Matrix
Product
State

MPS applied to the analysis of open quantum systems

- Methodology and thermalization -

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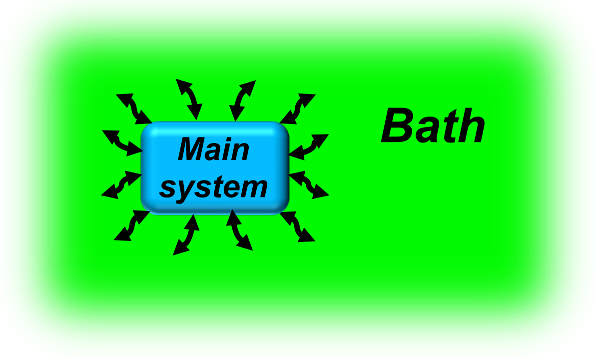
Introduction



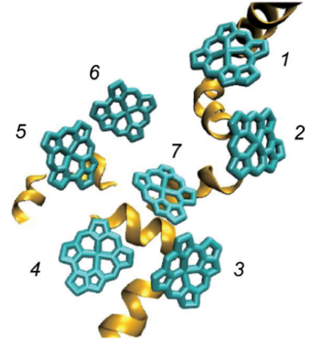
$$\mathcal{H}_{\mathrm{tot}} = \mathcal{H}_S \otimes \mathcal{H}_B$$

Bath effects:
- Fluctuation
- Dissipation
- Decoherence
- Relaxation

How do they affect the main system dynamics?

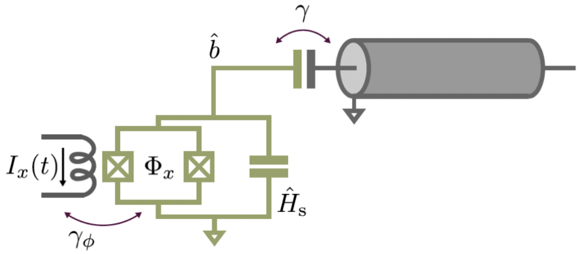
e.g.

Chemical dynamics in a condensed phase



A. Ishizaki and G. R. Fleming, Proc. Natl. Acad. Sci. U.S.A. 106, 17255 (2009)

Superconducting circuits



A. Blais, A. L. Grimsmo, S. M. Girvin, and A. Wallraff Rev. Mod. Phys. 93, 025005 (2020)

- ▶ Model Hamiltonian
- ▶ 2 numerical methods
- ▶ Application: thermalization

Bath oscillator model

$$H = H_S + H_B + H_I$$

$$U_t \equiv e^{-iHt/\hbar}$$

$$H_B = \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2 x_i^2}{2} \right] - E_0$$

Zero-point energy

$$H_I = V_S \otimes \sum_i c_i x_i$$

$$\begin{cases} |\Psi(t)\rangle = U_t |\Psi(0)\rangle \\ \rho(t) = U_t \rho(0) U_t^\dagger \end{cases}$$

- We assume $\rho(0) = \rho_S(0) \otimes \frac{e^{-\beta H_B}}{\mathrm{tr}_B[e^{-\beta H_B}]}$. We want $\rho_S(t) \equiv \mathrm{tr}_B[\rho(t)]$

- Spectral density: $J(\omega) \equiv \frac{\pi}{2} \sum_i \frac{c_i^2}{m_i \omega_i} [\delta(\omega - \omega_i) - \delta(\omega + \omega_i)]$

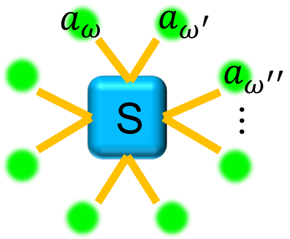
  We assume a *smooth* $J(\omega)$ to describe irreversible behavior

Wave-function approach: TEDOPA

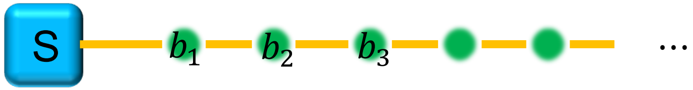
$$H = H_S + H_B + H_I \quad \begin{cases} H_B = \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2 x_i^2}{2}\right] - E_0 \sim \int_0^\Omega d\omega\, \hbar\omega a_\omega^\dagger a_\omega \\ H_I = V_S \otimes \sum_i c_i x_i \sim V_S \otimes \int_0^\Omega d\omega \sqrt{K(\omega)}\, (a_\omega + a_\omega^\dagger) \end{cases}$$

$K(\omega) \propto J(\omega)$ (spectral density)

Star



Mapping!



N-N coupling 1D chain

$$H_B = \sum_{n=1}^{\infty} \left[\hbar\epsilon_n b_n^\dagger b_n + \hbar t_n \left(b_{n+1}^\dagger b_n + b_n^\dagger b_{n+1}\right)\right]$$

$$H_I = V_S \otimes g\left(b_1 + b_1^\dagger\right)$$

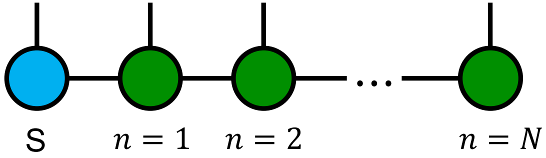
Possible with orthogonal polynomials for $\langle f_1, f_2 \rangle_K \equiv \int_0^\Omega d\omega\, K(\omega) f_1(\omega) f_2(\omega)$!

Alex W. Chin, Ángel Rivas, Susana F. Huelga, and Martin B. Plenio, J. Math. Phys. 51, 092109 (2010)
Javier Prior, Alex W. Chin, Susana F. Huelga, and Martin B. Plenio, Phys. Rev. Lett. 105, 050404 (2010)

Time **E**volving **D**ensity matrix with **O**rthogonal **P**olynomials **A**lgorithm (**TEDOPA**)

More about TEDOPA

$|\Psi(t)\rangle =$



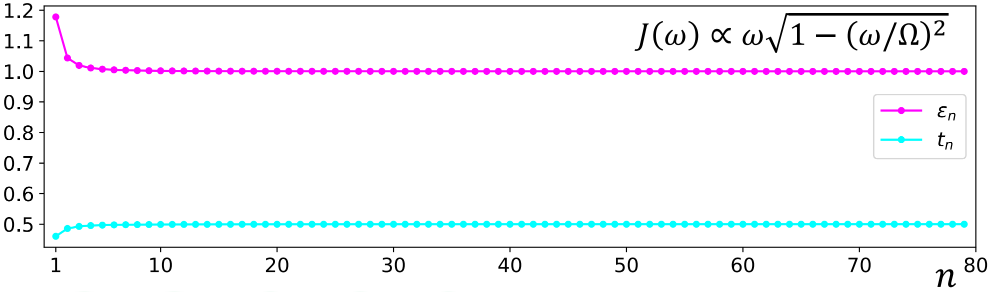
Open source packages are now available!

MPSDynamics.jl

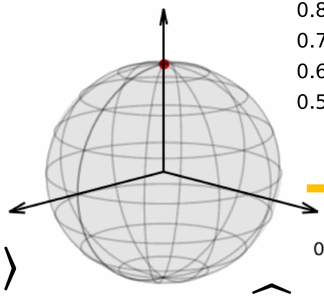
Thibaut Lacroix, Brieuc Le Dé, Angela Riva, Angus J. Dunnett, and Alex W. Chin, J. Chem. Phys. 161, 084116 (2024)

For "a wide class" of $J(\omega)$ …

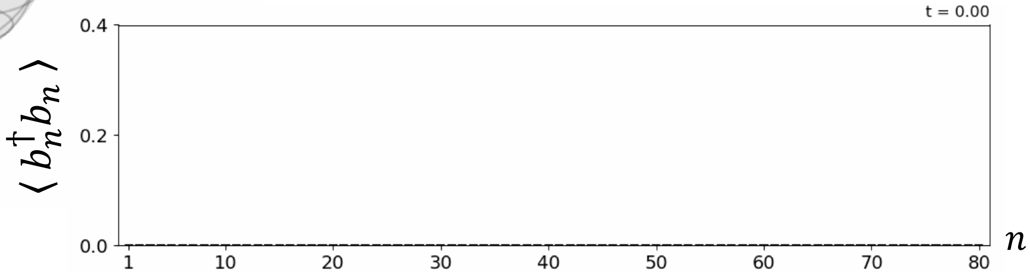
$$\epsilon_n,\ t_n \xrightarrow{n\to\infty} \text{constant}$$



e.g. Qubit system ($\beta = \infty$)



$$|\Psi(0)\rangle = |\uparrow\rangle \otimes |0_\omega 0_{\omega'} \cdots\rangle$$
$$= |\uparrow\rangle \otimes |0_{n=1} 0_{n=2} \cdots\rangle$$



Infinitely long recurrence time

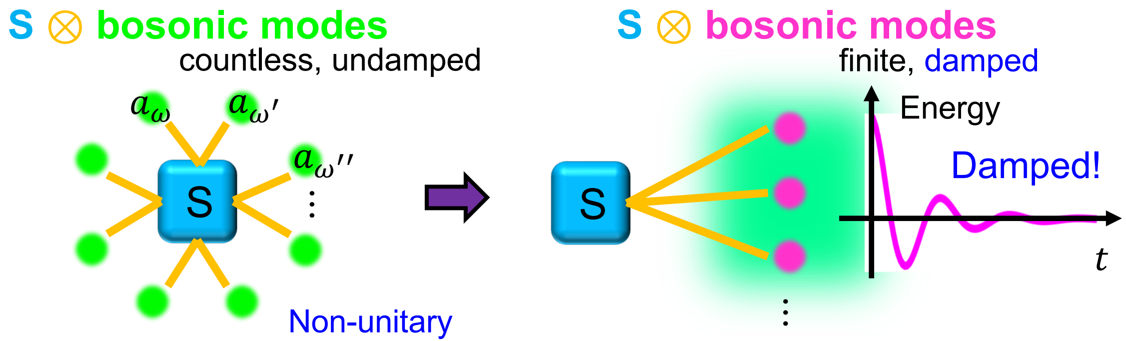
$\Rightarrow$ Irreversible loss!

Auxiliary mode approach: pseudomode / HEOM

Basic ideas

$$\mathcal{H}' = \mathcal{H}_S \otimes \mathcal{H}_{\text{aux}}$$

$$\mathcal{H}_{\text{aux}} = \mathcal{H}_{\text{aux},1} \otimes \mathcal{H}_{\text{aux},2} \cdots$$



Non-unitary

$$\frac{d}{dt}\rho'(t) = -\frac{i}{\hbar}[H_{S+\text{aux}}, \rho'(t)] + \mathcal{D}\rho'(t) \equiv \mathbb{L}\rho'(t)$$

Pseudomode

B. M. Garraway, Phys. Rev. A 55, 2290 (1997)
D. Tamascelli, et al., Phys. Rev. Lett. 120, 030402 (2018)

Hierarchical Equations Of Motion (HEOM)

Y. Tanimura and R. Kugo, J. Phys. Soc. Japan. 58, 101 (1989)
Meng Xu, et al., arXiv:2307.16790 [quant-ph]

Properties

- $\rho_S(t) = \mathrm{tr}_{\text{aux}}[\rho'(t)]$
- $\lambda \in \mathrm{spec}(\mathbb{L})$ has a real part $(\mathrm{Re}\lambda \le 0) \Rightarrow$ Existence of a steady state

Unlike TEDOPA, where a part of the chain keeps evolving

Why MPS?

A large number of modes are required for complex spectral densities

Q. Shi, Y. Xu, Y. Yan, M. Xu, J. Chem. Phys. 148, 174102 (2018)
R. Borrelli, J. Chem. Phys. 150, 234102 (2019)

Thermalization?

Evolution of the total state: $\rho(t) = U_t \left\{ \rho_S(0) \otimes \frac{e^{-\beta H_B}}{\mathrm{tr}_B[e^{-\beta H_B}]} \right\} U_t^\dagger$ $\quad U_t = e^{-iHt/\hbar}$

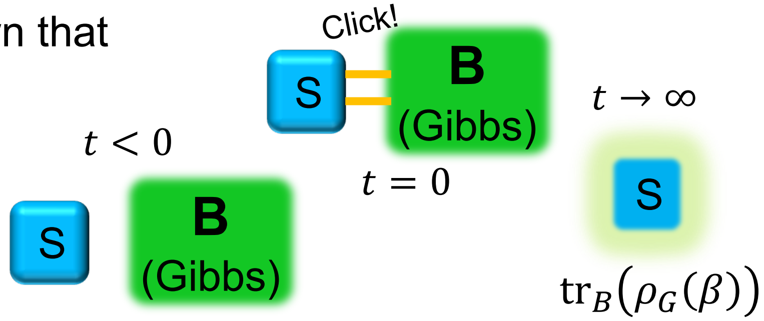
$\rho(t)$ in the long time limit?

According to **pseudomode / HEOM**, it is empirically known that

Y. Tanimura, J. Chem. Phys. 141, 044114 (2014)

$$\lim_{t\to\infty} \mathrm{tr}_B[\rho(t)] = \mathrm{tr}_B\left[\frac{e^{-\beta H}}{\mathrm{tr}[e^{-\beta H}]}\right] \quad \equiv \rho_G(\beta)$$

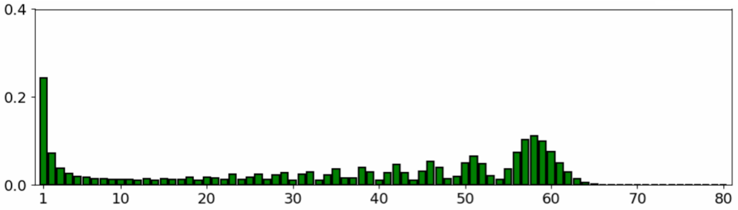
(independent of $\rho_S(0)$)



Thermalization!

However, it doesn't mean $\lim_{t\to\infty} \rho(t) = \rho_G(\beta)$.

According to **TEDOPA**, the wave function keeps evolving



How are these reconciled?

Thermalization with TEDOPA ①

TEDOPA cannot describe thermalization?

Harmonic oscillator: $H_S = \frac{p^2}{2} + \frac{q^2}{2} + \lambda q^2,\ V_S = q$

Analytic expressions are known;

$$\langle \mathcal{O} \rangle_{\mathrm{Gibbs}} = \mathrm{tr}[\mathcal{O}\rho_G(\beta)]$$

$$C_{\mathcal{O}}^{\mathrm{Gibbs}}(t) = \mathrm{tr}\left[e^{iHt}\mathcal{O}e^{-iHt}\mathcal{O}\rho_G(\beta)\right]$$

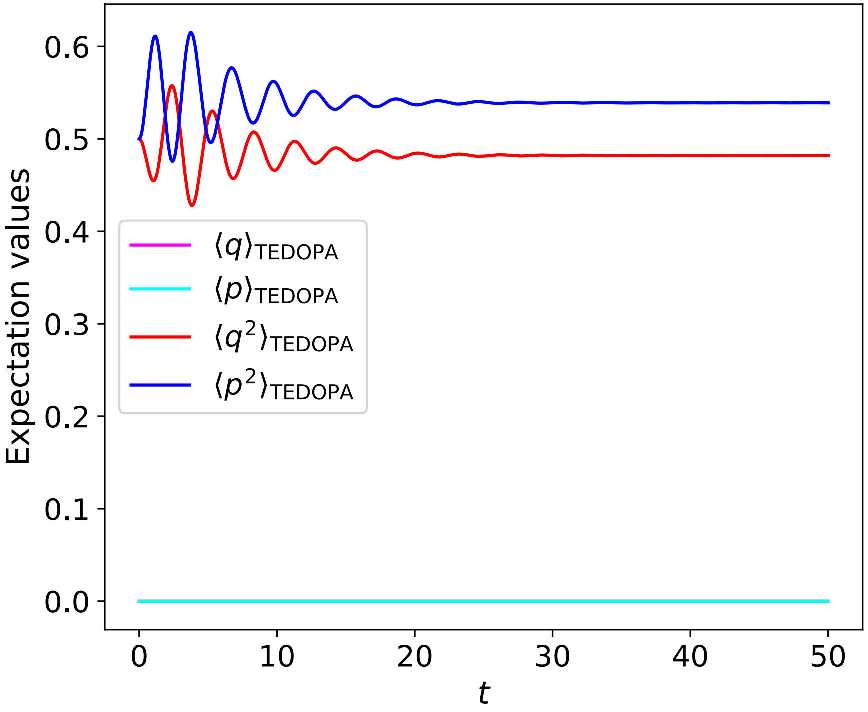
$\mathcal{O}$: system operator

H. Grabert, P. Schramm, G-L Ingold, Physics Reports 168, 115 (1988)

$\mathcal{O}$	$\langle \mathcal{O} \rangle_{\mathrm{Gibbs}}$	$\langle \mathcal{O} \rangle_{\mathrm{TEDOPA}}$
$\boldsymbol{q}$	0	$\sim 10^{-6}$
$\boldsymbol{p}$	0	$\sim 10^{-6}$
$\boldsymbol{q}^2$	0.48199	0.48198
$\boldsymbol{p}^2$	0.53903	0.53905

Good agreement!

$\beta = \infty$ and $|\Psi(0)\rangle = |0\rangle \otimes |00\cdots\rangle$



Thermalization with TEDOPA ②

TEDOPA cannot describe thermalization?

Harmonic oscillator: $H_S = \frac{p^2}{2} + \frac{q^2}{2} + \lambda q^2$, $V_S = q$

$$C_{\mathcal{O}}^{\mathrm{Gibbs}}(t) = \mathrm{tr}\left(e^{iHt}\mathcal{O}e^{-iHt}\mathcal{O}\rho_G(\beta)\right)$$

H. Grabert, P. Schramm, G-L Ingold, Physics Reports 168, 115 (1988)

Compute the asymptotic state

$$|\Phi\rangle = e^{-iHt_f/\hbar}|\Psi(0)\rangle$$

and then

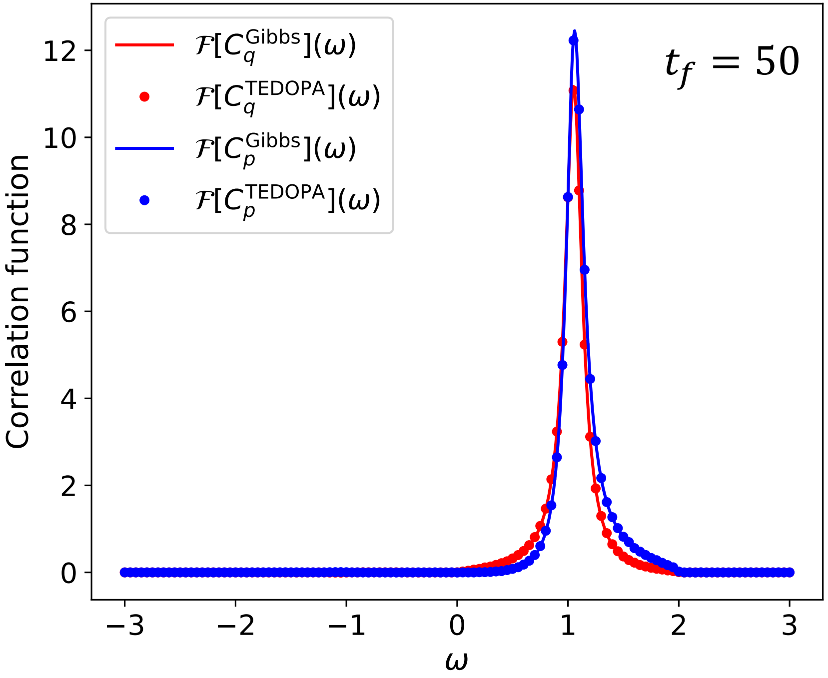
$$C_{\mathcal{O}}^{\mathrm{TEDOPA}}(t) = \mathrm{tr}\left(e^{iHt}\mathcal{O}e^{-iHt}\mathcal{O}|\Phi\rangle\langle\Phi|\right)$$
$$= \langle\Phi(t)|\mathcal{O}|\Phi_{\mathcal{O}}(t)\rangle$$

with

$$|\Phi(t)\rangle = e^{-iHt/\hbar}|\Phi\rangle$$
$$|\Phi_{\mathcal{O}}(t)\rangle = e^{-iHt/\hbar}\mathcal{O}|\Phi\rangle$$

Fourier transform $\mathcal{F}[C_{\mathcal{O}}](\omega) = \int_{-\infty}^{\infty} dt\, C_{\mathcal{O}}(t)e^{i\omega t} \in \mathbb{R}$

$\beta = \infty$ and $|\Psi(0)\rangle = |0\rangle \otimes |00\cdots\rangle$

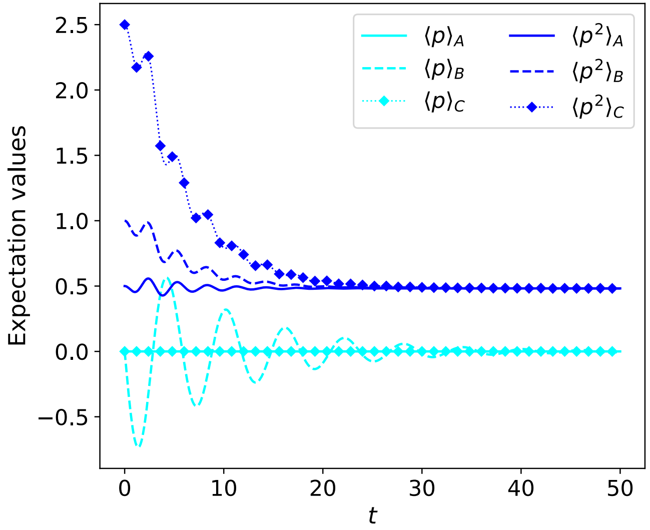


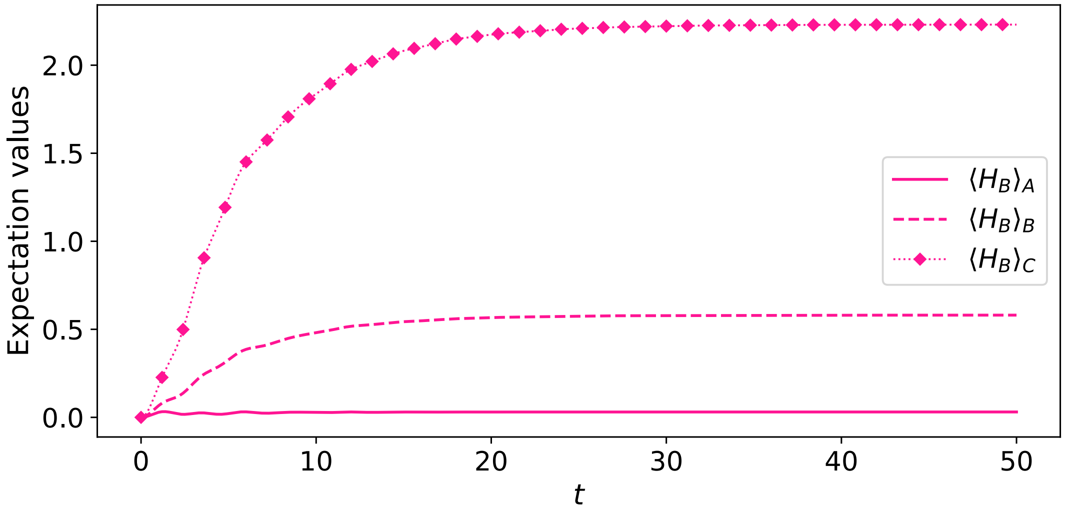
⇨ Thermalization occurs!

Thermal equilibrium state"s"

What about $\rho_S(0)$-dependence?

$$|\Psi_A(0)\rangle = |0\rangle \otimes |00\cdots\rangle \qquad |\Psi_B(0)\rangle = \frac{(|0\rangle + |1\rangle)}{\sqrt{2}} \otimes |00\cdots\rangle \qquad |\Psi_C(0)\rangle = |2\rangle \otimes |00\cdots\rangle$$





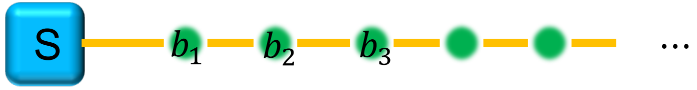
Resulting in different total states!

These can all be considered thermal equilibrium states, just like the Gibbs state!

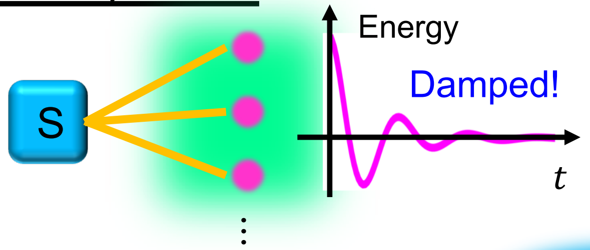
Summary

$$H = H_S + \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2 x_i^2}{2} \right] + V_S \otimes \sum_i c_i x_i$$

TEDOPA



Pseudomode, HEOM



✓ Thermalization of an open system

E. Leviatan, et al., arXiv:1702.08894 [cond-mat.stat-mech]
S. Goto and I. Danshita, Phys. Rev. B 99, 054307 (2019)

❖ Quantum thermodynamics

- 2nd law
  S. Sakamoto and Y. Tanimura, J. Chem. Phys. 153, 234107 (2020)
  S. Koyanagi and Y. Tanimura, J. Chem. Phys. 157, 014104 (2022)
- Thermodynamic relations
  S. Koyanagi and Y. Tanimura, J. Chem. Phys. 160, 234112 (2024)