Process Tensor Networks for non-Markovian Many-Body Open Quantum Systems

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IQTN – Workshop on the 9th of January, 2023 in Dundee (UK):

"Numerical Methods for many-body quantum systems"

Outline

1. Process Tensor - Framework Introduction

quantum Markovianity

multi-time correlations

many-body quantum systems

2. Process Tensor - Numerical Tools

overview on the numerical methods based on the process tensor

3. Process Tensor & Time Evolving Block Decimation

for chains of non-Markovian open quantum systems

- XY chain with boson baths
- XYZ chain with thermal leads

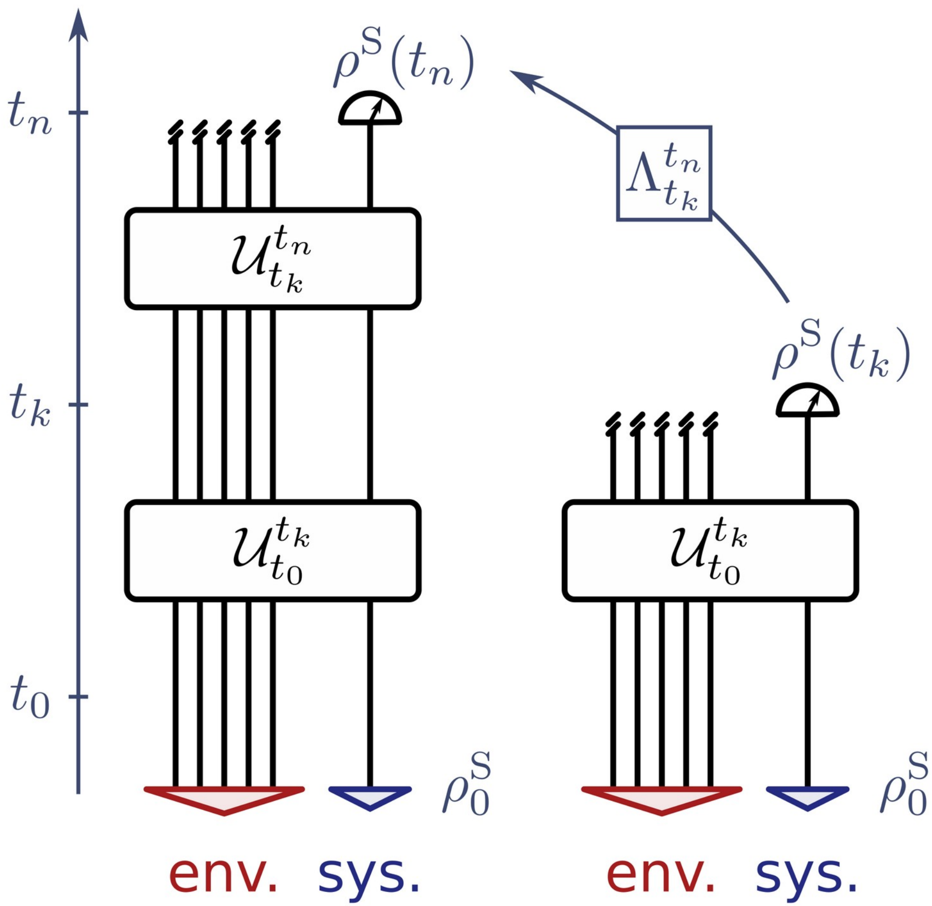
4. Closing Remarks

python package OQuPy

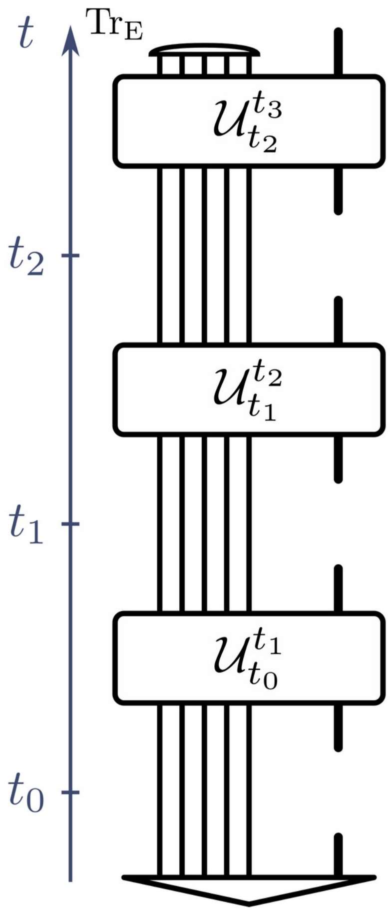
acknowledgements

summary

Dynamical Maps

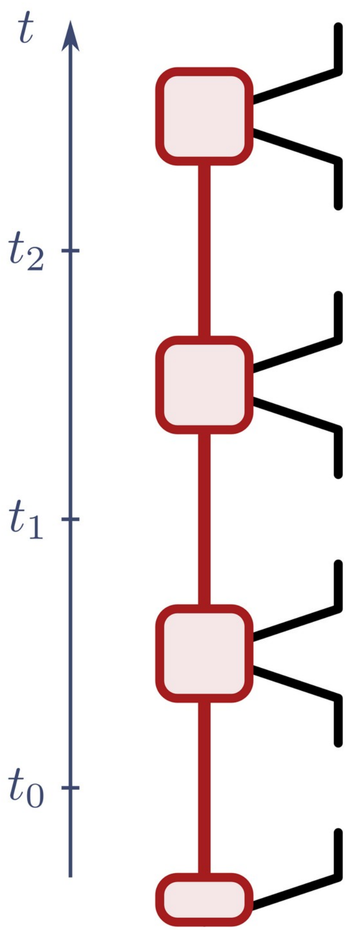


Process Tensor Framework [2]



[2] Pollock, Rodríguez-Rosario, Frauenheim, Paternostro, and Modi,
Non-markovian quantum processes: Complete framework and efficient characterization,
Phys. Rev. A 97, 012127 (2018)

Process Tensor Framework [2]



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process tensor
in matrix product operator form
(**PT-MPO**)

[2] Pollock, Rodríguez-Rosario, Frauenheim, Paternostro, and Modi,
Non-markovian quantum processes: Complete framework and efficient characterization,
Phys. Rev. A 97, 012127 (2018)

Process Tensor Framework [2]

The **process tensor** …

- encodes the dynamics *and* multi-time correlations,
- scales exponentially with the number of time steps, but
- can often be represented efficiently as an MPO.

The process tensor is related to :

quantum comb, *influence functional*, *process matrix*, ...

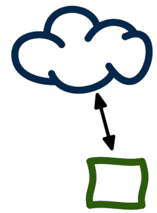
The necessary bond dimension of the PT-MPO is connected to the “degree of non-Markovianity” [3].
In particular[4]:

PT-MPO is a product operator	$\Rightarrow$ $\not\Leftarrow$	Dynamical map is CP-divisible

[2] Pollock et al. (2018) PRA, 97(1), p.012127.
[3] Pollock et al. (2018) PRL 120, 040405.
[4] Milz et al. (2019) PRL 123, 040401.

Process Tensor Framework + Trotterization

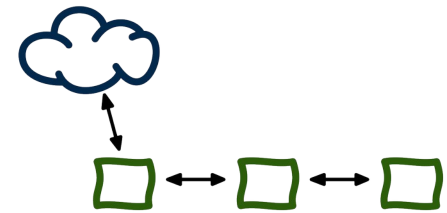
$$\hat{H} = \hat{H}^{\mathrm{S}} + \hat{H}^{\mathrm{E}} + \hat{H}^{\mathrm{I}}$$



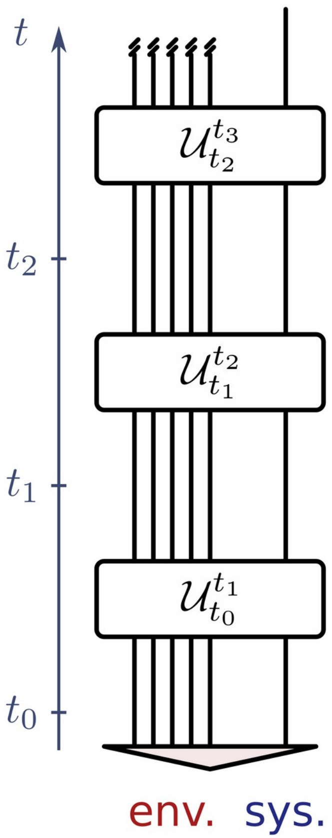
$\hat{H}^{\mathrm{E}}$ environment

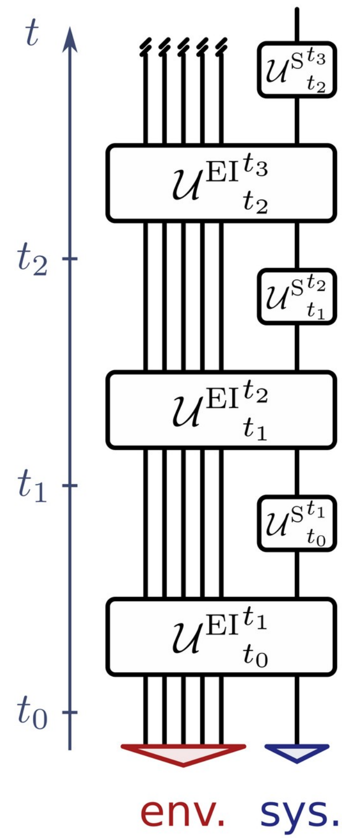
$\hat{H}^{\mathrm{I}}$ interaction

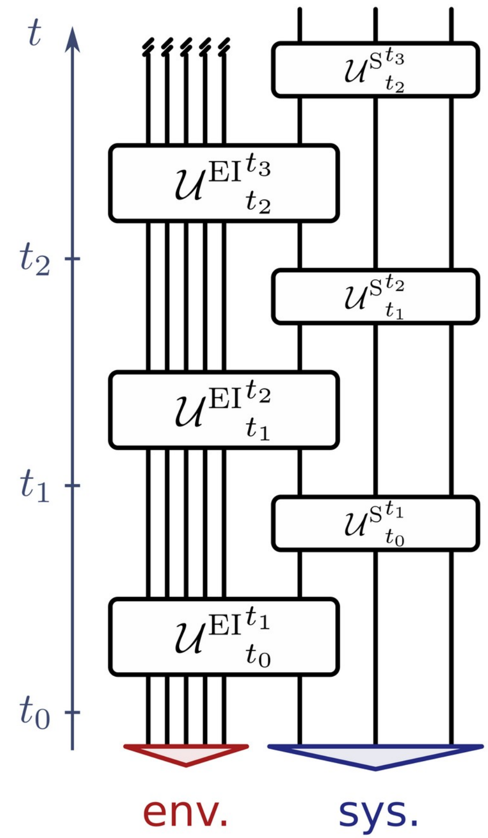
$\hat{H}^{\mathrm{S}}$ system



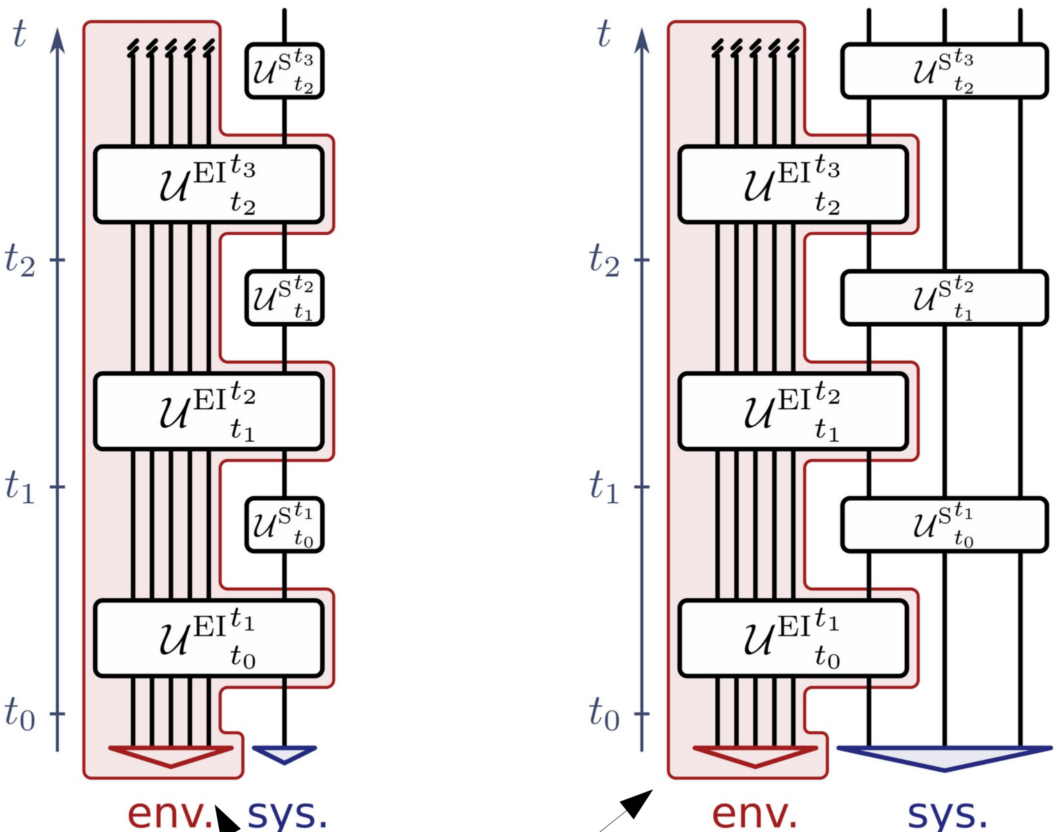
$$\hat{U} = \left[e^{-iH\delta t}\right]^N \approx \left[e^{-iH^{\mathrm{S}}\delta t}\, e^{-iH^{\mathrm{EI}}\delta t}\right]^N$$







Process Tensor Framework - Trotterization



many body system

$\simeq$

probing multi-time correlations of $\hat{H}^{\mathrm{EI}} = \hat{H}^{\mathrm{E}} + \hat{H}^{\mathrm{I}}$

process tensor for $\hat{H}^{\mathrm{EI}} = \hat{H}^{\mathrm{E}} + \hat{H}^{\mathrm{I}}$

Methods to yield a PT-MPO

From explicit TEBD-like environment tensor networks:
- [5] Bañuls et al. (2009) PRL 102, 240603.
- [6] Müller-Hermes et al. (2012) New J. Phys. 14, 075003.
- [7] Sonner et al. (2021) Ann. Phys. (N. Y.) 435, 168677.
- [8] Lerose et al. (2021) PRX 11, 021040.
- [9] Ye et al. (2021) J. Chem. Phys. 155, 044104.

Continuous gaussian bosonic environments:
- [10] Strathearn et al. (2018) Nat. Commun. 9, 3322.
- [11] Jørgensen and Pollock (2019) PRL 123, 240602.

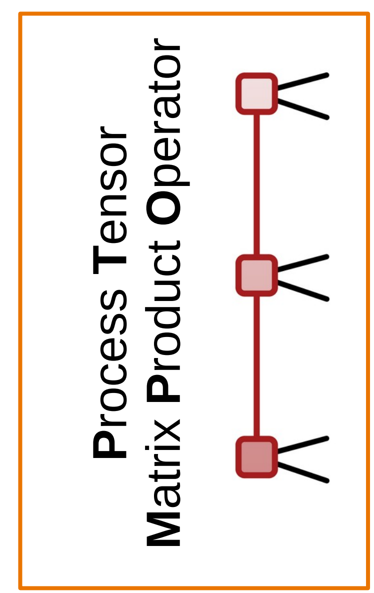
"TEMPO"

Continuous gaussian fermionic Environment:
- [12] Thoenniss et al. arXiv:2205.04995
- [13] Thoenniss et al. arXiv:2211.10272
- [14] Ng et al. arXiv:2211.10430.

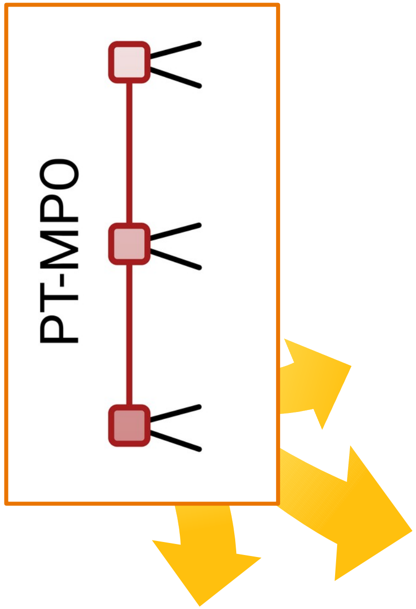
Any discrete set of non interacting environment modes
(Gaussian / non-Gaussian - bosonic / fermionic, spin env.)
- [15] Cygorek et al. (2022) Nat. Phys. 10.1038/s41567-022-01544-9.

"ACE"

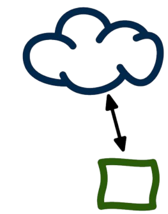
Process Tomography
- [16] White et al. PRX Quantum 3, 020344 (2022)



Methods to apply a PT-MPO

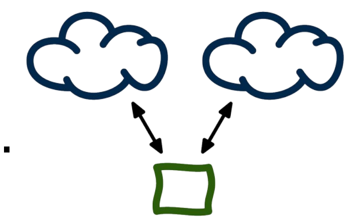


Optimal control of non-M. systems:
[17] GEF, Butler et al. (2021) PRL 126, 200401.
[18] Butler, GEF, et al. *in preparation*.

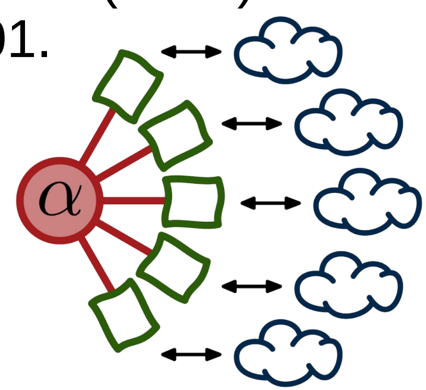


Environment dynamics of non-M. systems:
[19] Gribben et al. (2022) Quantum, 6, p.847.

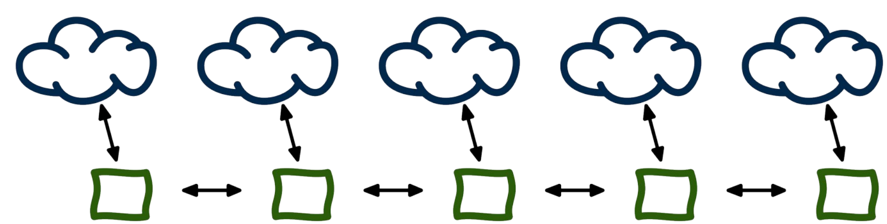
Non-M. systems with multiple environments:
[20] Gribben et al. (2022) PRX Quantum 3, 10321.



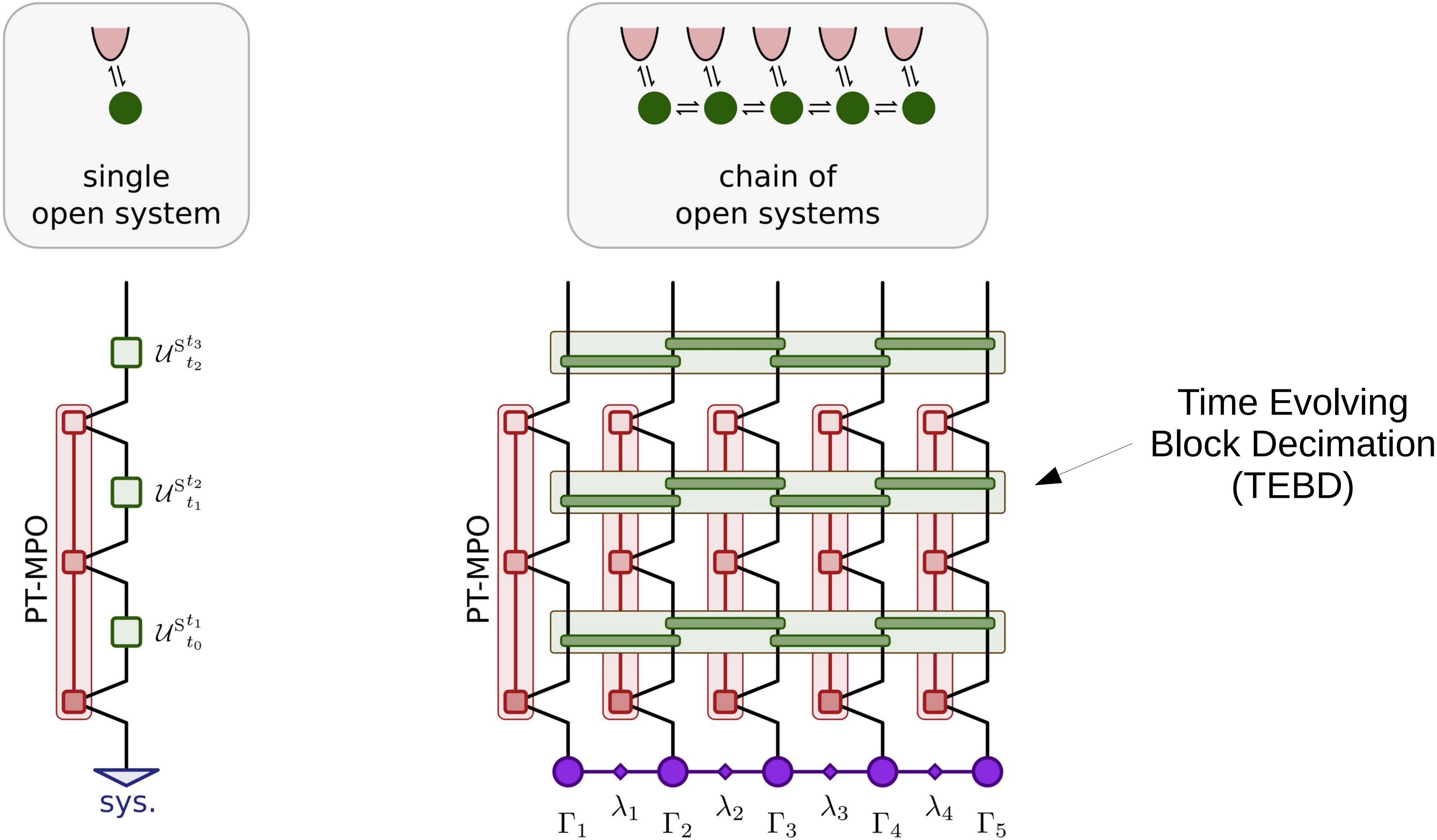
Mean-field of non-M. systems:
[21] Fowler-Wright et al. (2022)
PRL 129, 173001.



Chains of non-M. systems:
[22] GEF et al. arXiv:2201.05529.

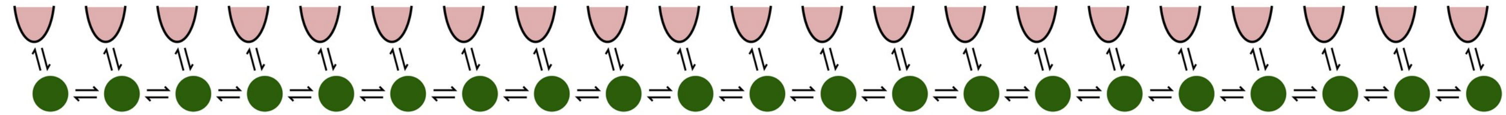


Chains of non-M. Open Quantum Systems [22]



[22] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529

XY Spin Chain with Environments [23]

Total Hamiltonian: 

$$\hat{H} = \boxed{\hat{H}_{\mathrm{XY}}} + \sum_{n=-10}^{10} \hat{H}_n^{\mathrm{E}}$$

Anisotropic XY Chain:

anisotropy

$$\hat{H}_{\mathrm{XY}} = \sum_{n=-10}^{10} \hat{s}_n^z + \sum_{n=-10}^{9} \left[(1-\eta)\hat{s}_n^x \hat{s}_{n+1}^x + (1+\eta)\hat{s}_n^y \hat{s}_{n+1}^y \right]$$

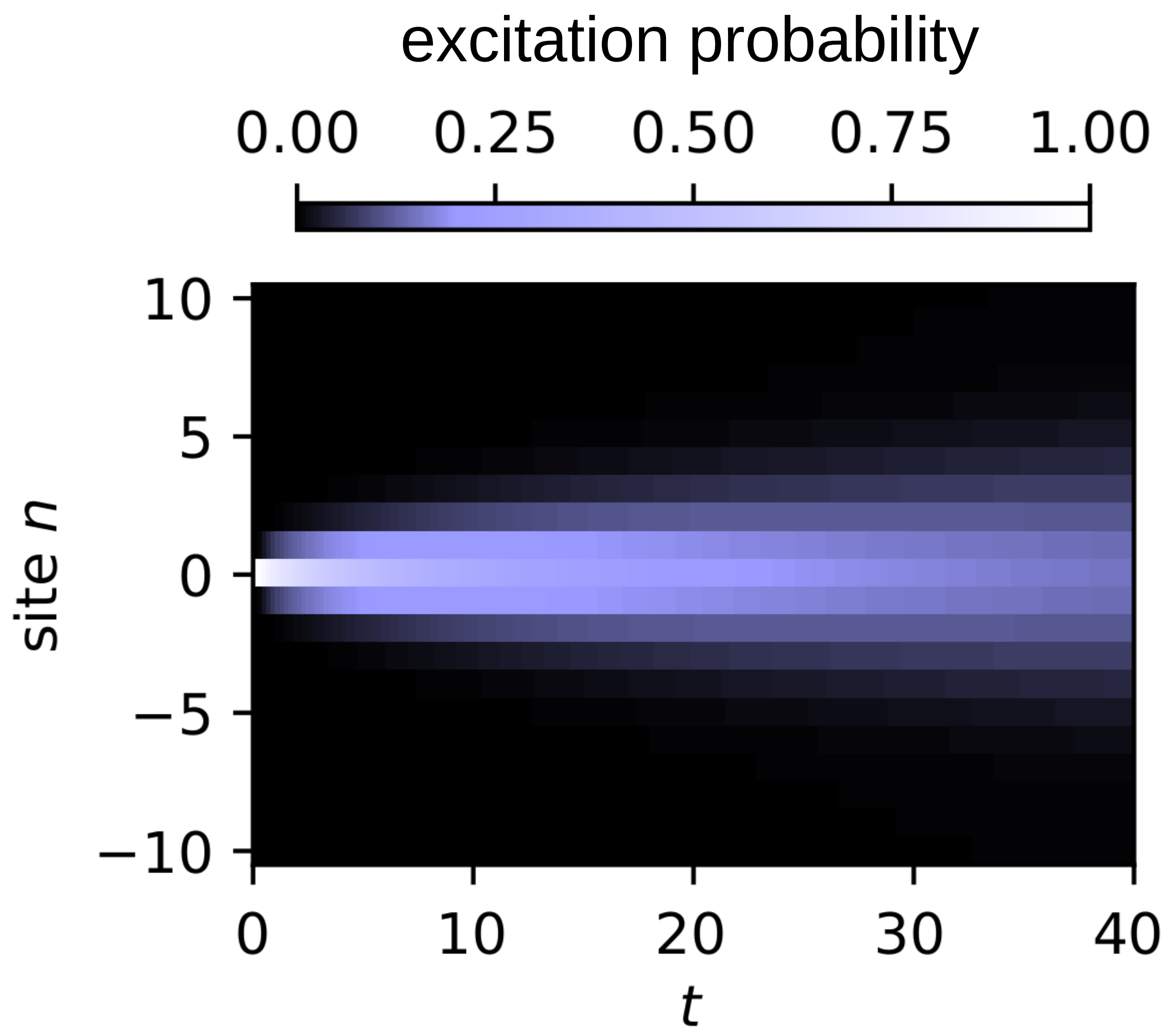
Strongly coupled bosonic environments (at finite temperature):

$$\hat{H}_n^{\mathrm{E}} = \sum_{k=0}^{\infty} \left[\hat{s}_n^z \left(g_{n,k} \hat{b}_{n,k}^\dagger + g_{n,k}^* \hat{b}_k \right) + \omega_{n,k} \hat{b}_{n,k}^\dagger \hat{b}_{n,k} \right]$$

$$J_n(\omega) = \sum_k |g_{n,k}|^2 \delta(\omega - \omega_{n,k}) = 2\alpha\, \omega\, e^{-\frac{\omega^2}{\omega_c^2}}$$

[23] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529 v2 (*in preparation*)

XY Spin Chain with Environments [23]



$\eta = 0.04$

$\alpha = 0.32$

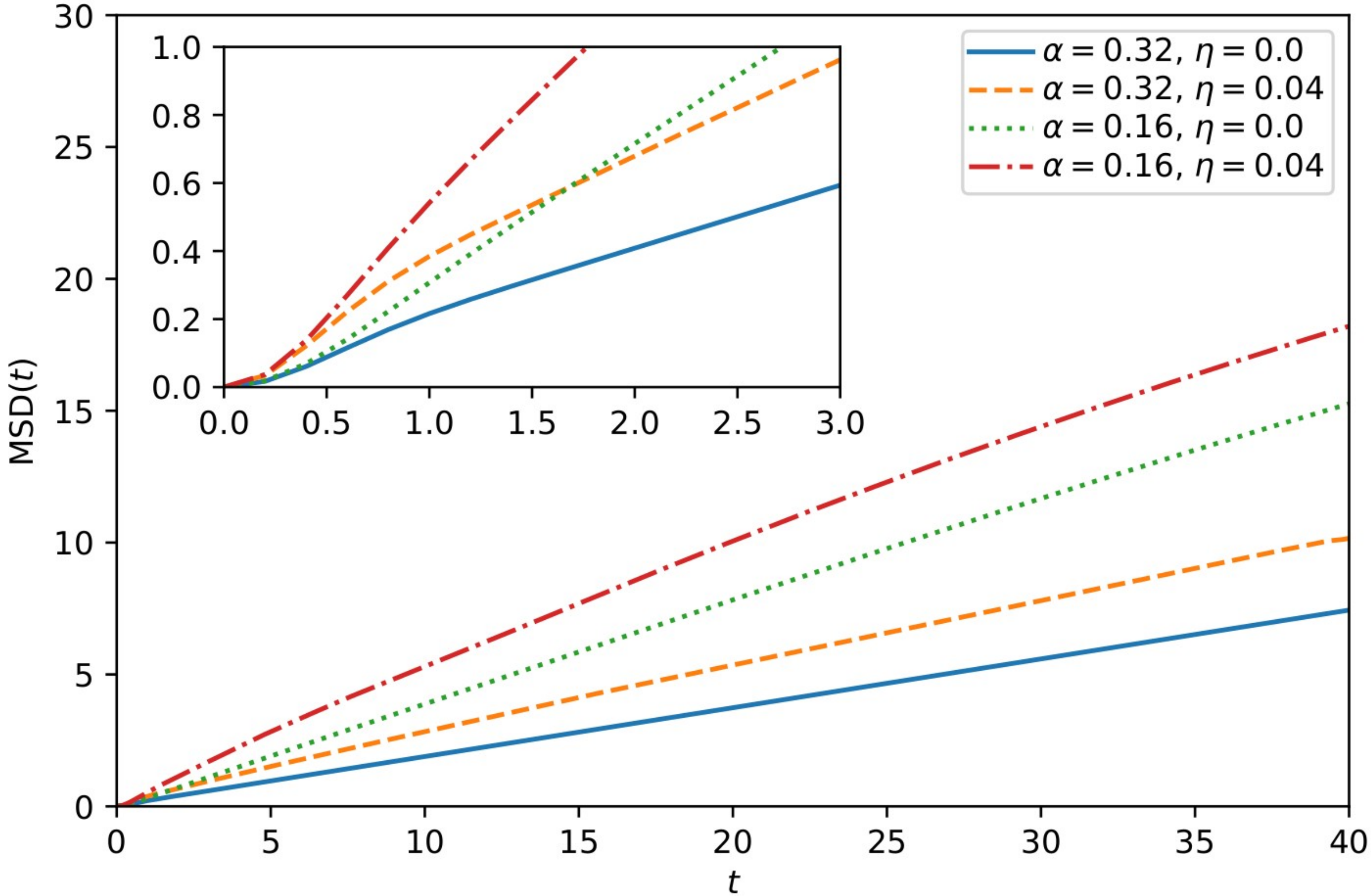
$\omega_c = 4.0$

$T = 1.6$

[23] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529 v2 (*in preparation*)

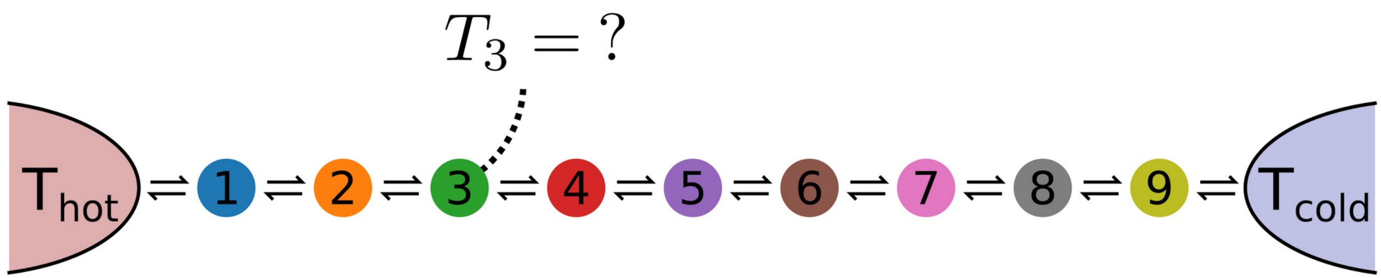
XY Spin Chain with Environments [23]

Mean Squared Displacement: $\mathrm{MSD}(t) = \frac{1}{p_n(t)} \sum_{n=-10}^{10} p_n(t) \times n^2$



[23] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529 v2 (*in preparation*)

XYZ Spin Chain with Thermal Leads [22]



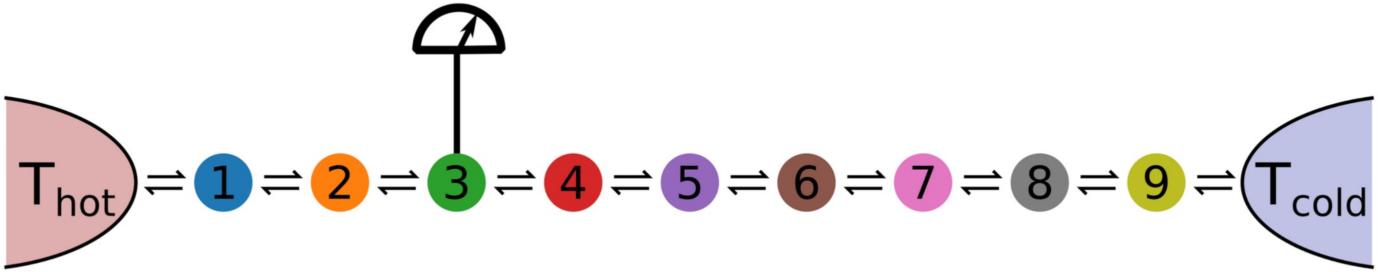
Naive approach:

Compare **reduced state** with **“local” Gibbs state**

$$\tilde{\rho}_{\mathrm{spin3}} \neq \rho^{\mathrm{local}}_{\mathrm{spin3}} = \frac{1}{Z} \exp\left(- \frac{\hat{H}_{\mathrm{spin3}}}{k_B T_3} \right)$$

[22] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529

Fluctuation Dissipation Theorem



Check Fluctuation Dissipation Theorem:

$$S(t) = \frac{1}{2}\langle\{\sigma_z(t), \sigma_z(0)\}\rangle_{\text{ss}}$$

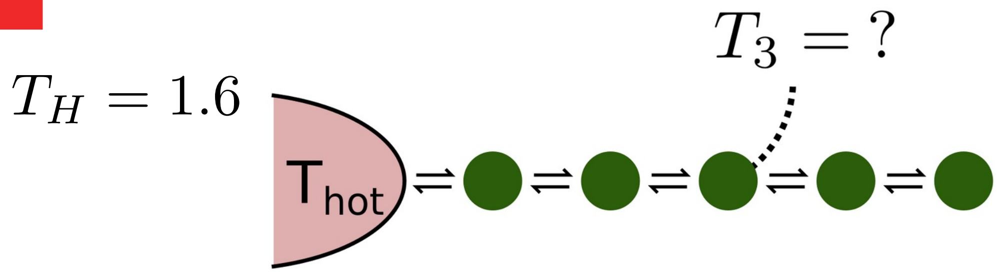
$$\chi(t) = i\Theta(t)\langle[\sigma_z(t), \sigma_z(0)]\rangle_{\text{ss}}$$

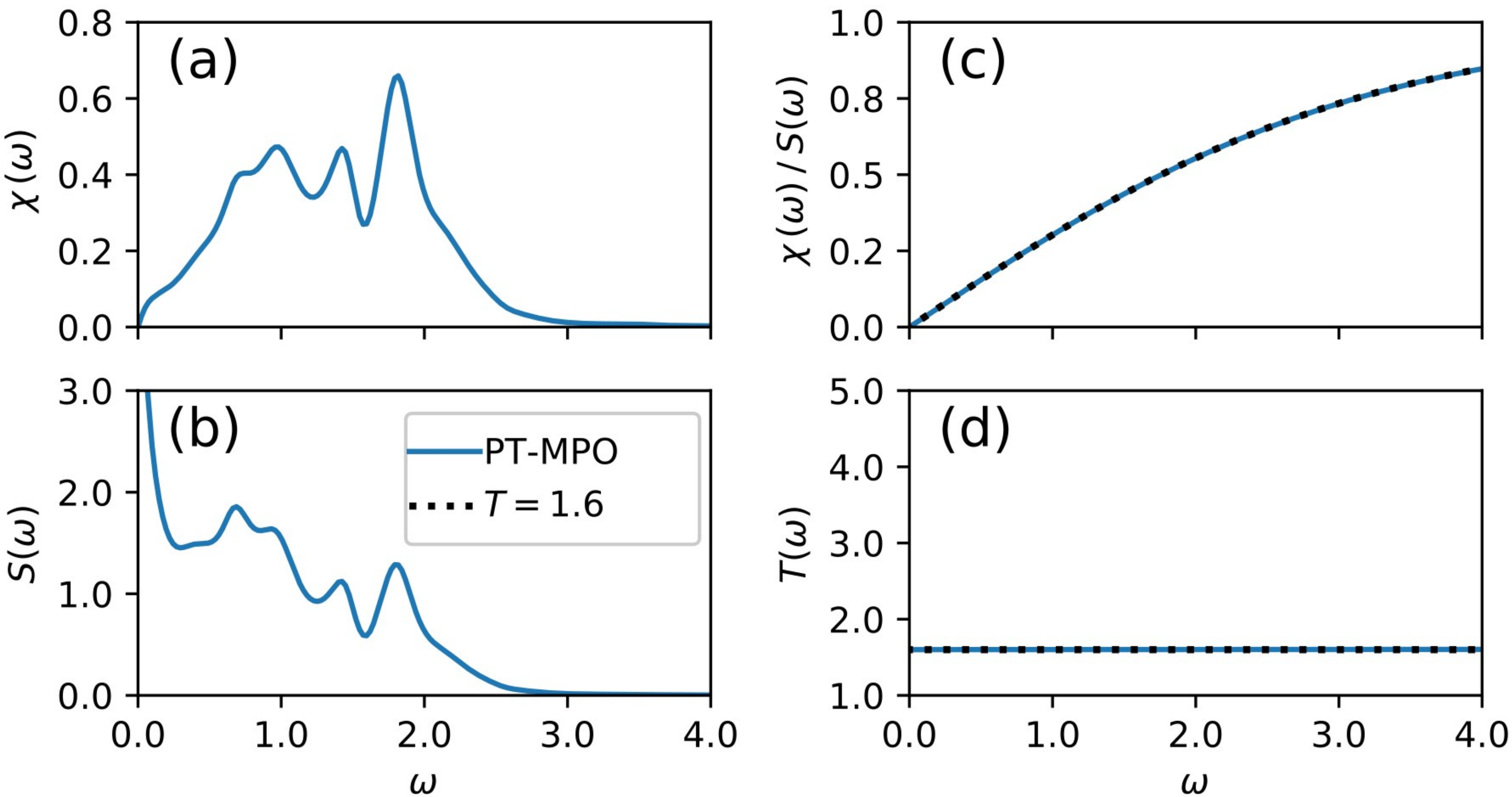
$$\mathrm{Re}\, S(\omega) = \frac{1}{2}\int_{-\infty}^{+\infty} dt\, \langle\{\sigma_z(t), \sigma_z(0)\}\rangle_{\text{ss}} e^{i\omega t}$$

$$\mathrm{Im}\, \chi(\omega) = \int_{-\infty}^{+\infty} dt\, \langle[\sigma_z(t), \sigma_z(0)]\rangle_{\text{ss}} e^{i\omega t}$$

$$\boxed{\frac{\mathrm{Im}\, \chi(\omega)}{\mathrm{Re}\, S(\omega)} = \tanh\left(\frac{\omega}{2T}\right)}$$

Chain with a Single Thermal Lead [22]

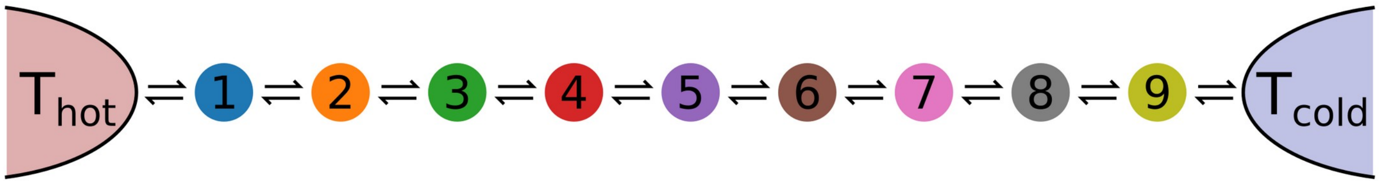


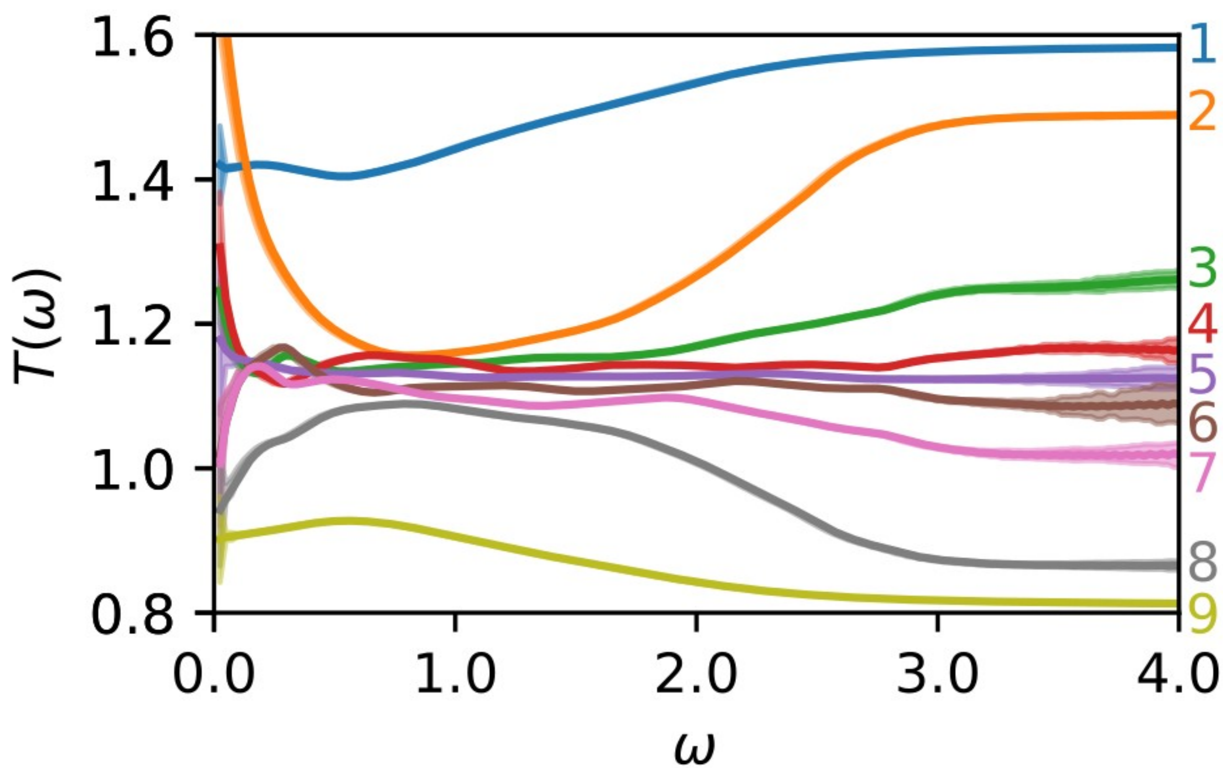


[22] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529

Chain with Thermal Leads [22]

$T_H = 1.6$ $T_C = 0.8$



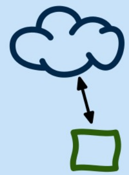


[22] GEF, Kilda, Lovett, Keeling, arXiv:2201.05529

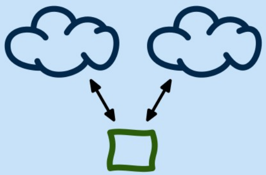
OQuPy

Open Quantum Systems in Python

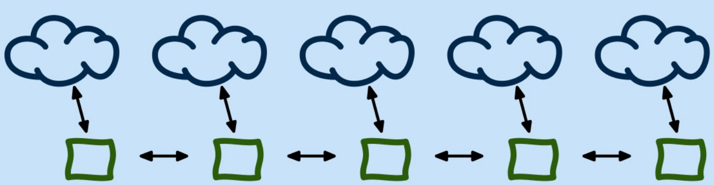
Sys. and Env. Dynamics [1-6]:



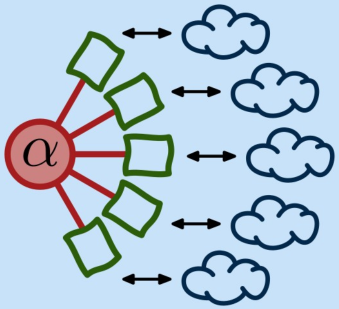
Multiple Environments [7]:



Chain of Open Quantum Systems [8]:



Mean-Field Dynamics [9]:



[1] Strathearn et al. (2017) New J. Phys. 19(9), p.093009.
[2] Strathearn et al. (2018) Nat. Commun. 9, 3322.
[3] Pollock et al. (2018) Phys. Rev. A 97, 012127.
[4] Jørgensen and Pollock (2019) Phys. Rev. Lett. 123, 240602.
[5] Fux et al. (2021) Phys. Rev. Lett. 126, 200401.
[6] Gribben et al. (2021) arXiv:2106.04212.
[7] Gribben et al. (2022) PRX Quantum 3, 10321.
[8] Fux et al. (2022) arXiv:2201.05529.
[9] Fowler-Wright at al. (2021) arXiv:2112.09003.

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OQuPy

Open Quantum Systems in Python

latest

Search docs

INTRODUCTION

Installation

TUTORIALS

Quickstart

Time dependence and PT-TEMPO

Environment Dynamics

⊟ Chains and PT-TEBD

⊞ Example - Heisenberg spin chain

Mean-Field Dynamics

API REFERENCE

API Outline

All Modules

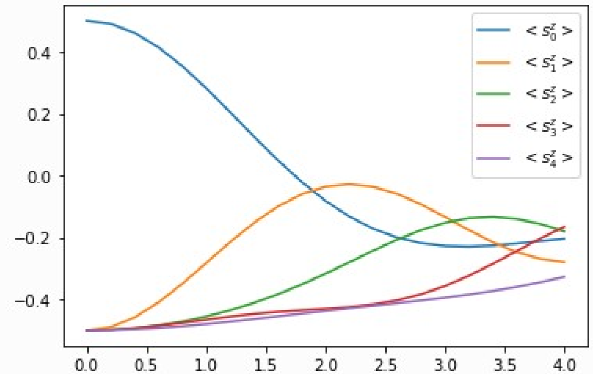
DEVELOPMENT

Contributing

Authors & Acknowledgements

How to Cite this Project

Bibliography



Yay! We can observe how the excitation travels along the chain.

2. Open Heisenberg spin chain

Now, let's add a strongly coupled and structured environment to the chain. We will couple a ohmic bosonic environment to the first spin through the environment Hamiltonian

$$H^E = \sum_k^\infty s_1^y \left(g_k b_k^\dagger + h.c\right) + \omega_k b_k^\dagger b_k \,,$$

where $b_k^{(\dagger)}$ are the bosonic lowering (raising) operators, and s_1^y is the y spin operator of the first site. The coupling constants g_k and frequencies ω_k are determined by the spectral density

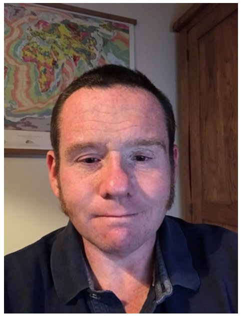
$$J(\omega) = \sum_k^\infty |g_k|^2 \delta(\omega - \omega_k) = 2\alpha\, \omega\, e^{-\frac{\omega}{\omega_c}} \,.$$

We choose the values $\alpha = 0.32$ and $\omega_c = 4.0$, and specify that the bosonic environment is initially at temperature $T = 1.6$.

```
alpha = 0.32
```

Acknowledgements

Jonathan Keeling
(St Andrews)
[PhD Supervisor]



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[PT-TEBD]

Felix Pollock
(formerly Monash)
[Process Tensors]

<u>Major contributions to OQuPy:</u>

Dominic Gribben (Mainz)

Piper Fowler-Wright (St Andrews)

<u>Collaboration on closely related topics:</u>

Paul Eastham (Trinity College Dublin) → optimal control
Eoin Butler (Trinity College Dublin) → optimal control
Dominic Gribben (Mainz) → environment dynamics & long time behaviour
Rosario Fazio (ICTP) → unraveling of many-body quantum trajectories

Summary

quantum (non)-Markovianity

multi-time correlations

many-body q. systems

Process **T**ensor
Matrix **P**roduct **O**perator