How to represent a quantum bath for Tensor Network simulation?

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How to discretize a quantum bath for real-time evolution

Inés de Vega, Ulrich Schollwöck, and F. Alexander Wolf
Phys. Rev. B **92**, 155126 – Published 15 October 2015

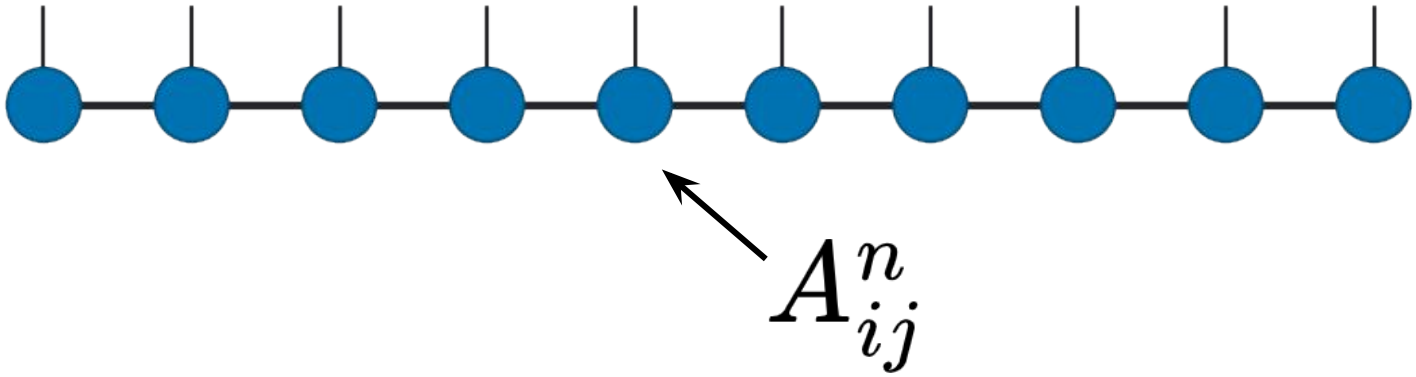
ABSTRACT

Many numerical techniques for the description of quantum systems that are coupled to a continuous bath require the discretization of the latter. To this end, a wealth of methods has been developed in the literature, which we classify as (i) direct discretization, (ii) orthogonal polynomial, and (iii) numerical optimization strategies. We recapitulate strategies (i) and (ii) to clarify their relation. For quadratic Hamiltonians, we show that (ii) is the best strategy in the sense that it gives the numerically exact time evolution up to a maximum time t_{max}, for which we give a simple expression. For nonquadratic Hamiltonians, we show that no such best strategy exists. We present numerical examples relevant to open quantum systems and strongly correlated systems, as treated by dynamical mean-field theory (DMFT).

Bath representation and computational cost

- Bath discretization aims for having smaller bath modes
- Why? It assumes smaller bath modes allow lower computational cost
- What determines the computational cost? It depends on the method
- Today, I will focus on the variational wavefunction method
  In particular, with Tensor Network Ansatz

Matrix Product State (MPS)



Parameterize wavefunction with low rank tensors

Computational cost / memory - linear to number of tensors

Key factor - bond dimensions, physically relevant to entanglement structure

Tensor network for dynamics is generally hard

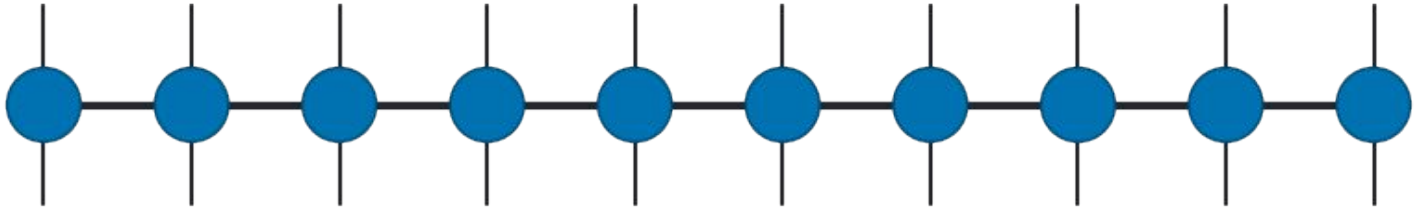
- In general, entanglement grows linearly over time
- Bond dimension $\chi \propto e^{S}$ Worst case, exponential complexity
- However, open quantum system has particular structure

  both in the Hamiltonian and initial states
- We will here assume Gaussian bath. It gives us freedom for choosing bath

  representation through Gaussian rotations.
- Choosing a proper basis and ordering can reduce lots of entanglement

Density operator or wavefunction?

1. Matrix product density operator

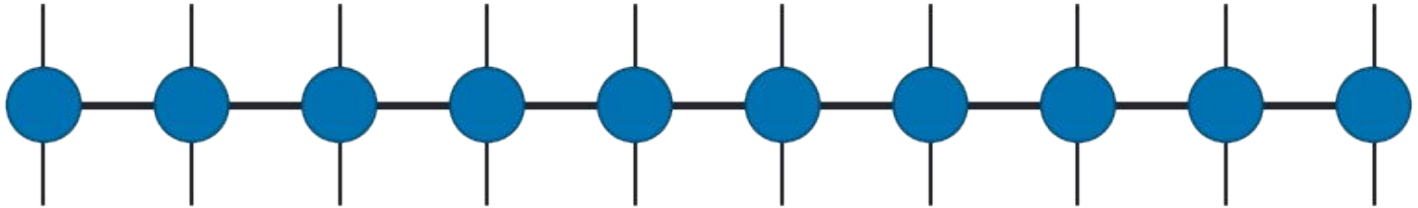


Directly parameterize density operator with Tensor Network

as Matrix Product Operator

Density operator or wavefunction?

1. Matrix product density operator



2. Purification based wavefunction (only for unitary Hamiltonian dynamics)

Also known as ancilla method

In practice, it often provides lower entanglement

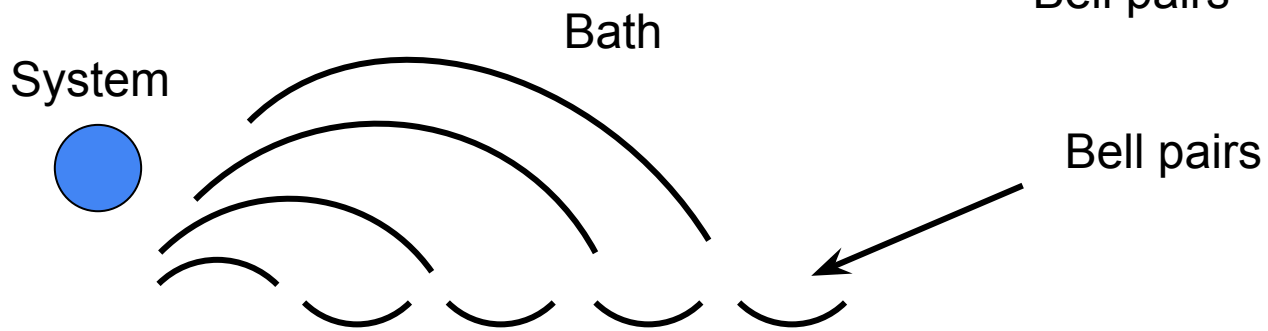
Unitary operator is only applied to ‘ket’ part

Feiguin and White, PRB 72, 220401 (2005).

Purification for (Gaussian) thermal bath

$$\hat{\rho} \propto e^{-\beta E_k c_k^\dagger c_k} \longrightarrow |\Omega\rangle \propto e^{-\frac{\beta}{2} c_k^\dagger b_k^\dagger} |0\rangle$$

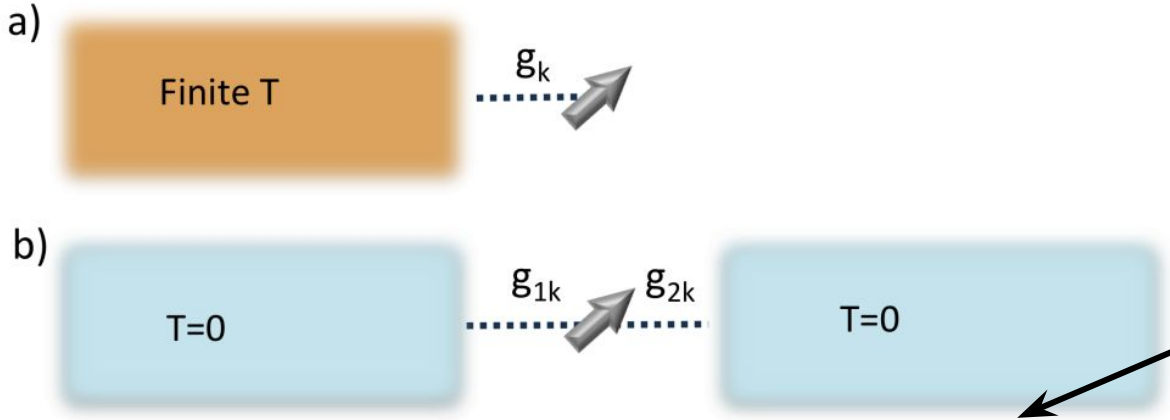
Bell pairs



Initially entangled state with long range interactions

Entanglement quickly grows over time evolution

Thermofield-based bath representation



Bogoliubov transformation

Find canonical transformation

$$|\Omega\rangle = e^{-iG}|0\rangle$$

which is Gaussian

$$\hat{H} \rightarrow \hat{H}' = e^{iG}\hat{H}e^{-iG}$$

Starting from the vacuum (zero temperature)

Less entanglement, better for Tensor Network

Vega and Banuls, PRA 92, 052116 (2015).

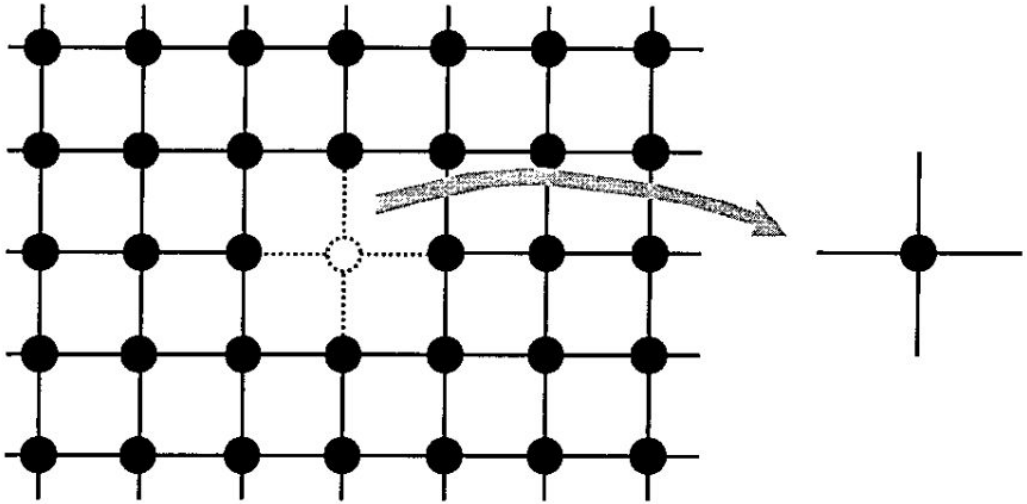
Sagas for Anderson impurity model

Fermionic Open quantum system

Starting point of

dynamical mean field theory

(DMFT)

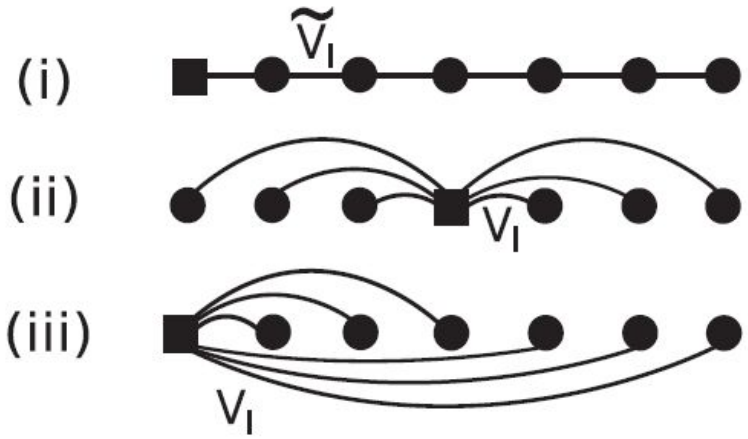


$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{\sigma} \epsilon_\sigma d^\dagger_\sigma d_\sigma + U d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow + \sum_{k,\sigma} V_k (d^\dagger_\sigma c_{k\sigma} + c^\dagger_{k\sigma} d_\sigma),$$

Computes dynamical properties (Green's function)

Georges, Kotliar, Krauth, and Rozenberg, RMP 68, 13 (1996).

Chain geometry and Star geometry



Chain geometry $\sum_{l=0}^{L_b-1} \sum_{\sigma} \left(\widetilde{V}_l c^{\dagger}_{l+1,\sigma} c_{l\sigma} + \text{H.c.} \right)$

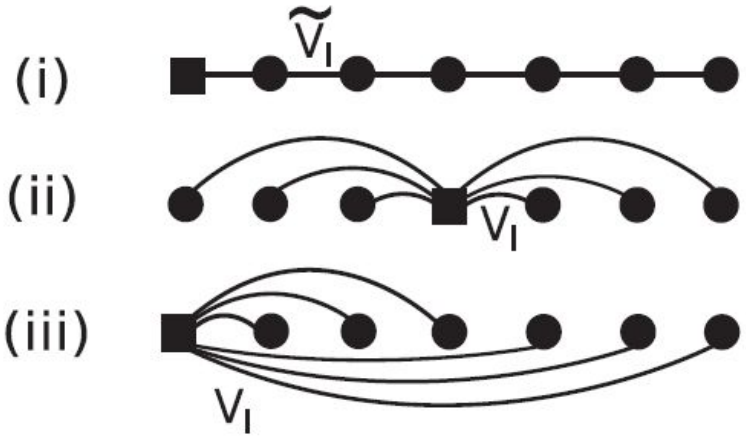
Star geometry $\sum_{l=1}^{L_b} \sum_{\sigma} \left(V_l c^{\dagger}_{0\sigma} c_{l\sigma} + \text{H.c.} \right)$

Chain geometry - Related to Orthogonal Polynomial / Lanczos / Krylov based bath discretization methods

Only has local interactions - low entanglement?

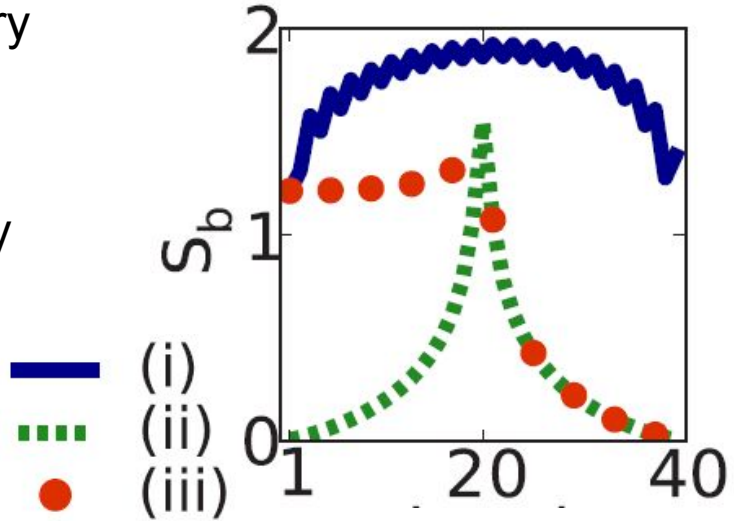
Wolf, McCulloch, and Schollwock, PRB 90, 235131 (2014).

Chain geometry and Star geometry



Chain geometry

Star geometry

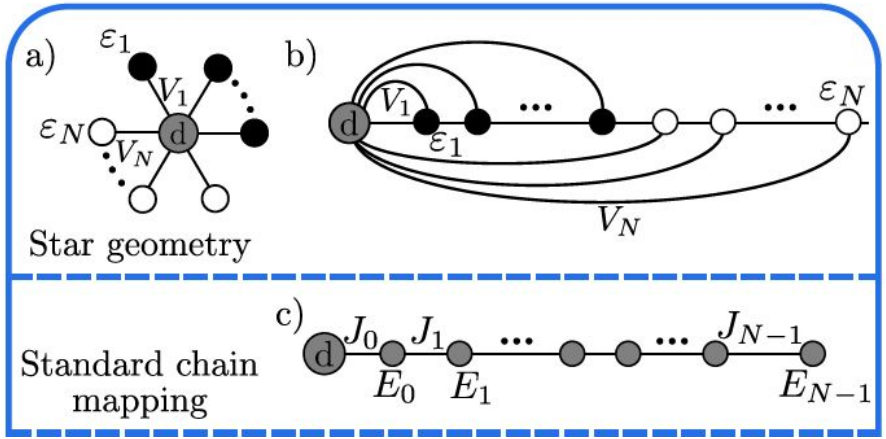


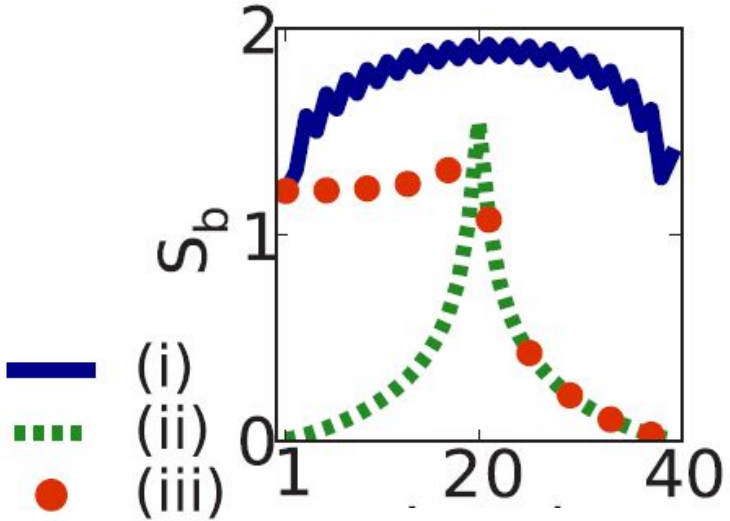
Chain geometry has larger entanglement than star!

Requires larger bond dimension

Wolf, McCulloch, and Schollwock, PRB 90, 235131 (2014).

Chain geometry and Star geometry

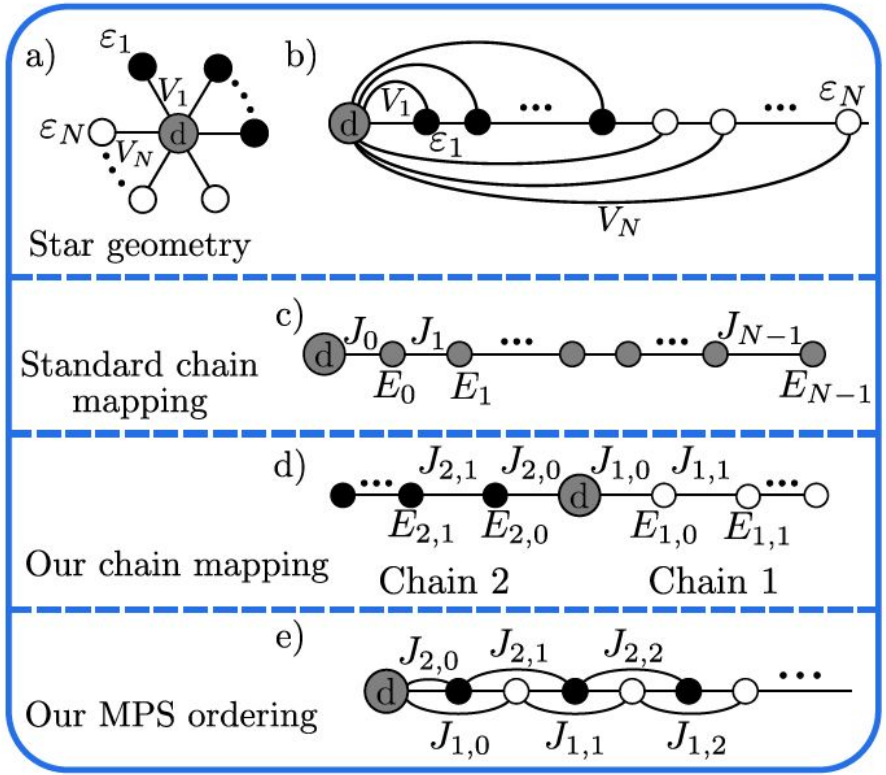




High entanglement - mainly because of mixing between occupied and empty modes

Wolf, McCulloch, and Schollwock, PRB 90, 235131 (2014).

Chain geometry from thermofield transformation



- Thermal bath

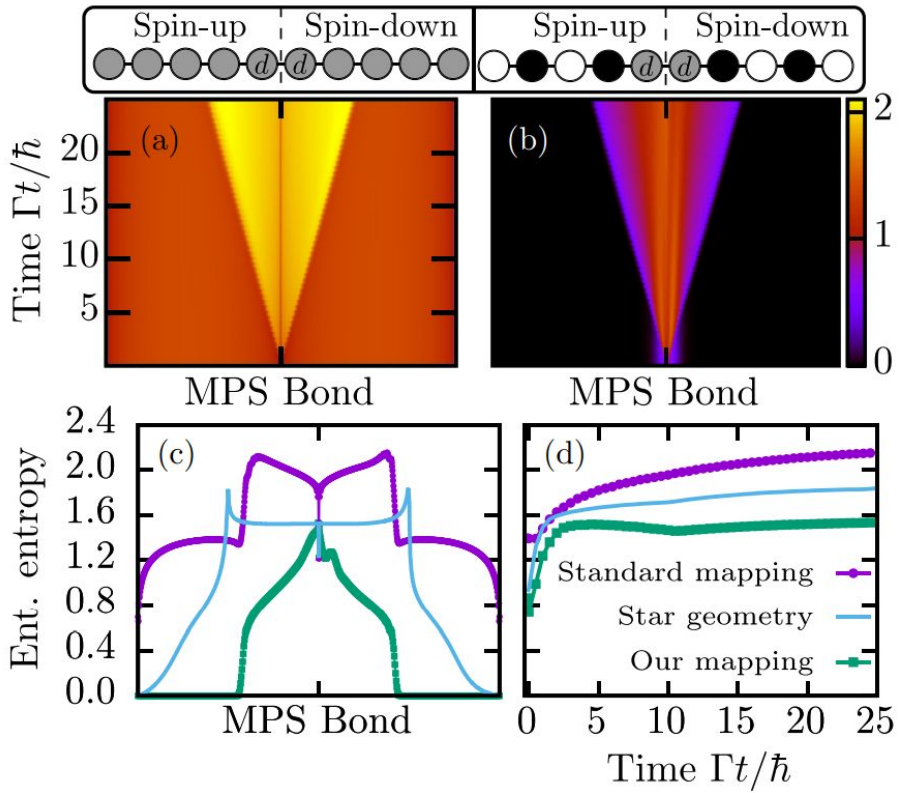
After thermofield transformation, two chains with fully occupied and empty modes are separated

No mixing

Thermofield

Kohn and Santoro, PRB 104, 014303 (2021).

Entanglement profile



Chain mapping over occupied/empty modes has low entanglement

Entanglement is spreading over light-cone

Almost no entanglement increase over time

Kohn and Santoro, PRB 104, 014303 (2021).

Entanglement - Unitary vs Dissipative dynamics

- General many-body unitary dynamics

  Entanglement entropy grows linearly over time $S(t) \propto t$

- Dissipative dynamics

  Either from imaginary time evolution or Lindblad dissipators

  Constant entanglement entropy in the long-time limit $S(t) \sim C$

- Can we use this structure for open quantum system dynamics?

Equivalence between Unitary and Lindbladian bath

Unitary

$$\hat{H}_{SE} = \hat{H}_S + \hat{H}_E + \sum_{j=1}^{\kappa} \hat{A}_{S,j} \otimes \hat{G}_{E,j},$$

$$\rho_S^U(t) = \mathrm{Tr}_E \left\{ e^{-i\hat{H}_{SE}t} \left(\rho_S(0) \otimes \rho_E(0)\right) e^{i\hat{H}_{SE}t} \right\},$$

Lindbladian

$$\hat{H}_{SR} = \hat{H}_S + \hat{H}_R + \sum_{j=1}^{\kappa} \hat{A}_{S,j} \otimes \hat{F}_{R,j},$$

$$\dot{\rho}_{SR}(t) = \mathcal{L}_{SR}\left[\rho_{SR}(t)\right] = -i\left[\hat{H}_{SR}, \rho_{SR}(t)\right] + \mathcal{D}_R\left[\rho_{SR}(t)\right], \quad (2)$$

where

$$\mathcal{D}_R[\rho] = \sum_{j=1}^{\ell} \gamma_j \left(\hat{L}_{R,j} \rho \hat{L}_{R,j}^{\dagger} - \frac{1}{2} \left\{ \hat{L}_{R,j}^{\dagger} \hat{L}_{R,j}, \rho \right\} \right) \quad (3)$$

$$\rho_S^L(t) = \mathrm{Tr}_R \left\{ e^{\mathcal{L}_{SR}t} \left[\rho_S(0) \otimes \rho_R(0)\right] \right\}.$$

Equivalence between these two dynamics

Tamascelli, Smirne, Huelga, Plenio, PRL 120, 030402 (2018).

Equivalence between Unitary and Lindbladian bath

Unitary

$$C^U_{jj'}(t+s,s) = \mathrm{Tr}_E \left\{ e^{i\hat{H}_E(t+s)} \hat{G}_{E,j} e^{-i\hat{H}_E(t+s)} e^{i\hat{H}_E s} \hat{G}_{E,j'} e^{-i\hat{H}_E s} \rho_E(0) \right\}.$$

Lindbladian

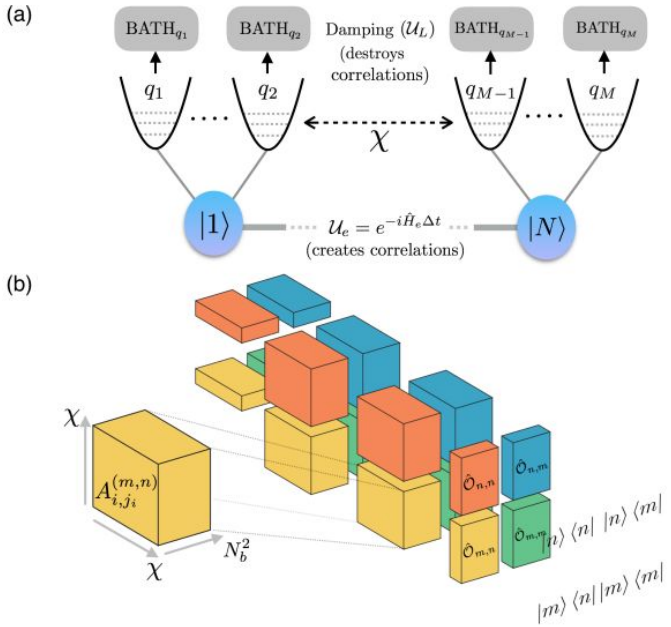
$$C^L_{jj'}(t+s,s) = \mathrm{Tr}_R \left\{ \hat{F}_{R,j} e^{\mathcal{L}_R t} \left[\hat{F}_{R,j'} e^{\mathcal{L}_R s} \left[\rho_R(0) \right] \right] \right\}$$

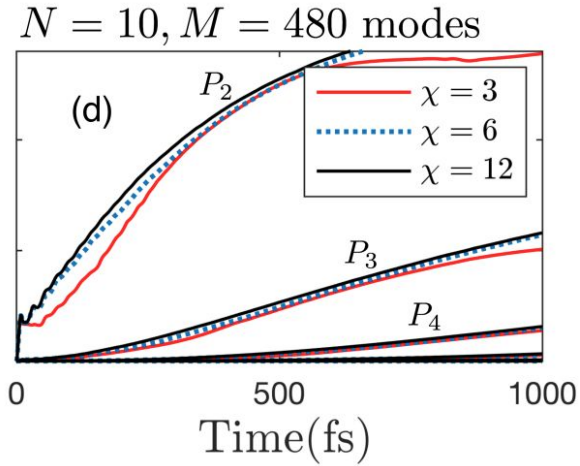
$$\left.\begin{array}{rcl} F_{R,j}(t) & = & G_{E,j}(t) \\ C^L_{jj'}(t+s,s) & = & C^U_{jj'}(t+s,s) \end{array}\right\} \ \forall j, j', t, s \geq 0$$

$$\Longrightarrow \quad \rho^L_S(t) = \rho^U_S(t) \ \ \forall t.$$

Tamascelli, Smirne, Huelga, Plenio, PRL 120, 030402 (2018).

Dissipation assisted matrix product factorization



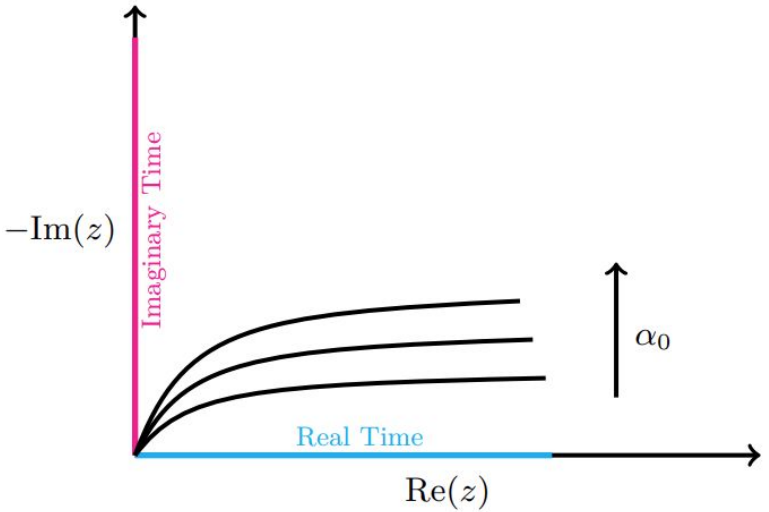


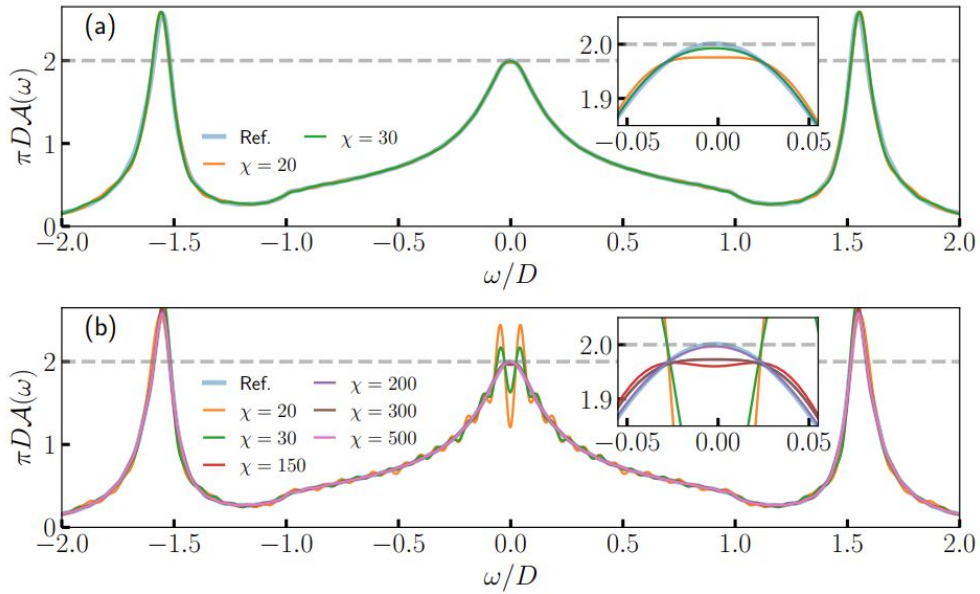
10-site excitation coupled to 48 vibrational modes each (480 modes in total)

Lindblad dissipation allows MPS with only bond dimension 12

Somoza, Marty, Lim, Huelga, Plenio, PRL 123, 100502 (2019).

Complex Time evolution





Time evolution in complex plane with analytical continuation can allow us to get system green's function with much lower bond dimension

Cao et. al., arXiv 2311.10909 (2023).
Grundner et. al., arXiv 2312.11705 (2023).

Topics that are not covered today

- Tree Tensor Network (Hierarchical Tucker) wavefunction in MCTDH
- Tensor Network for HEOM
- Time-dependent bath representation
- Space-time Tensor Network with influence functional
- Tensor Train for Diagrammatic Monte Carlo sampling

Take-away Message

- When concerning bath discretization, we often aim to minimize the number of bath modes, but, with Tensor Network, smaller bath modes ≠ lower computational cost (if it has larger entanglement)

- With same entanglement, the bath mode only contributes to linear time complexity $\mathcal{O}(n_b)$

- Even with the fixed bath modes, we should choose a proper bath representation for the proper evaluation of computational cost