M_j^0 = \begin{pmatrix}1&0\\0&0\end{pmatrix}$, $M_j^1 = \begin{pmatrix}0&0\\0&1\end{pmatrix}$ (bond dim. $= 2$)

- Importantly, the MPS representation is not unique:

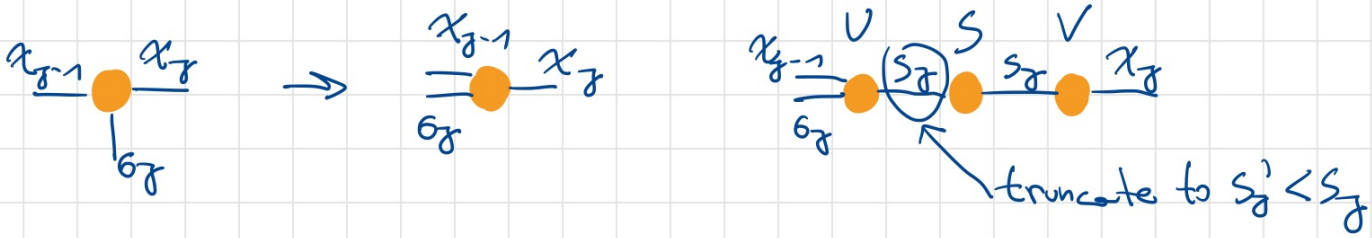
$$M^{\sigma_j} M^{\sigma_{j+1}} = \underbrace{M^{\sigma_j} C}\,\underbrace{C^{-1} M^{\sigma_j}} = N^{\sigma_j} N^{\sigma_{j+1}}.$$

- Fundamental MPS manipulation is compression.

It is based on singular value decomposition (SVD):

$M = USV^\dagger$ with U, V unitary and S diagonal with real entries ordered descendingly. Truncation: discard the smallest s_α until $\sum_\alpha |s_\alpha|^2 = \epsilon$. Sweep through the MPS & truncate every site.

Truncation for left→right sweep: [2]



• Why? Consider a bipartition $\overset{A}{\uparrow}\overset{}{\downarrow}|\overset{B}{\uparrow}\overset{}{\downarrow}$

$$|\psi\rangle = \sum_{jk} C_{jk} |j\rangle_A |k\rangle_B \xrightarrow[\text{Schmidt form}]{\text{SVD}} |\psi\rangle = \sum_\alpha s_\alpha |\alpha\rangle_A |\alpha\rangle_B$$

and $\rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi| = \sum_\alpha s_\alpha^2 |\alpha\rangle_A \langle\alpha|$

large Schmidt values → large contribution to RDM

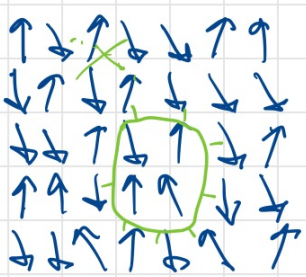
Also von Neumann entropy: $S = -\mathrm{Tr}\,\rho_A \log \rho_A = -\sum_\alpha s_\alpha^2 \log s_\alpha^2$

- 1 Schmidt value = 1 : no entanglement
- all " " with same magnitude : maximal entanglement

- Remember that the von Neumann entropy for a χ-dimensional matrix is bounded by $S \leq \log(\chi) \Rightarrow \chi \geq \exp(S)$, i.e. the bond dimension between j and $j+1$ grows exponentially with the entanglement w.r.t. the bipartition.

• Luckily, many physically-interesting states are lowly-entangled.

Area law [3]: for ground states of gapped Hamiltonians with local interactions, the entanglement scales as the boundary of the bipartition.



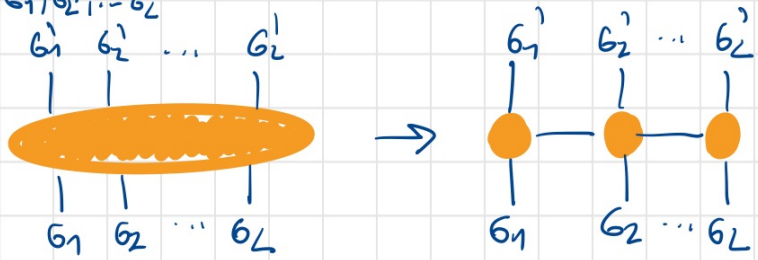
spins know only about NN, => only the spins on the boundary contribute

=> In 1D, the entanglement of GS of gapped, local Hamiltonians is independent of L!

Matrix product operators

- In a similar way, any operator can be written as

$$\hat{O} = \sum_{\substack{\sigma_1 \sigma_2 \dots \sigma_L \\ \sigma_1' \sigma_2' \dots \sigma_L'}} W^{\sigma_1 \sigma_1'} W^{\sigma_2 \sigma_2'} \cdots W^{\sigma_L \sigma_L'} |\sigma_1, \sigma_2, \dots \sigma_L\rangle\langle\sigma_1', \sigma_2', \dots \sigma_L'|$$



- Importantly: applying an MPO to an MPS results in an MPS with $\chi'_{MPS} = \chi_{MPO}\,\chi_{MPS}$ → truncation needed $\tilde{M}^{\sigma_j}_{(a,b),(a',b')} = \sum_{\sigma_j'} N^{\sigma_j \sigma_j'}_{aa'} M^{\sigma_j'}_{bb'}$

[4]

- Example:

$$\hat{O} = h \sum_j \hat{\sigma}^z_j \quad \Rightarrow \quad W^i = \begin{pmatrix} \mathbb{1} & 0 \\ h\hat{\sigma}^z & \mathbb{1} \end{pmatrix}$$

2 sites: $\begin{pmatrix} \hat{\sigma}_1^z & \mathbb{1} \end{pmatrix} \begin{pmatrix} \mathbb{1} \\ \hat{\sigma}_1^z \end{pmatrix} = \hat{\sigma}_1^z + \hat{\sigma}_2^z$

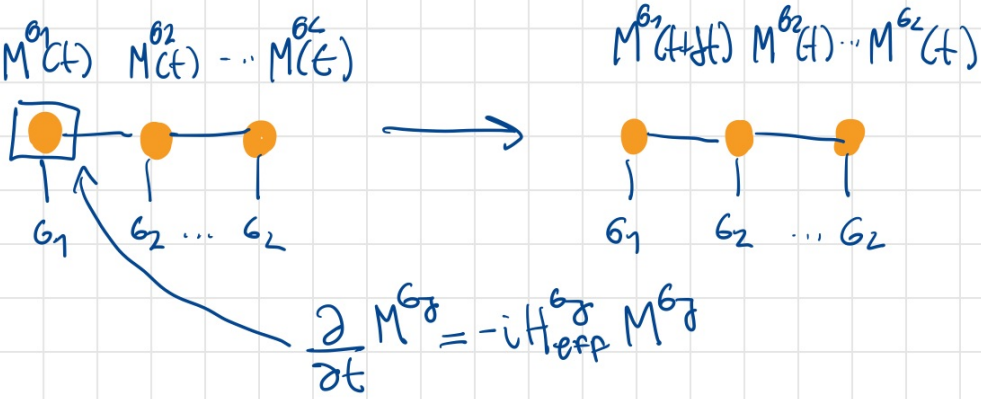
Ground state search: The density matrix renormalization group (DMRG) algorithm

- approximate global energy minimization with local energy minimization [1]: sweep through MPS & optimize 1 at a time

$$\frac{\partial}{\partial M^{\sigma_1}}\left(\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle\right) = 0 \Rightarrow H_{\text{eff}}^{\sigma_1} M^{\sigma_1} = \lambda M^{\sigma_1}$$

Time evolution: The time-dependent variational principle (TDVP) [2]

- global Schrödinger equation → local Schrödinger equation



2A) Dissipative time evolution

We want to solve for the full Lindblad dynamics when we are interested in timescales: → decoherence, → thermalization, → state preparation, → ...

There are two main approaches

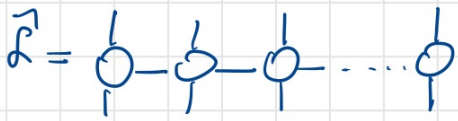
1) Direct propagation of $\hat{\rho}$ [5] $\quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \to \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}$

We make use of vectorization:

$\hat{\rho} \to |\rho\rangle\rangle$ (column stacking) $\quad |\rho\rangle\rangle =$  MPS

$\hat{\mathcal{L}} \to \hat{\mathcal{L}} = -i\hat{H}\otimes\mathbb{1} + \mathbb{1}\otimes i\hat{H} + \sum_k \hat{L}_k^\dagger \otimes \hat{L}_k - \frac{1}{2}\hat{L}_k^\dagger \hat{L}_k \otimes \mathbb{1} - \frac{1}{2}\mathbb{1}\otimes \hat{L}_k^\dagger \hat{L}_k$

$\mathrm{vec}(M_1 M_2 M_3) = (M_3^T \otimes M_1)\,\mathrm{vec}(M_2)$

$\hat{\mathcal{L}} =$  MPO

Then, the Lindblad equation simply reduces to an imaginary-time, non-Hermitian Schrödinger equation:

$$|\dot{\rho}\rangle\rangle = \hat{\mathcal{L}}\,|\rho\rangle\rangle \;, \quad |\rho(t)\rangle\rangle = e^{\hat{\mathcal{L}}t}\,|\rho(0)\rangle\rangle$$

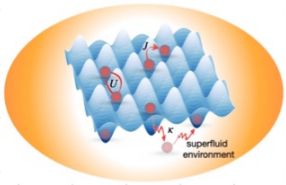
- Main difficulty: TDVP works only for Hermitian Hamiltonians

Possible solution: $\hat{\mathcal{L}} = \frac{\hat{\mathcal{L}}+\hat{\mathcal{L}}^\dagger}{2} + \frac{\hat{\mathcal{L}}-\hat{\mathcal{L}}^\dagger}{2} \equiv \hat{\mathcal{L}}_s + \hat{\mathcal{L}}_a \equiv \hat{\mathcal{L}}_s + i\hat{\mathcal{L}}_{\bar{s}}$

$$\Rightarrow |\rho(\delta t)\rangle\rangle \approx e^{\hat{\mathcal{L}}_s \delta t} \cdot e^{i\hat{\mathcal{L}}_{\bar{s}}\delta t}\,|\rho(0)\rangle\rangle + \mathcal{O}(\delta t^2)$$

ie: alternate a real and an imaginary timestep with two Hermitian Hamiltonians.

Example: the dissipative preparation of a Bose-Einstein condensate



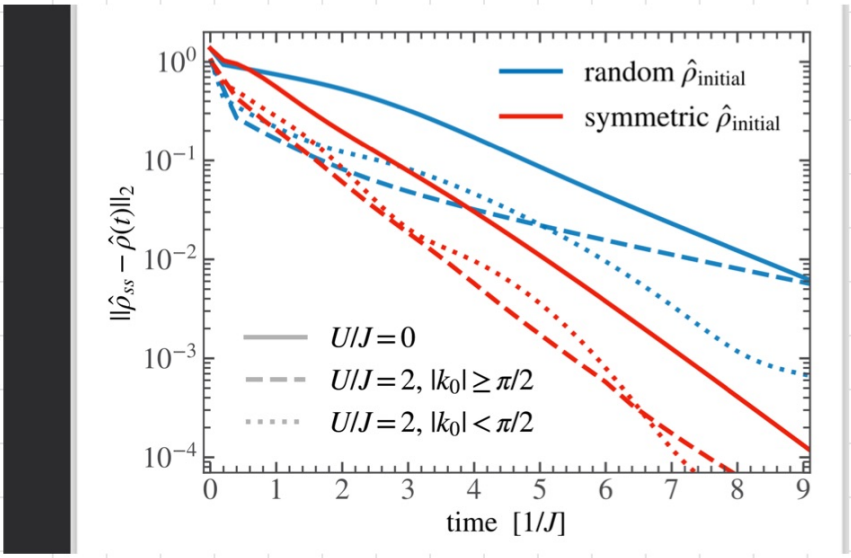
- Consider bosons hopping on an optical lattice:

$$\hat{H} = -J\sum_{j=1}^{L-1}\left(\hat{b}_{j+1}^{\dagger}\hat{b}_j + \text{h.c.}\right) + \frac{U}{2}\sum_{j=1}^{L}\hat{b}_j^{\dagger 2}\hat{b}_j^2$$

- It can be shown that the jump operators $\hat{L}_j = \sqrt{\kappa}\,(\hat{b}_j^{\dagger} + \hat{b}_{j+1})(\hat{b}_j - \hat{b}_{j+1}^{\dagger})$ drive any initial state to $\hat{\rho}_{ss} = |BEC\rangle\langle BEC|$, $|BEC\rangle = \frac{(\hat{b}_{k_0}^{\dagger})^N}{\sqrt{N!}}|vac\rangle$

- These jump operators describe the immersion of the lattice in a superfluid.

- Q: how fast do different initial configurations converge to the BEC? AND SYSTEM SIZE?



2) Pure state unravelings

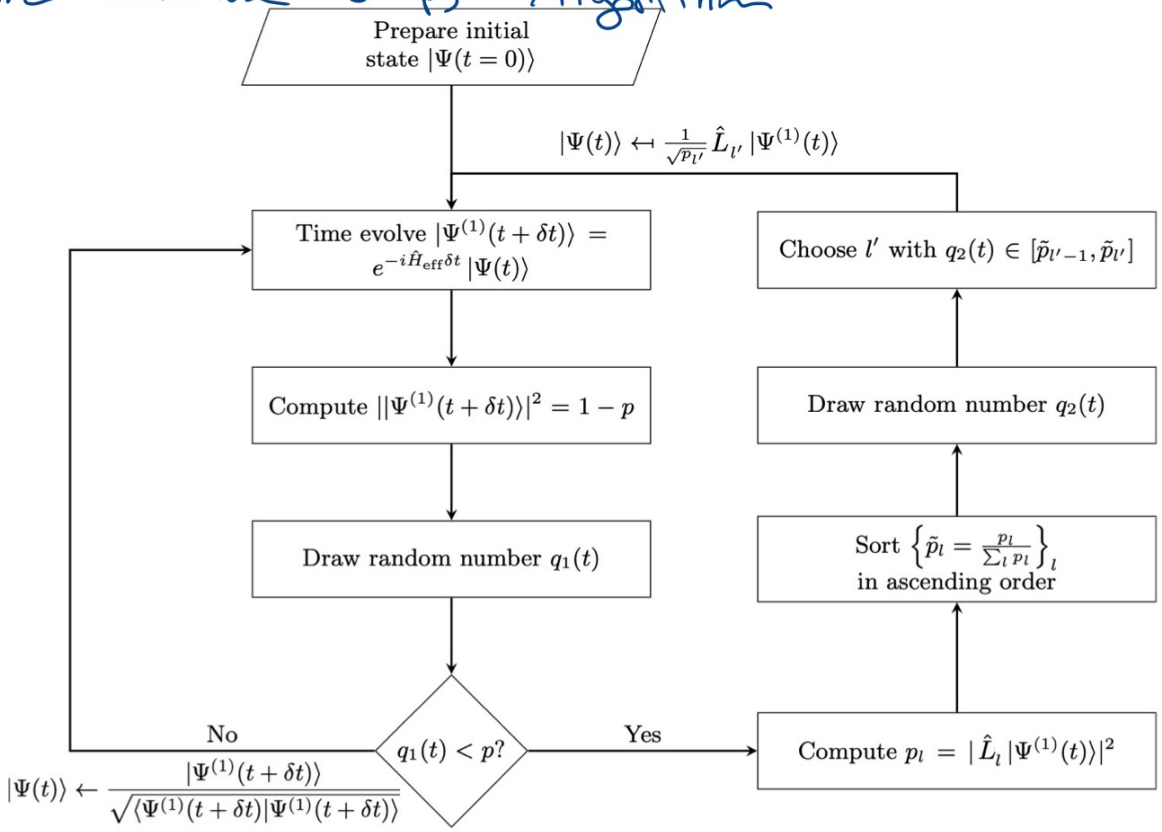
- 1 deterministic propagator of a mixed state $\hat{\rho} \rightarrow$ N stochastic evolutions of pure states $|\psi_q\rangle$ reduce dimensionality $\dim(\hat{\mathcal{L}}) = D^2 \rightarrow \dim(\hat{H}) = D$

- Consider a pure initial state $\hat{\rho}(0) = |\psi(0)\rangle\langle\psi(0)|$ and define $\hat{H}_{eff} \equiv \hat{H} - \frac{i}{2}\sum_e \hat{L}_e^+ \hat{L}_e$ => The Lindblad eq. becomes

$$\dot{\hat{\rho}} = \underbrace{-i(\hat{H}_{eff}\hat{\rho} - \hat{\rho}\hat{H}_{eff}^+)}_{\text{non-unitary evolution } e^{-iH_{eff}t}|\psi(0)\rangle \text{ (deterministic)}} + \underbrace{\sum_e \hat{L}_e \hat{\rho} \hat{L}_e^+}_{\text{"jumps" } \hat{L}_e|\psi(t)\rangle \text{ (stochastic)}}$$

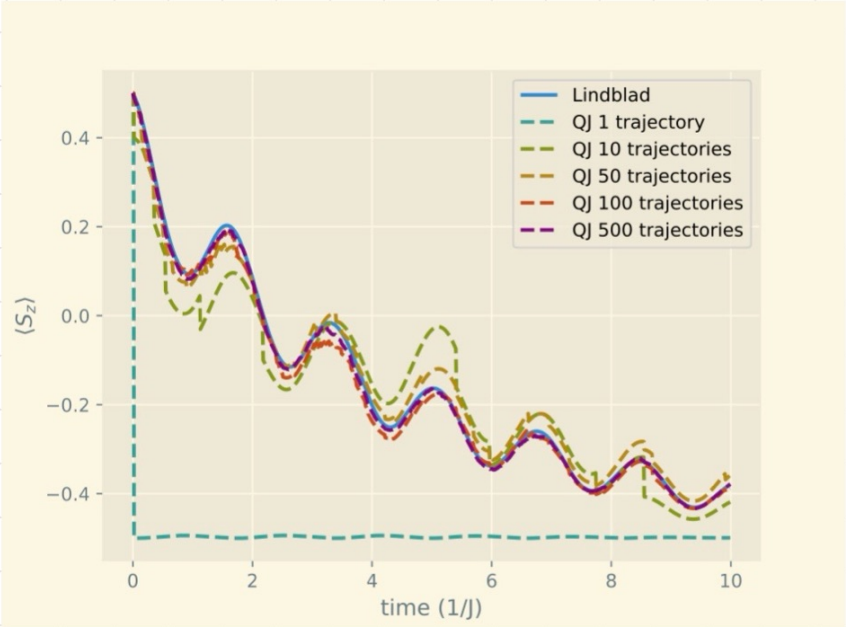
- Idea: monitor the norm decrease of $|\psi(t)\rangle$, as a measure of the strenght of the influence of the environment.

The Quantum Jumps Algorithm

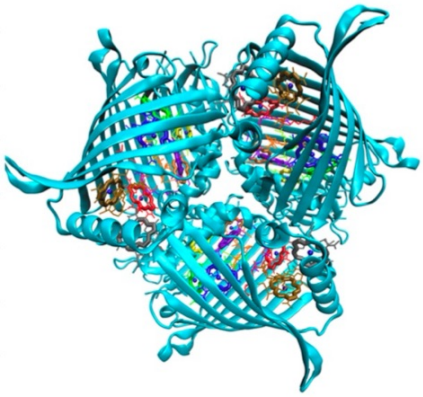


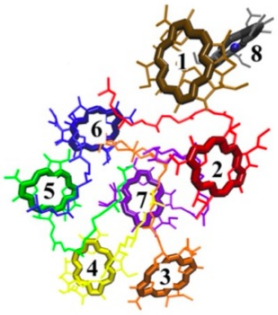
[6]

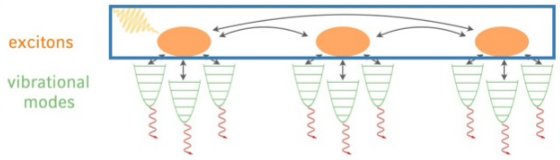
$$\frac{1}{N}\sum_{q=1}^{N} |\psi(t)_q\rangle\langle\psi(t)_q| = \hat{\rho}_N(t) \xrightarrow{N\to\infty} \hat{\rho}(t)$$



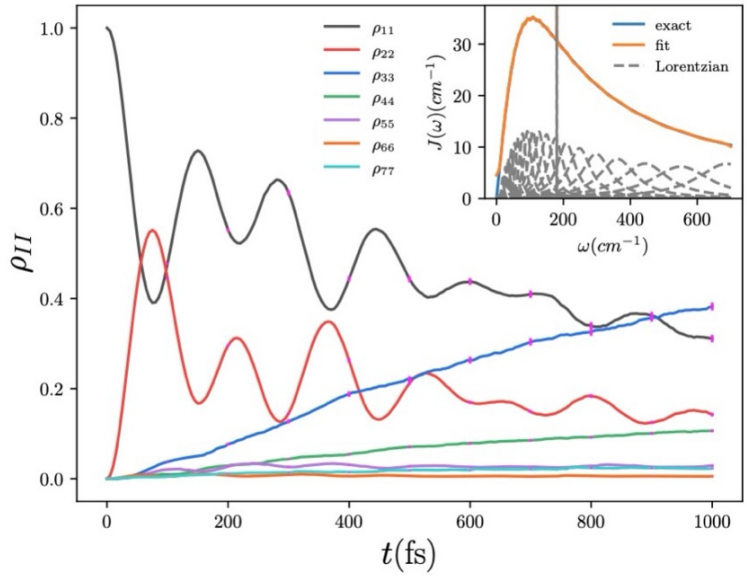
	advantages	disadvantages
direct propagation	- single time evolution - large timestep	- large dimensionality - positivity issues
unraveling	- small dimensionality - trivially parallelizable	- many time evolutions - small timesteps







More than 250 modes with d=16



2B) Direct steady state computation

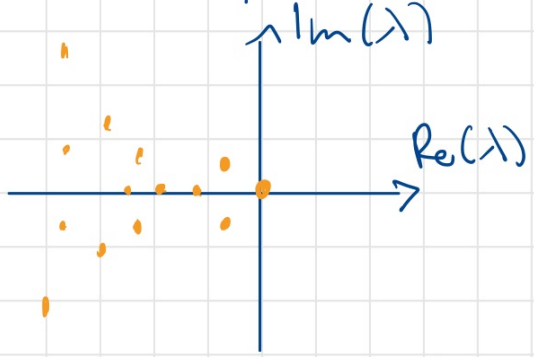
- If we are not interested in equilibration timescales and transient dynamics, but only in steady-state properties, we can avoid computing the dynamics.
- Consider a Lindbladian with a unique steady state. Then

$\mathcal{L} = \sum_k \lambda_k |r_k\rangle\rangle\langle\langle l_k|$, arrange $\lambda_1 = 0 < |\mathrm{Re}(\lambda_2)| \leq |\mathrm{Re}(\lambda_3)|$

$|r_1\rangle\rangle$ corresponding to λ_1 is the steady state.

- Long time evolution

→ diagonalization → DMRG?



- Problem: $\mathcal{L}$ is non-Hermitian => DMRG doesn't work (no variational principle)

[7]

=> $\mathcal{L} \to \mathcal{L}^\dagger \mathcal{L} \geq 0$. The eigenvector corresponding to the zero-eigenvalue is the steady-state

Difficulties: $\mathcal{L}^\dagger \mathcal{L}$ has:
- large bond dim
- it is non-local
- gap can become very small

2C) Computing Lindbladian spectra

(Part of) the spectrum of the Lindbladian is needed for:
- dissipative phase transition (closing of Liouvillian gap)
- anomalous thermalizations, e.g. the Mpemba effect
- metastability

• Main idea: compute a few time evolution steps, build a small subspace in which to approximate the full $\mathcal{L}$, and diagonalize it $\mathcal{L} \to \mathcal{L}^{\text{eff}}$

Following Miyanti, Huybrects: [8]

1) Represent vectorized Lindbladian as MPO & vectorized initial state as MPS.
2) compute a set of N time evolved states: $\{|\psi_n\rangle = \mathcal{E}^n|\psi_0\rangle\}_{n=0}^{N-1}$ with $\mathcal{E} = \exp(\underline{\underline{\mathcal{L}}}\delta t)$ with TDVP
3) Orthogonalize these states with (Gram-Schmidt) to obtain a basis $\{|\psi_i\rangle\}$
4) Compute the approximated, N lowest eigenvalues of $\underline{\underline{\mathcal{L}}}$ in this subspace: $\mathcal{L}^{\text{eff}}_{ij} = \langle\psi_i|\underline{\underline{\mathcal{L}}}|\psi_j\rangle$ & diagonalize

- Why is $\{|\Psi_i\rangle\}$ a good basis?

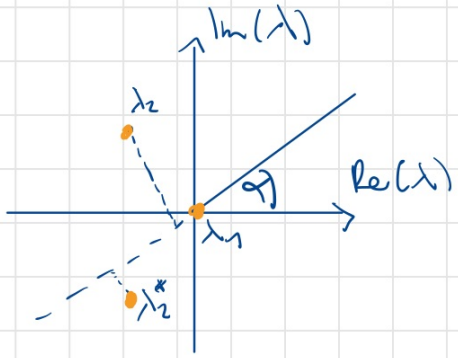
$$|\rho(t)\rangle\rangle = \mathcal{E}|\rho(0)\rangle\rangle = a_0|\rho_{ss}\rangle\rangle + \sum_{k=2}^{\Delta^2} e^{\lambda_k t} \langle\langle \ell_k|\rho(0)\rangle\rangle |r_k\rangle\rangle$$

$\Rightarrow$ the contribution of each Lindbladian mode is suppressed exponentially as $\propto e^{\mathrm{Re}(\lambda_k)t}$

Thus, the states $|\Psi_i\rangle$ have a large overlap with the lowest-dec. modes $|r_k\rangle\rangle$.

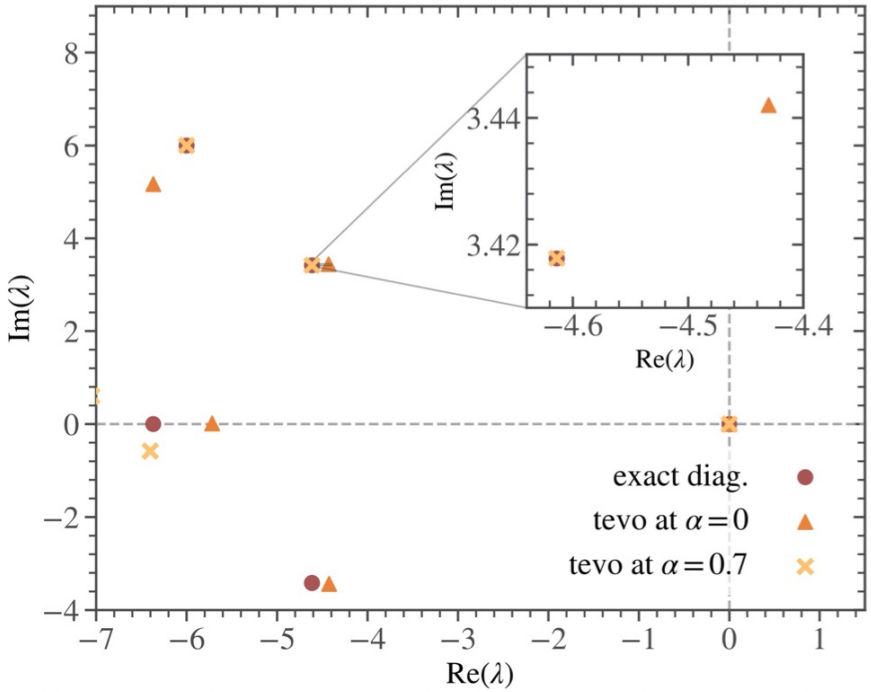
- If we are interested also in higher-order modes, it is convenient to use a complex-time evolution: $t \to z = e^{i\alpha}t$

$$\Rightarrow e^{\mathrm{Re}(\lambda_k)t} \to e^{\mathrm{Re}(\lambda_k)z}, \quad \mathrm{Re}(\lambda_k z) = t[\mathrm{Re}(\lambda_k)\cos(\alpha) + \mathrm{Im}(\lambda_k)\sin\alpha]$$



a positive α moves eigenvalues in the upper-half plane closer to zero

$\Rightarrow$ they are less suppressed!


8
6
4
2
0
−2
−4
Im(λ)
−7
−6
−5
−4
−3
−2
−1
0
1
Re(λ)
3.44
3.42
Im(λ)
−4.6
−4.5
−4.4
Re(λ)
exact diag.
tevo at α = 0
tevo at α = 0.7

References

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[2] S. Paeckel et al., 'Time-evolution methods for MPS'.

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[8] F. Minganti, D. Huybrechts 'Arnoldi-Lindblad time evolution'