QuTiP:
Applications from quantum technology and quantum biology

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Resources: https://arxiv.org/abs/2412.04705, Lambert at al., v5 review.
www.qutip.org
https://qutip2024.wordpress.com/ v5 release developer's conference
https://github.com/nwlambert/AutumnSchool/ Python code and more details adapted from here

QuTiP development recently supported by:

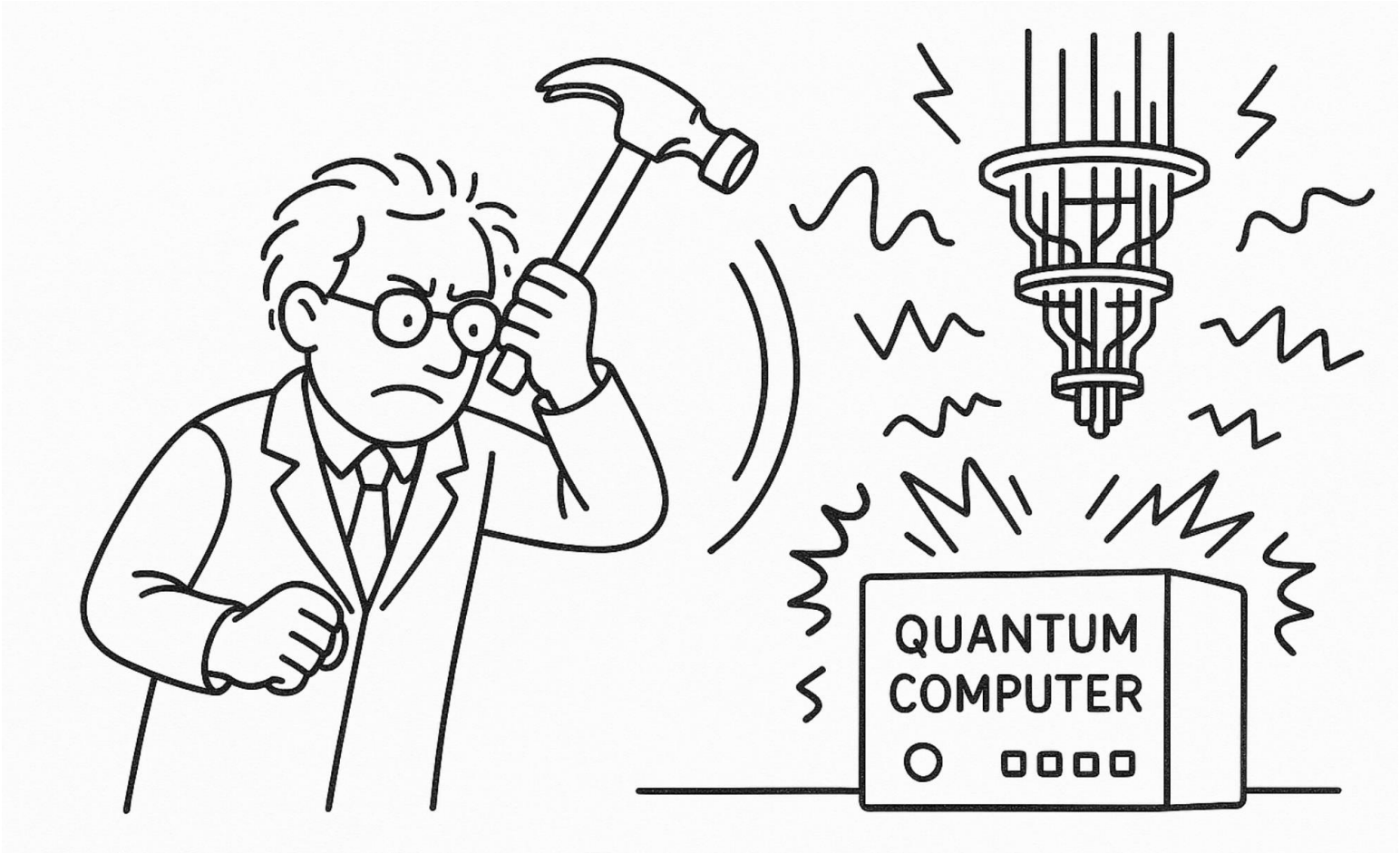
Here begins our new MIRAI
MOONSHOT
RESEARCH & DEVELOPMENT PROGRAM

RIKEN

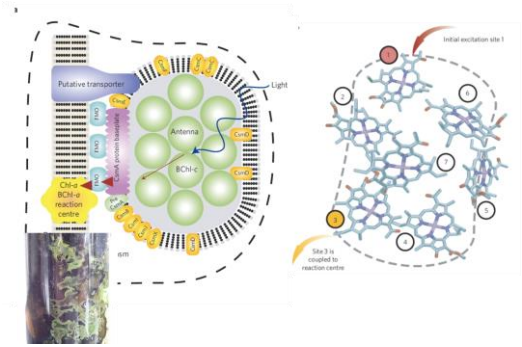
INSTITUT QUANTIQUE
UNIVERSITÉ DE SHERBROOKE

Google Summer of Code

Part 3: non-Markovian methods continued with input-output HEOM and pseudomodes + some additional QuTiP features with ENR states and more…

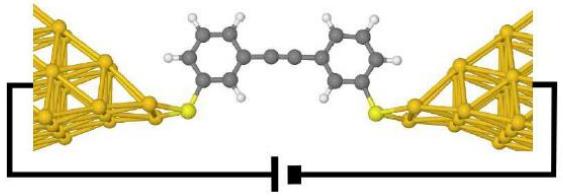


Certain systems exist in a difficult regime where system energies, bath energies, and coupling strengths all coincide: **no perturbative parameter**



Physical Chemistry: E.g., Energy transfer in photosynthetic complexes:

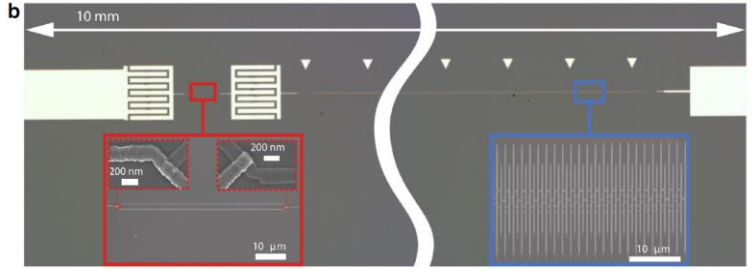
Electrical excitations strongly couple to nuclear motion, thermal energy is on the same order as reorganization energy, electronic coupling, etc.



C. Schinabeck, PhD. thesis 2019

Quantum dots, molecular electronics:

electronic levels can strongly couple to vibrational modes and macroscopic leads.



Circuit/waveguide quantum electro-dynamics (QED):
open transmission lines, SQUID arrays, meta-materials can directly realize engineered quantum environments.

E.g., Martinez et al., NPJ QI 2019, Kuzmin et al. NPJ QI 2019, L. Magazzù et al., Nat. Comms 2018

Part 3: non-Markovian methods continued, ENR states, optimal control, and other features

- **A few more comments on noise with driven systems, HEOM and Bloch-Redfield master equations**

- More applications of non-Markovian noise:
  - Dynamical decoupling of noise
  - Extending the HEOM (input output HEOM)
  - Pseudomodes for dissipative state engineering
  - Fermions

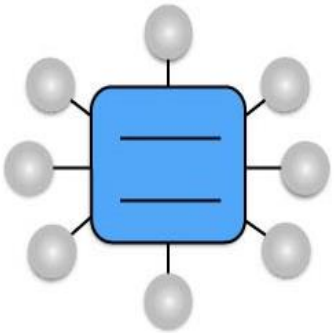
- Hidden QuTiP features that might be useful for you
  - ENR states
  - Optimal control libraries

- Conclusion and summary

Spin-boson model

- **A quick recap,** we argued that noise can be derived from a bosonic bath model, and simulated approximately (lindblad) or with some more exact methods (HEOM)

$$H_{\mathrm{SB}} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k g_k(a_k + a_k^\dagger)$$



Environment characterized by spectral density and temperature, which gives correlation functions or power spectrum

$$J(\omega) = \pi \sum_k |g_k|^2 \, \delta(\omega - \omega_k).$$

$$X = \sum_k g_k(a_k + a_k^\dagger).$$

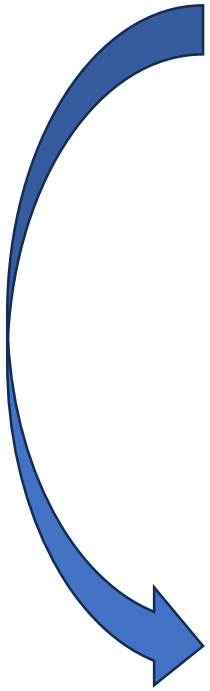
$$C(\tau) = \langle \bar{X}(t+\tau)\bar{X}(t) \rangle = \int_0^\infty d\omega \frac{J(\omega)}{\pi} [\coth(\beta\omega/2)\cos(\omega\tau) - i\sin(\omega\tau)]$$

$$S(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t \, C(t) \, \mathrm{e}^{\mathrm{i}\omega t},$$

$\beta = k_B T$

Hierarchical equations of motion

$$H_{\mathrm{SB}} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k \frac{g_k}{\sqrt{2\omega_k}}(a_k + a_k^\dagger)$$



$$\frac{\partial}{\partial t}\tilde{\rho}(t) = -i[\tilde{H}_I(t), \tilde{\rho}(t)]$$

$$\tilde{\rho}(t) = \rho(0) - i\int_0^t ds[\tilde{H}_I(s), \tilde{\rho}(s)]$$

$$\frac{\partial}{\partial t}\tilde{\rho}_S(t) = -i\mathrm{Tr}_E[\tilde{H}_I(t), \tilde{\rho}(0)] - \int_0^t ds\mathrm{Tr}_E[\tilde{H}_I(t), [\tilde{H}_I(s), \tilde{\rho}(s)]$$

Lindblad equation: Bloch-Redfield form

With a bit more work (!) one can arrive at something like

For eigenstates $|\psi_j\rangle$ of H_S, and $c_{j,l} = \langle\psi_j|\sigma_z|\psi_l\rangle$ $\Delta_{j,l} = E_j - E_l$ is the difference in eigenenergies.

$$\frac{\partial}{\partial t}\rho_S(t) = -i[H_S, \rho(t)]$$

$$+\sum_{j>l,l} \pi J(\Delta_{j,l})|c_{j,l}|^2 \left(n(\Delta_{j,l})+1\right)\left[2|\psi_l\rangle\langle\psi_j|\rho_S(t)|\psi_j\rangle\langle\psi_l| - \{|\psi_j\rangle\langle\psi_j|, \rho_S\}\right]$$

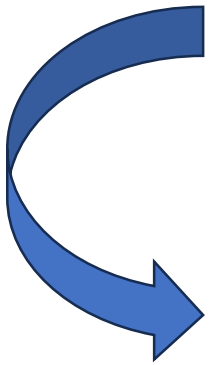
$$+\sum_{j>l,l} \pi J(\Delta_{j,l})|c_{j,l}|^2 n(\Delta_{j,l})\left[2|\psi_j\rangle\langle\psi_l|\rho_S(t)|\psi_l\rangle\langle\psi_j| - \{|\psi_l\rangle\langle\psi_l|, \rho_S\}\right]$$

The first part is the coherent system evolution, the second part describes spontaneous and stimulated emission, and the third part describes absorption. $n(\omega) = (e^{\omega/T}-1)^{-1}$

Hierarchical equations of motion

$$H_{\mathrm{SB}} = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k \frac{g_k}{\sqrt{2\omega_k}}(a_k + a_k^\dagger)$$

Keep repeating this process, arrive at Dyson series.



$$\tilde{\rho}(t) = \rho(0) - i\int_0^t ds[\tilde{H}_I(s), \tilde{\rho}(s)]$$

$$\frac{\partial}{\partial t}\tilde{\rho}_S(t) = -i\mathrm{Tr}_E[\tilde{H}_I(t), \tilde{\rho}(0)] - \int_0^t ds\mathrm{Tr}_E[\tilde{H}_I(t), [\tilde{H}_I(s), \tilde{\rho}(s)]$$

Hierarchical equations of motion

Dyson series contains higher-order products of bath operators:
Gaussian bath, so we can re-sum these and find Feynman-Vernon
Influence functional:

$$\bar{\rho}_{\mathrm{S}}(t) = \mathcal{T} \exp\left\{ -\int_0^t dt_2 \int_0^{t_2} dt_1 Q^{\times}(t_2) \left[C_R(t_2 - t_1) Q(t_1)^{\times} + i C_I(t_2 - t_1) Q^{o}(t_1) \right] \right\} \bar{\rho}_{\mathrm{S}}(0)$$

$A^{\times}B \equiv [A, B]$ and $A^{\circ}B = \{A, B\}$.

The HEOM!

$$\bar{\rho}_{\rm S}(t) = \mathcal{T} \exp\left\{ -\int_0^t dt_2 \int_0^{t_2} dt_1 Q^{\times}(t_2) \left[C_R(t_2 - t_1) Q(t_1)^{\times} + i C_I(t_2 - t_1) Q^{o}(t_1) \right] \right\} \bar{\rho}_{\rm S}(0)$$

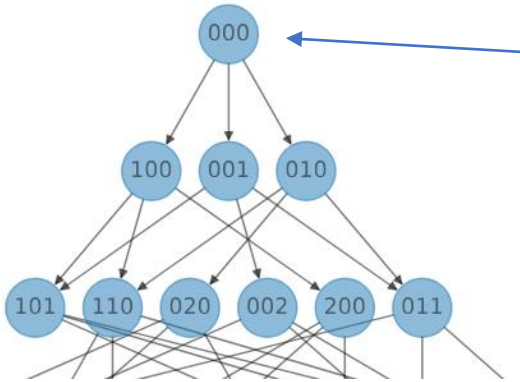
The HEOM assumes that the **correlation functions can be expressed as a sum of exponentials** (with complex parameters):

$$C(t) = C_R(t) + \mathrm{i} C_I(t), \qquad C_{R,I}(t) = \sum_{k=1}^{N_{R,I}} c_k^{R,I} \exp[-\nu_k^{R,I} t]$$

$n = \{n_1, n_2, .. n_m, \ldots, n_M\}$: it contains M indices, 0 to M, a cut-off in the number of exponentials.

$n_{jk} \in \{0..N_c\}$, and N_c is a cut-off parameter

$$\dot{\rho}^{n}(t) = \left(\mathcal{L} - \sum_{j=\mathrm{R,I}} \sum_{k=1}^{N_j} n_{jk} \gamma_k^j \right) \rho^{n}(t)$$
$$- \mathrm{i} \sum_{k=1}^{N_{\mathrm{R}}} c_k^{\mathrm{R}} n_{\mathrm{R}k} Q^{\times} \rho^{n_{\mathrm{R}k}^{-}}(t) + \sum_{k=1}^{N_{\mathrm{I}}} c_k^{\mathrm{I}} n_{\mathrm{I}k} Q^{\circ} \rho^{n_{\mathrm{I}k}^{-}}(t)$$
$$- \mathrm{i} \sum_{j=\mathrm{R,I}} \sum_{k=1}^{N_j} Q^{\times} \rho^{n_{jk}^{+}}(t)$$



$\rho_S(t)$

Driven dissipative example 1: weak driving

Time-dependent systems: Consider a standard example of a driven qubit with the time-dependent Hamiltonian

$$H = \frac{\Delta}{2}\sigma_z + \frac{A}{2}\sin(\omega_d t)\sigma_x ,$$

We also include dissipation with rate γ and zero temperature

Call Lindblad master equation with either just lists or QobjEvo()

```
# --- mesolve ---

c_ops_me = [np.sqrt(gamma) * qt.sigmam()]
me_result = qt.mesolve(H, psi0, tlist, c_ops=c_ops_me, e_ops=e_ops)
```

He we phenomenologically added a ‘collapse operator’ that is just the sigma_- operator: this happens to work out since the **driving amplitude was small compared to the energy splitting**

Driven dissipative example 1: weak driving

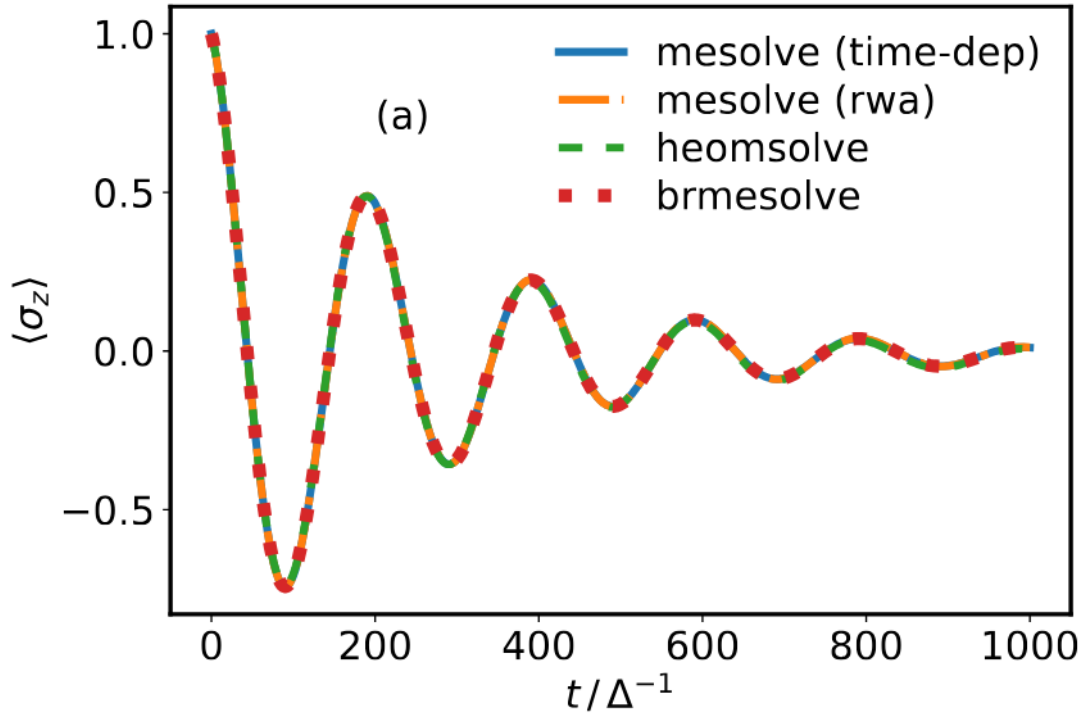
Time-dependent systems: Consider a standard example of a driven qubit with the time-dependent Hamiltonian

$$H = \frac{\Delta}{2}\sigma_z + \frac{A}{2}\sin(\omega_d t)\sigma_x$$

We also include dissipation with rate γ, and zero temperature

$$(A = 0.01\Delta)$$

$$\gamma = 0.005\Delta/(2\pi)$$



All 3 solvers align here:

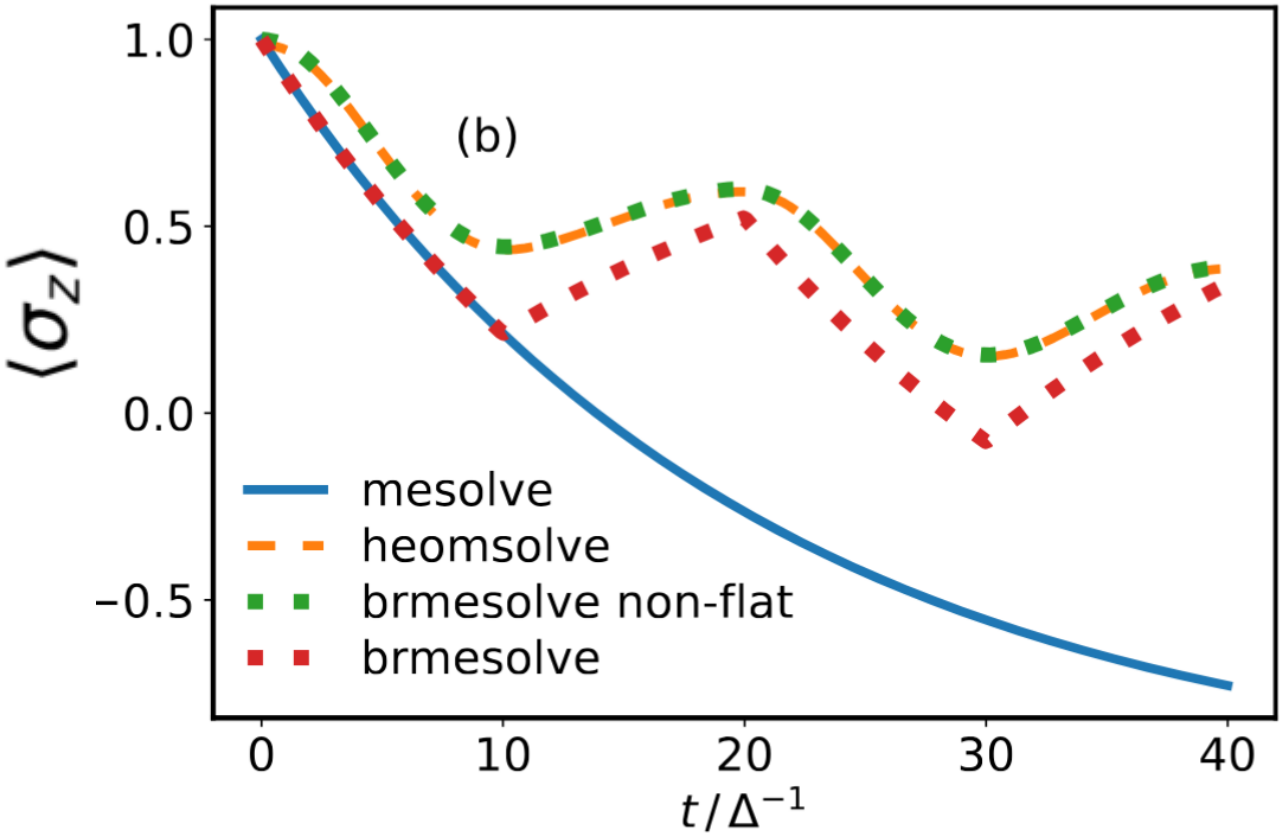
Bath power spectrum is weak and broad (Markovian)

Drive is weak amplitude and resonant

Driven dissipative example 1: ‘strong’ driving

Time-dependent systems: A second example, to illustrate where using naive local-basis collapse operators can fail, is that of a single qubit whose energies are switched between positive and negative values,

$$H = \frac{\Delta}{2}\sin(\omega_d t)\sigma_z\,. \qquad \omega_d = 0.05\Delta \qquad \gamma = 0.05\Delta/(2\pi).$$



Local operators Lindblad is insensitive to large changes in the energy of the system so fails

Brmesolve() diagonalizes the system H at each time step and constructs new collapse operators (numerically challenging)

Here HEOM and brmesolve align well, particularly if we explicitly use the ‘approximately flat’ power spectrum in both

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- More applications of non-Markovian noise:
  - **Dynamical decoupling of noise**
  - Extending the HEOM (input output HEOM)
  - Pseudomodes for dissipative state engineering
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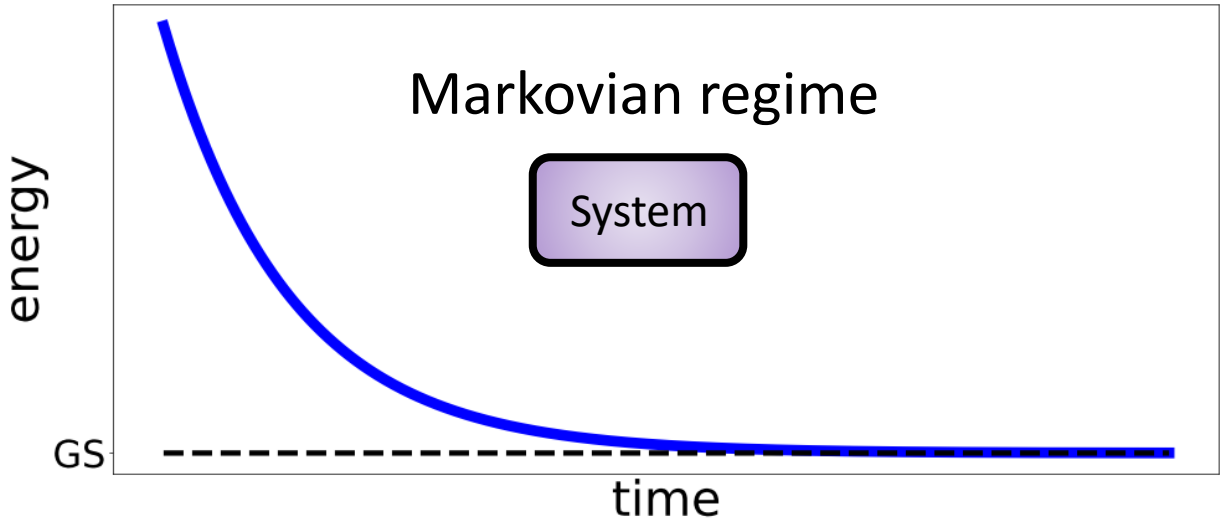
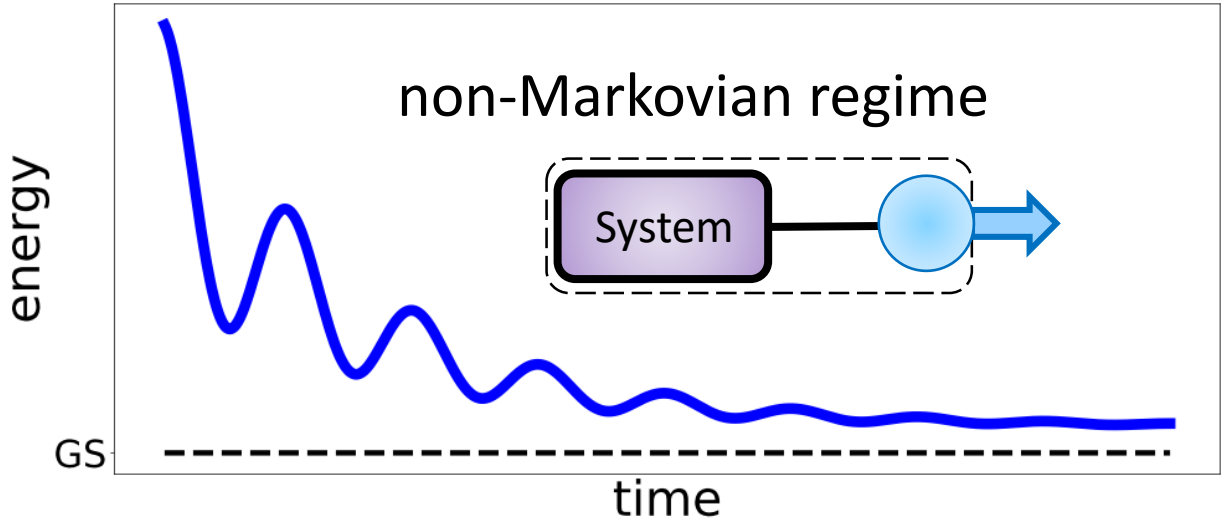
Dynamical decoupling of noise

In the Markovian limit noise tends to affect the system monotonically; it depletes populations/energies and coherence irreversibly

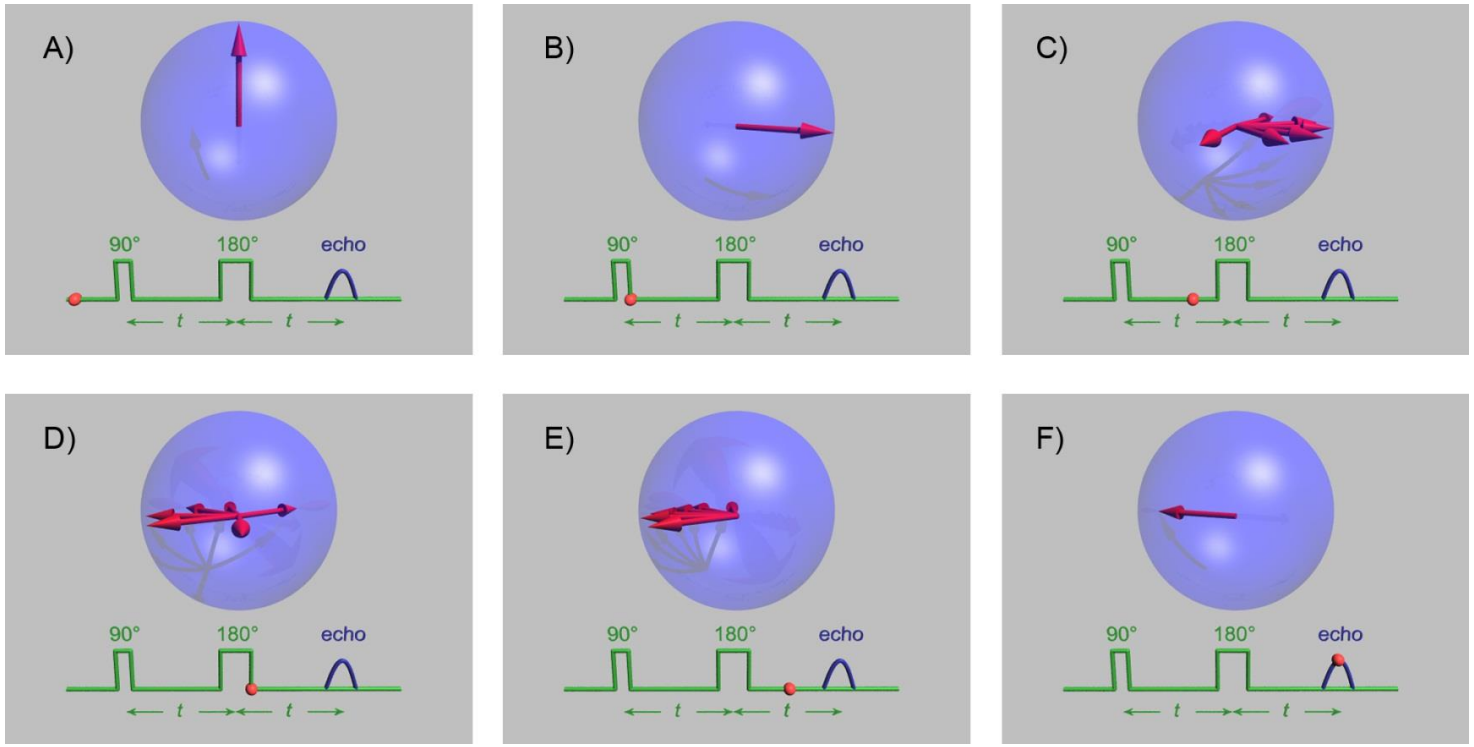
In the non-Markovian case all these things can ‘come back’ for a while (and in the extreme limit of a dissipation-less single mode, continue for ever)





Dynamical decoupling of noise

Dynamical decoupling relies on the idea that we can periodically manipulate the system so that coherence lost in the previous period is regained in the next:

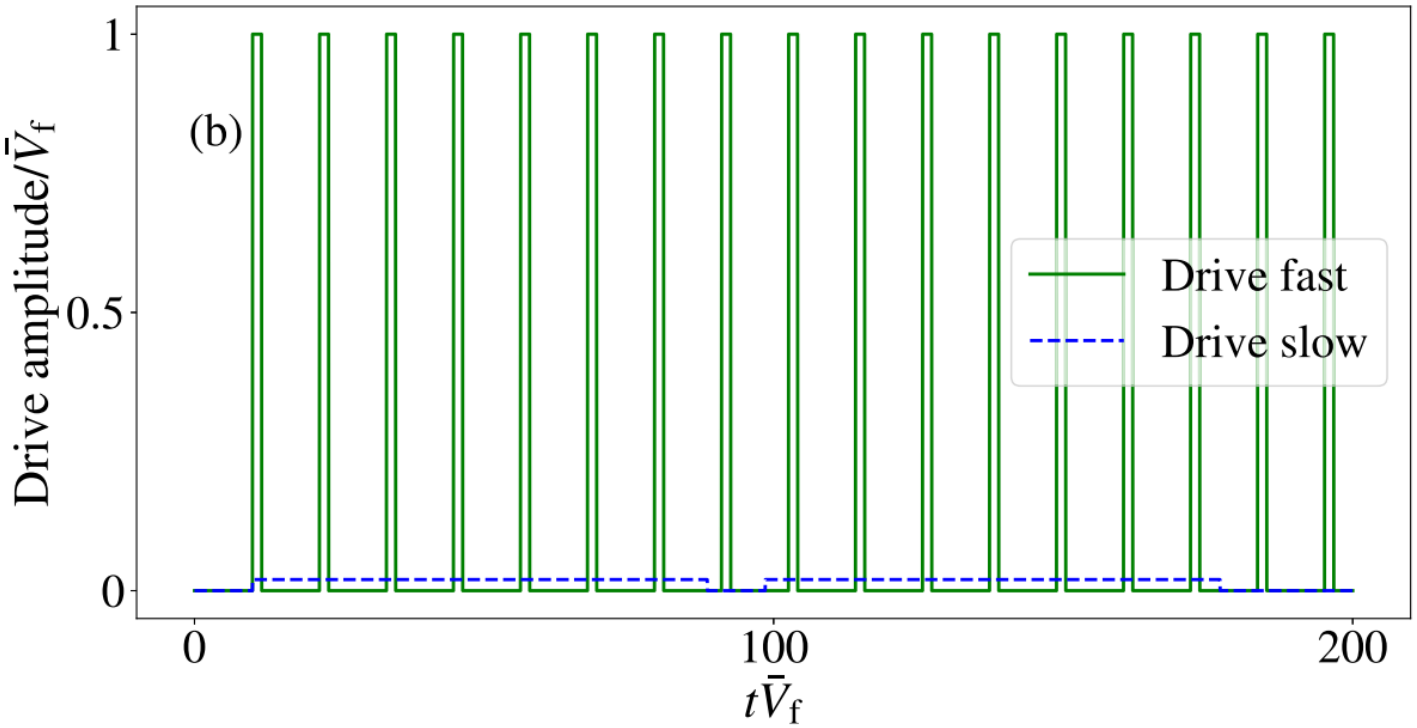


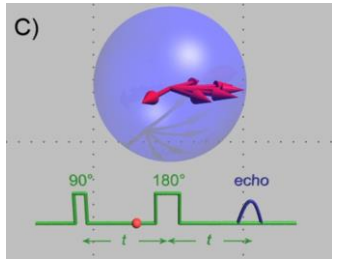
From Wikipedia!

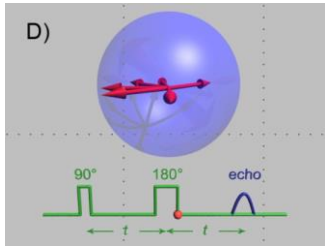
Dynamical decoupling of noise

Lets try and simulate this with the QuTiP HEOM solver and see if it works. We apply a resonant drive which Can be switched on and off with a controllable amplitude (following Viola and Lloyd arxiv:quant-ph/9803057)

$$H_S = \frac{\epsilon}{2}\sigma_z + H_D(t). \qquad \tilde{H}_D(t) = \sum_{n=1}^{n_p} V_n(t)\,\sigma_x.$$







$$\tau_p \bar{V} = \pi/2.$$

Dynamical decoupling of noise

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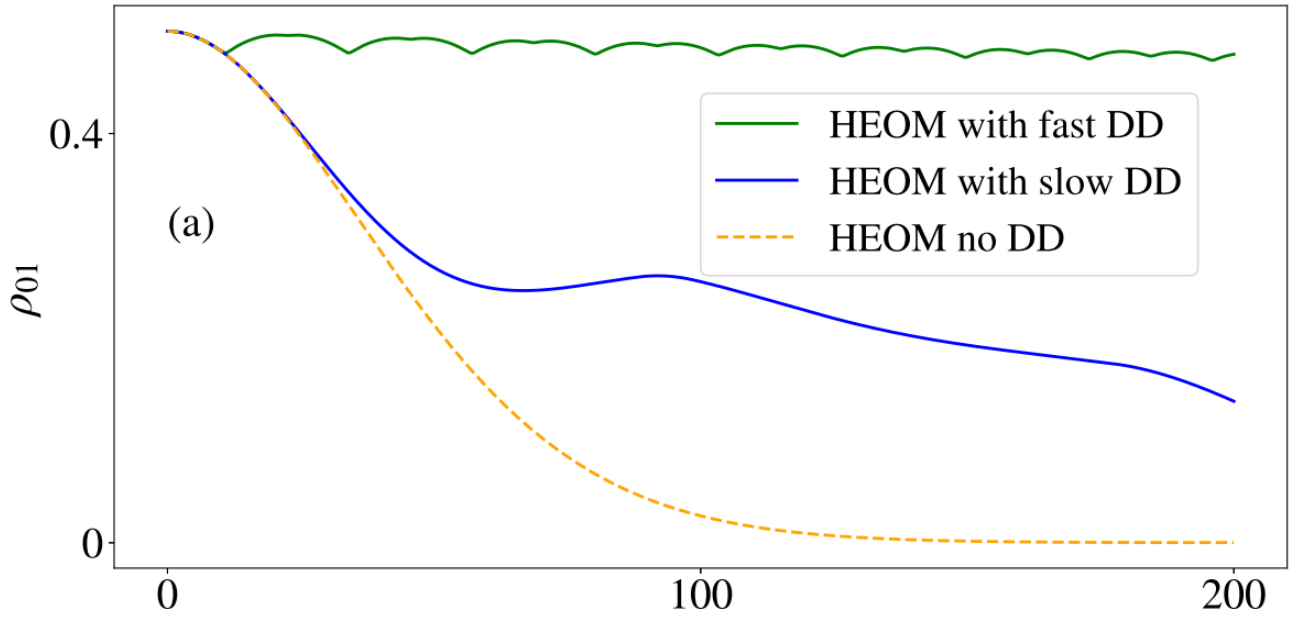


Seems to work!

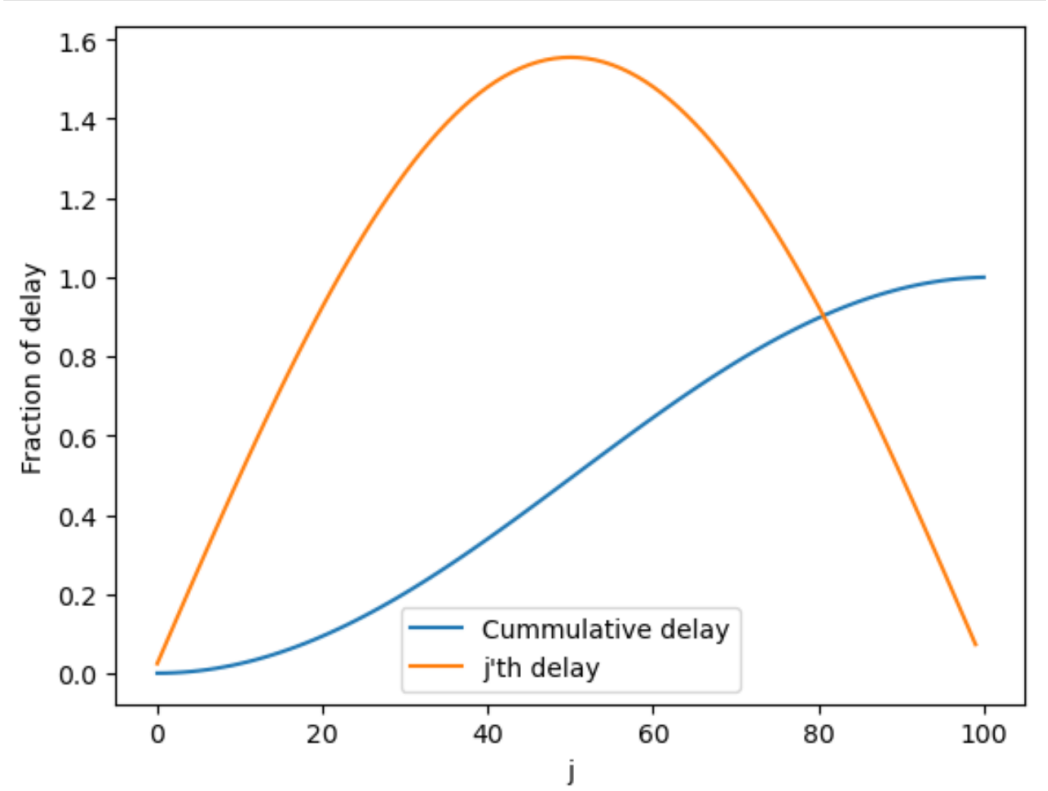
Is this (equally spaced) the optimal choice of pulse spacing?

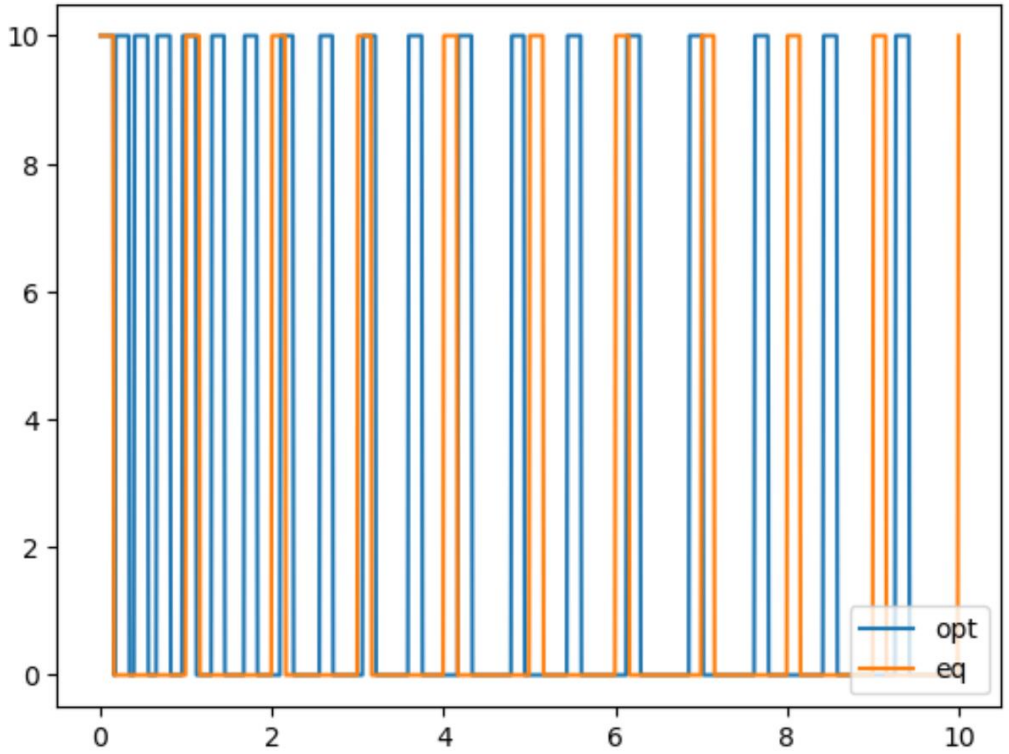
With HEOM we can try out alternatives, including realistic parameters

Dynamical decoupling of noise

$$\tilde{H}_D(t) = \sum_{n=1}^{n_p} V_n(t)\,\sigma_x.$$

Uhrig (PRL 2007) suggested $\sin^2\left(\frac{\pi}{2}\frac{j}{N+1}\right)$ is optimal (N = Total # of pulses, j = particular pulse in the range 0,… N).

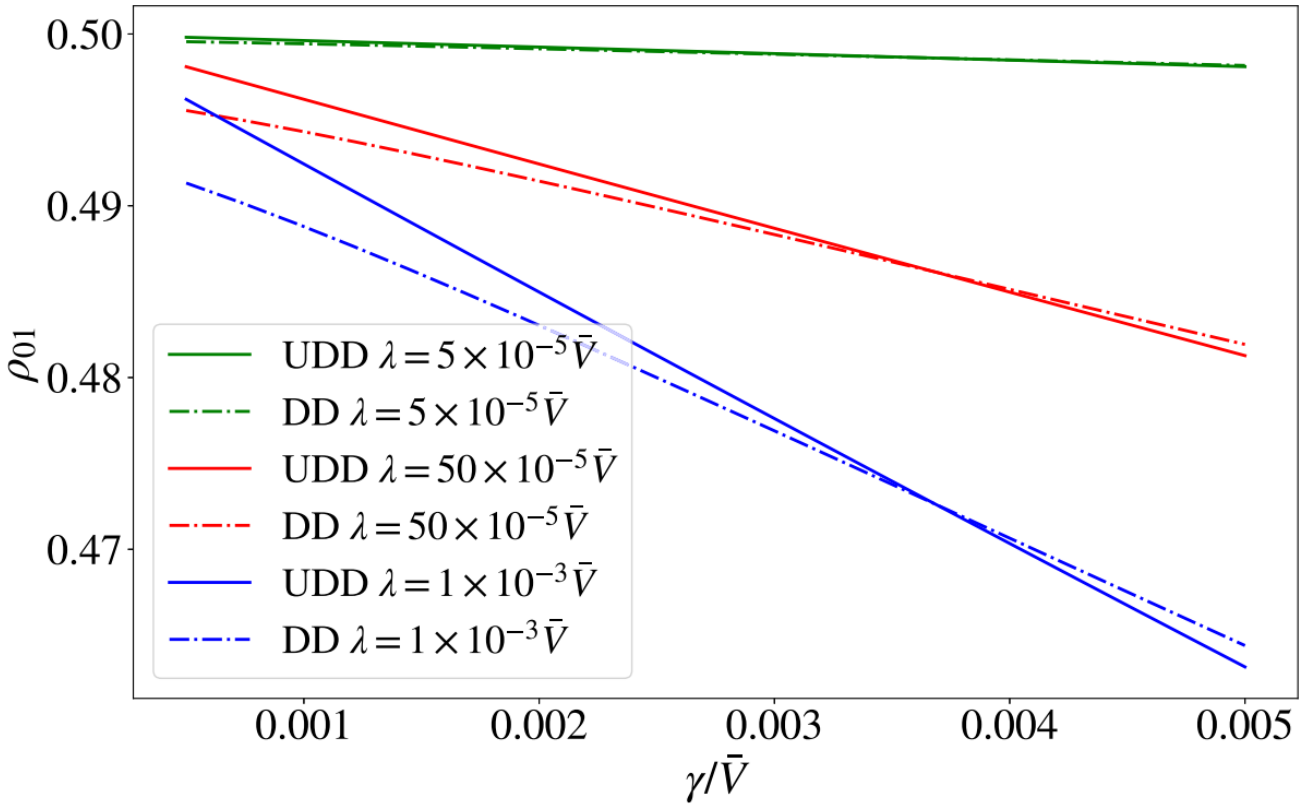




Dynamical decoupling of noise

$$\tilde{H}_D(t) = \sum_{n=1}^{n_p} V_n(t)\,\sigma_x.$$

To understand performance, we plot the final coherence after 100 pulses, and modify the bath properties



Uhrig assumed a sharp (step) function cut-off,
But the Drude-Lorentz SD we use here has a long tail.

This seems to affect the optimality of his scheme,
Where when the SD is very broad, evenly spaced scheme is more optimal.

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“input-output” Hierarchical Equations of Motion

Cirio, Liang, Lambert, arXiv:2408.12221

Code under review in QuTiP (https://github.com/qutip/qutip-tutorials/pull/118)

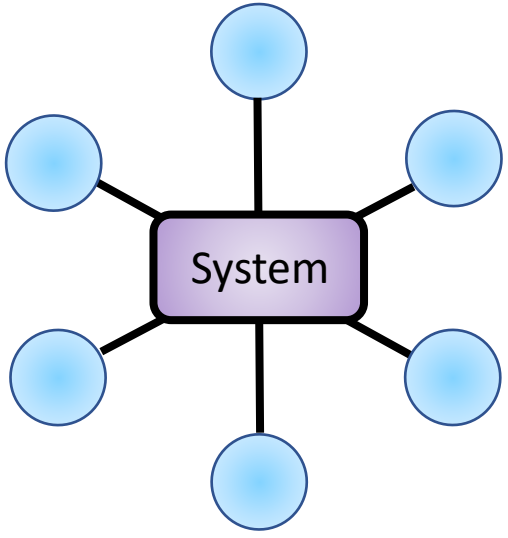
Normal HEOM ‘assumptions’:

- Bath initially in a Gaussian state
- HEOM can reproduce ‘system’ state, but only limited information about bath state/observables
- Coupling is linear in bath operators
- Free bath evolution preserves Gaussianity
- Free bath correlation functions can be decomposed as, or fit with, exponentials

‘Input output’ HEOM ‘assumptions’:

- ~~Bath initially in a Gaussian state~~
- ~~HEOM can reproduce ‘system’ state, but only limited information about bath state/observables~~
- Coupling is linear in bath operators
- Free bath evolution preserves Gaussianity
- Free bath correlation functions can be decomposed as, or fit with, exponentials
  - Still necessary for free-bath properties, not necessary for correlation encoding free-bath evolution and input/output observables.

Hierarchical Equations of Motion (HEOM)



$$H = H_S + \hat{s}X + \sum_k \omega_k a_k^\dagger a_k \text{ with } X = \sum_k g_k(a_k + a_k^\dagger)$$

$$\rho_S(t) = F[\hat{s}, C(t), \rho_S(0)]$$

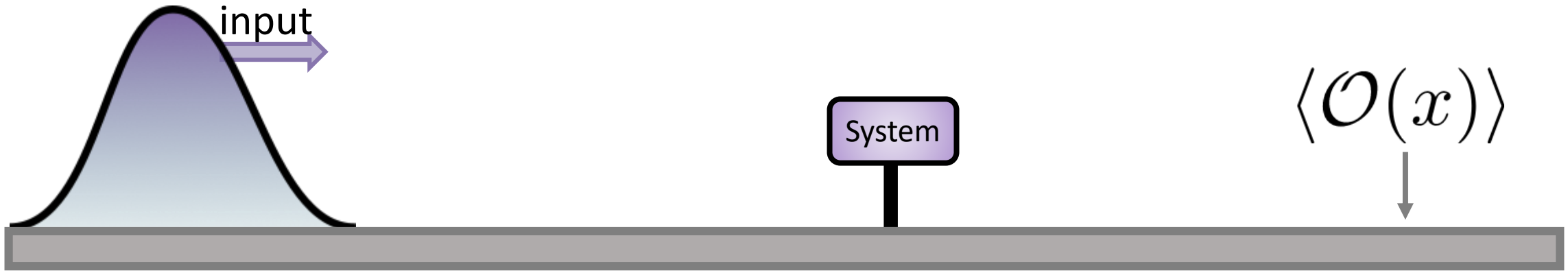
$$\boxed{\rho_S(t) = \mathcal{T} e^{\mathcal{F}_t} \rho_S(0)}$$

$$\mathcal{F}_t = -\int_0^t dt_2\, \mathcal{A}_{t_2} \int_0^{t_2} dt_1 \sum_\alpha C^\alpha(t_2 - t_1)\mathcal{B}^\alpha_{t_1}$$

Exponential ansatz

$$\sum_n c_n^\alpha e^{-\gamma_n^\alpha (t_2 - t_1)}$$

Input-output HEOM (relies on an 'extended' influence functional for bath operators)

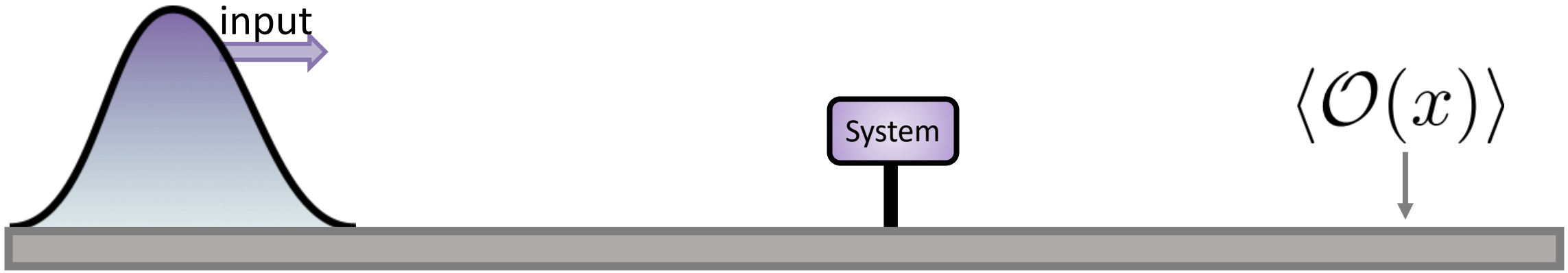


$$\langle \mathcal{O}(t) \rangle = \mathrm{Tr}_B \left\{ \phi_1^{\mathrm{out}}(t) \phi_2^{\mathrm{out}}(t) \mathcal{T} e^{-i \int_0^t d\tau \, [\hat{s}(\tau) X(\tau), \cdot]} \rho_S(0) \otimes \phi^{\mathrm{in}}(0)^\dagger \rho_B \phi^{\mathrm{in}}(0) \right\}$$

output state

non-Gaussian input state

Input-output HEOM



Auxiliary density matrices

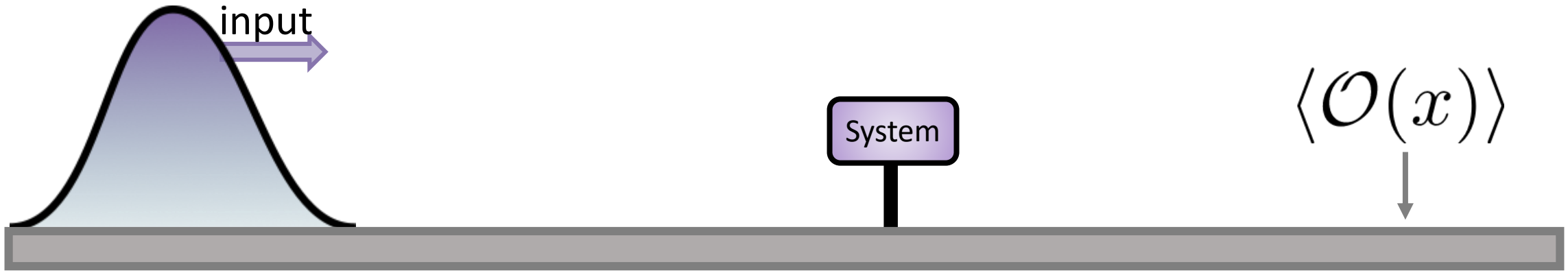
$$\dot{\rho}^{(N^{\mathrm{out}},N^{\mathrm{in}},N)}_{\vec{n}_1^{\mathrm{out}},\vec{n}_2^{\mathrm{out}},n_1^{\mathrm{in}},n_2^{\mathrm{in}},\vec{n}}$$

output indexes depend on the spectral ansatz

Input indexes are binary

Regular HEOM

Input-output HEOM



$$\dot{\rho}^{(N^{\rm out},N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}} = \mathrm{HEOM}_0\left[\rho^{(N^{\rm out},N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}}\right]$$

← Regular HEOM

$$+n_1^{\rm in}\mathcal{G}_t^1\,\rho^{(N^{\rm out},N^{\rm in}-1,N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in}-1,n_2^{\rm in},\vec{n}} + n_2^{\rm in}\mathcal{G}_t^2\,\rho^{(N^{\rm out},N^{\rm in}-1,N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in}-1,\vec{n}}$$

← Input (time-dependent function)

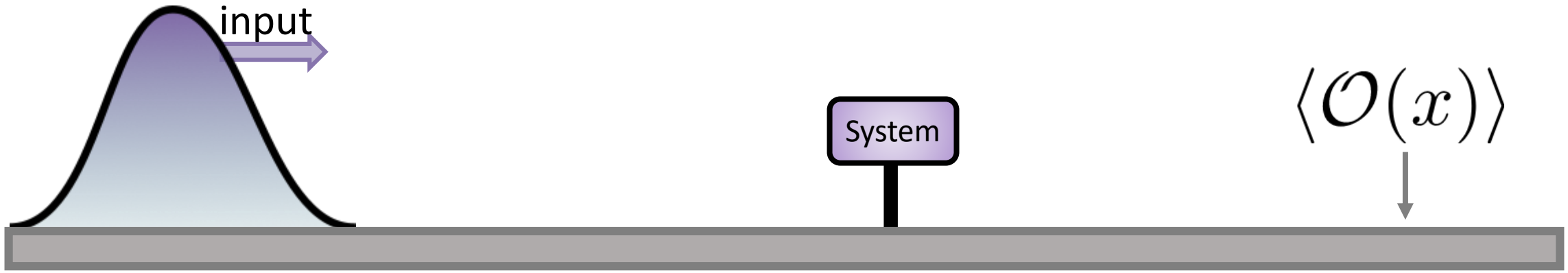
$$-\sum_{\alpha,k}\left[n^{\rm out}_{1\alpha k}\gamma^{1\alpha k} + n^{\rm out}_{2\alpha k}\gamma^{2\alpha k}\right]\rho^{(N^{\rm out},N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}}$$

$$+\sum_{\alpha,k} c^{1\alpha k}\mathcal{S}_t^{\alpha}\,\rho^{(N^{\rm out}-1N^{\rm in},N)}_{\vec{n}_1^{\rm out}-\vec{e}(\alpha,k),\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}}$$

← Output (similar to regular HEOM or written as a function)

$$+\sum_{\alpha,k} c^{2\alpha k}\mathcal{S}_t^{\alpha}\,\rho^{(N^{\rm out}-1,N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out}-\vec{e}(\alpha,k),n_1^{\rm in},n_2^{\rm in},\vec{n}}\ ,$$

Input-output HEOM



$$\dot{\rho}^{(N^{\rm out},N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}} = {\rm HEOM}_0\left[\rho^{(N^{\rm out},N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}}\right]$$

$$+n_1^{\rm in}\mathcal{G}_t^1\,\rho^{(N^{\rm out},N^{\rm in}-1,N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in}-1,n_2^{\rm in},\vec{n}} + n_2^{\rm in}\mathcal{G}_t^2\,\rho^{(N^{\rm out},N^{\rm in}-1,N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in}-1,\vec{n}}$$

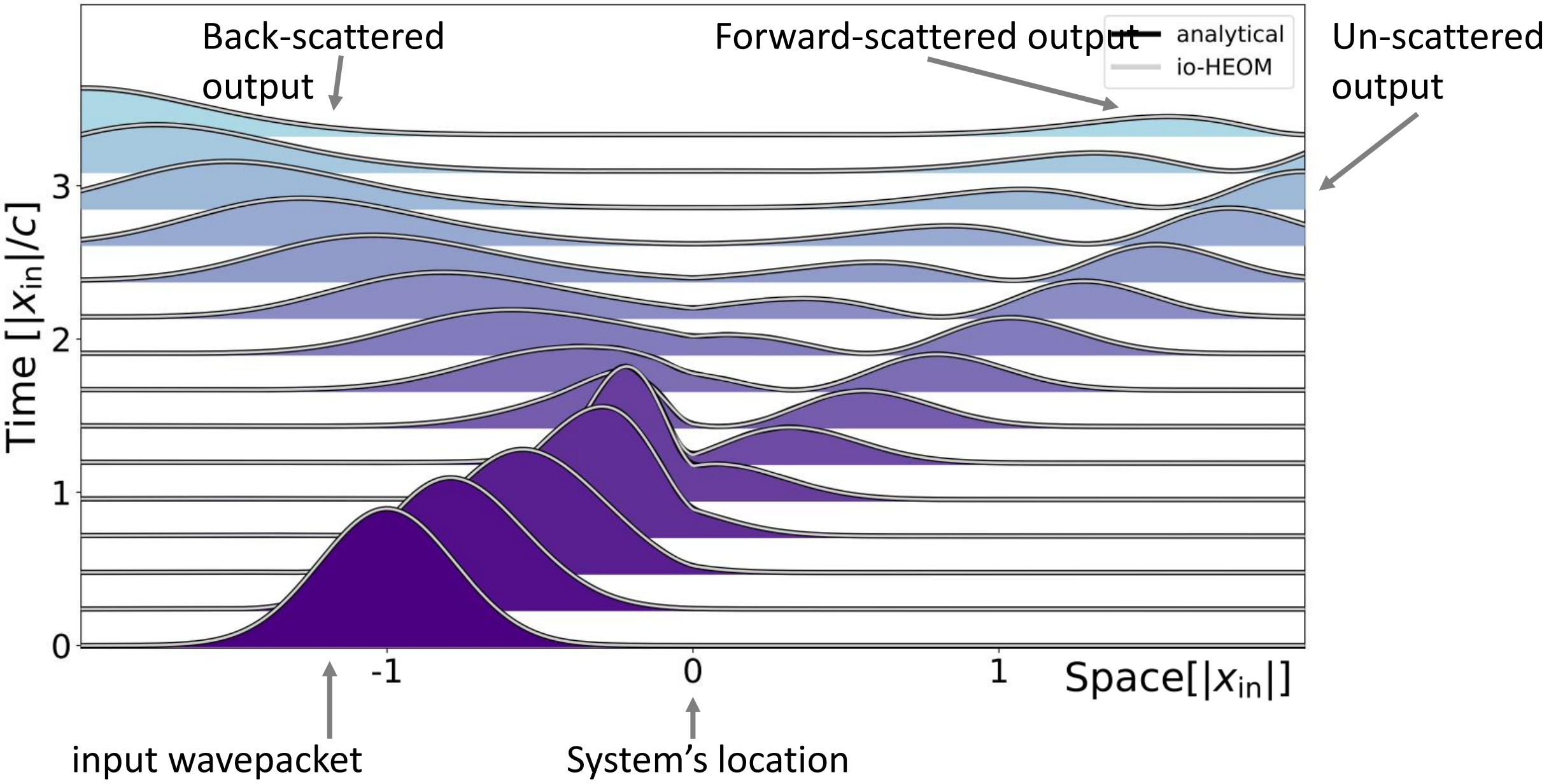
$$-\sum_{\alpha,k}\left[n^{\rm out}_{1\alpha k}\gamma^{1\alpha k}+n^{\rm out}_{2\alpha k}\gamma^{2\alpha k}\right]\rho^{(N^{\rm out},N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}}$$

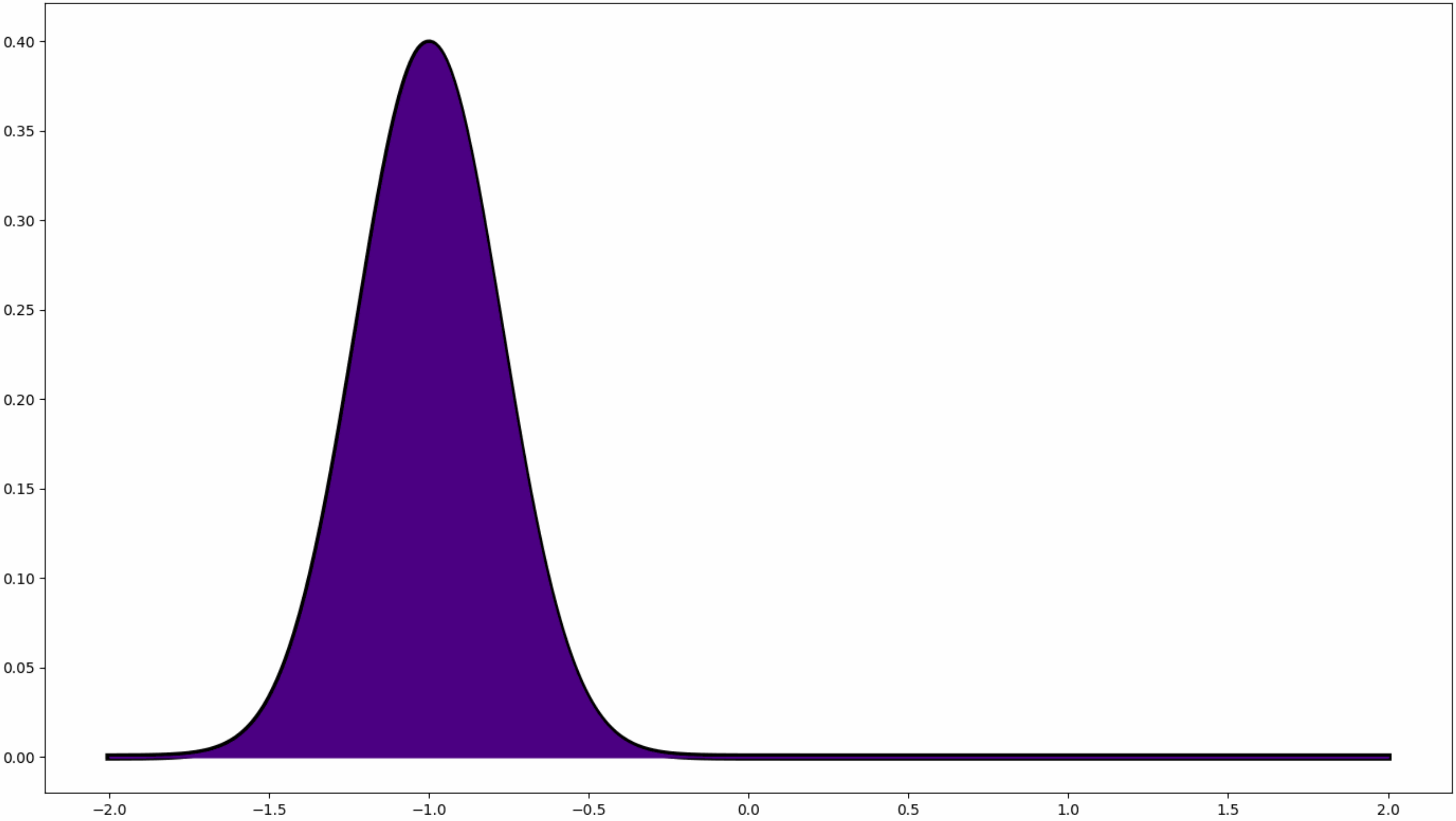
$$+\sum_{\alpha,k}c^{1\alpha k}\mathcal{S}_t^{\alpha}\,\rho^{(N^{\rm out}-1,N^{\rm in},N)}_{\vec{n}_1^{\rm out}-\vec{e}(\alpha,k),\vec{n}_2^{\rm out},n_1^{\rm in},n_2^{\rm in},\vec{n}}$$

$$+\sum_{\alpha,k}c^{2\alpha k}\mathcal{S}_t^{\alpha}\,\rho^{(N^{\rm out}-1,N^{\rm in},N)}_{\vec{n}_1^{\rm out},\vec{n}_2^{\rm out}-\vec{e}(\alpha,k),n_1^{\rm in},n_2^{\rm in},\vec{n}}\ ,$$

Only “tier-decreasing processes” in the input-output indexes

Example (benchmark since it is analytically solvable model)




0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

Part 3: non-Markovian methods continued, ENR states, optimal control, and other features

- A few more comments on noise with driven systems, HEOM and Bloch-Redfield master equations

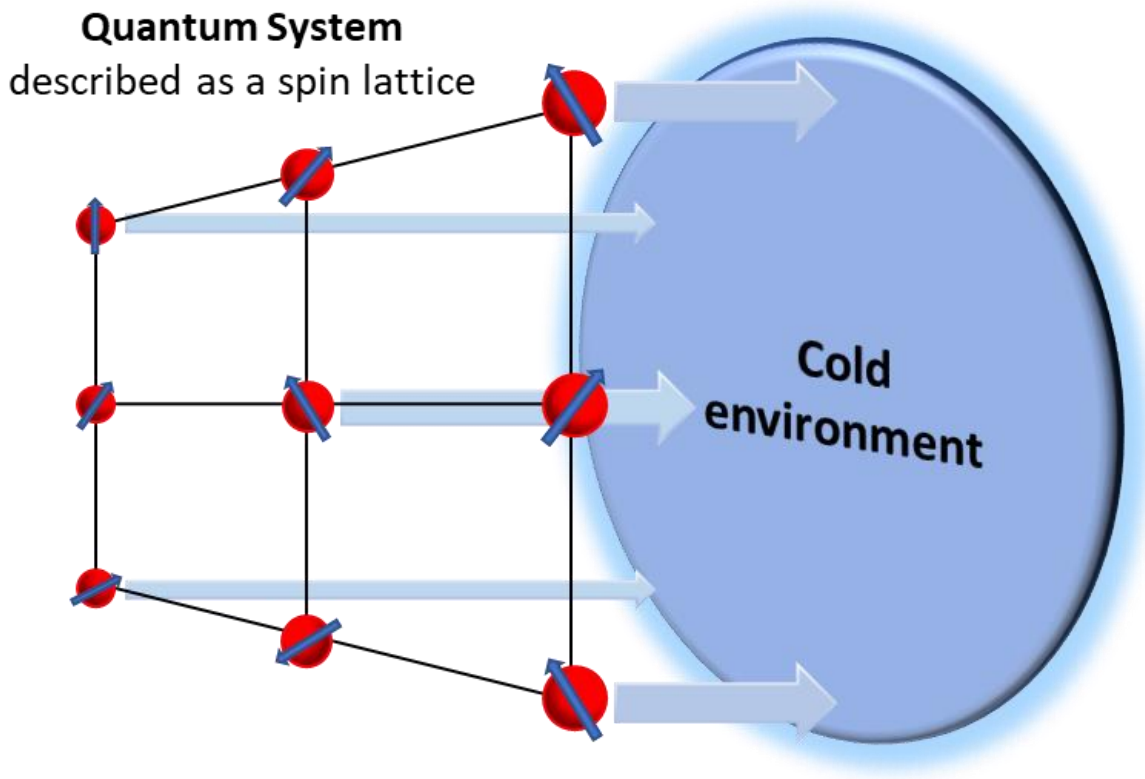
- More applications of non-Markovian noise:
  - Dynamical decoupling of noise
  - Extending the HEOM (input output HEOM)
  - **Pseudomodes for dissipative state engineering**
  - Fermions

- Hidden QuTiP features that might be useful for you
  - ENR states
  - Optimal control libraries

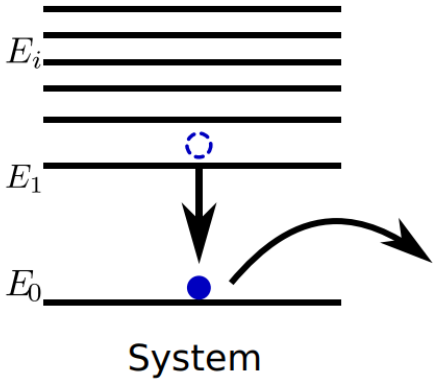
- Conclusion and summary

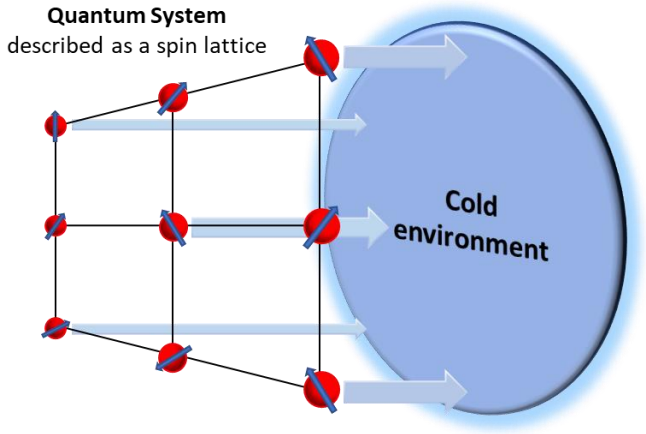
What is ‘dissipative state engineering’?

Can artificially simulated environments cool complex quantum systems to ground-states, and is this useful in practise?



Lindblad equations: A useful basis for DSE?

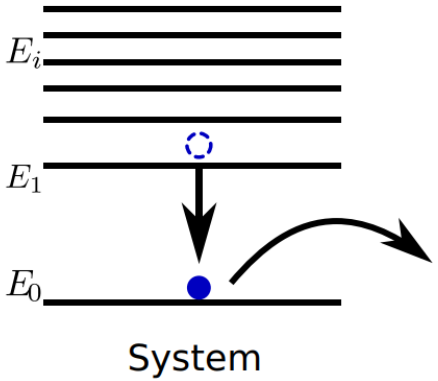


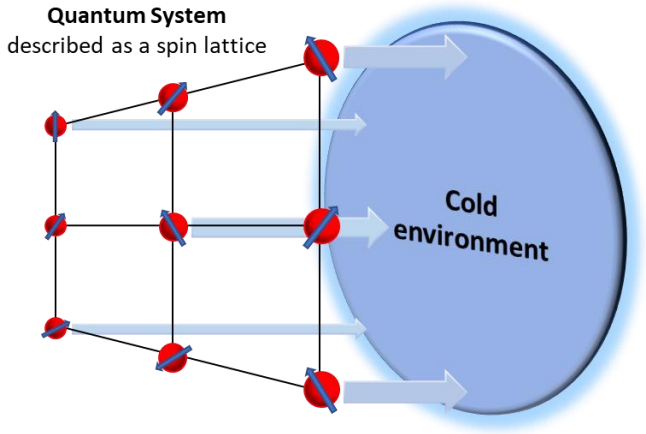


<u>Vestraete, Wolf, Cirac, Nature Physics 2009:</u>
Local (system) measurements/dissipation **for frustration-free Hamiltonians.**

$$\mathcal{L}(\rho) = \sum_k L_k \rho L_k^\dagger - \frac{1}{2}\left\{L_k^\dagger L_k, \rho\right\}_+ \qquad L_k \text{ acts locally}$$

Lindblad equations: A useful basis for DSE?





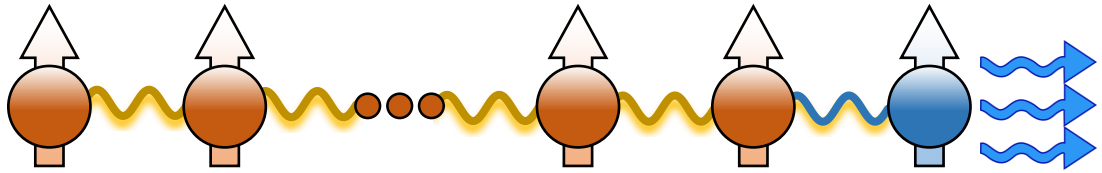
Dissipative state engineering: general case, we already **need to know the eigenstates** to even construct it

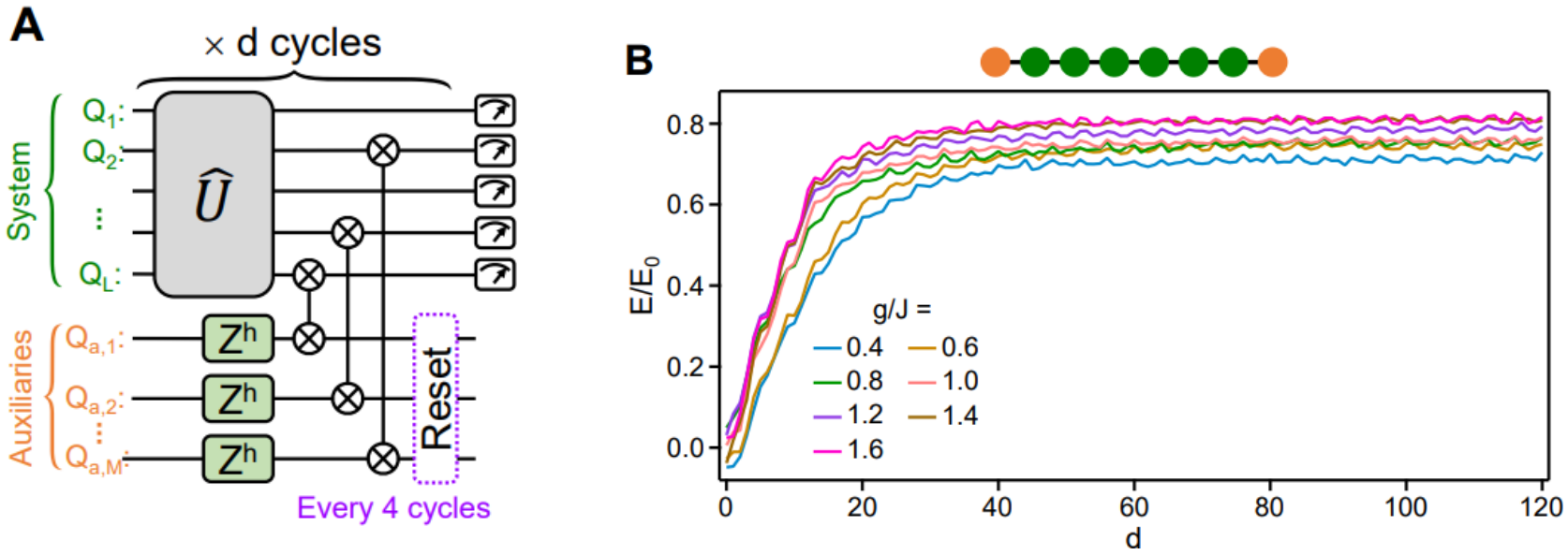
$$\dot{\rho}_s(t) = -i\left[H_s, \rho_s(t)\right] + \sum_{i,j>i} S(\Delta_{j,i}) c_{i,j} L[d_{ij}]\rho_s(t) + \sum_{i,j>i} S(-\Delta_{j,i}) c_{i,j} L[d_{ij}^\dagger]\rho_s(t),$$

$$c_{i,j} = |\langle\psi_i| Q |\psi_j\rangle|^2 \qquad d_{ij} = |\psi_i\rangle\langle\psi_j|$$

Are some other methods from open quantum systems useful for this task?

Similar ideas proposed by Raghunandan *et al., Sci. Adv. (2020)*
Experiment by Google, X. Mi *et. al.,* Science (2024)





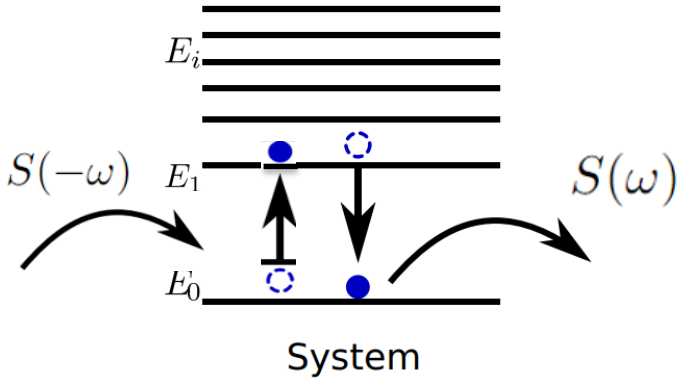
Use of ancilla acts like **structured environment**

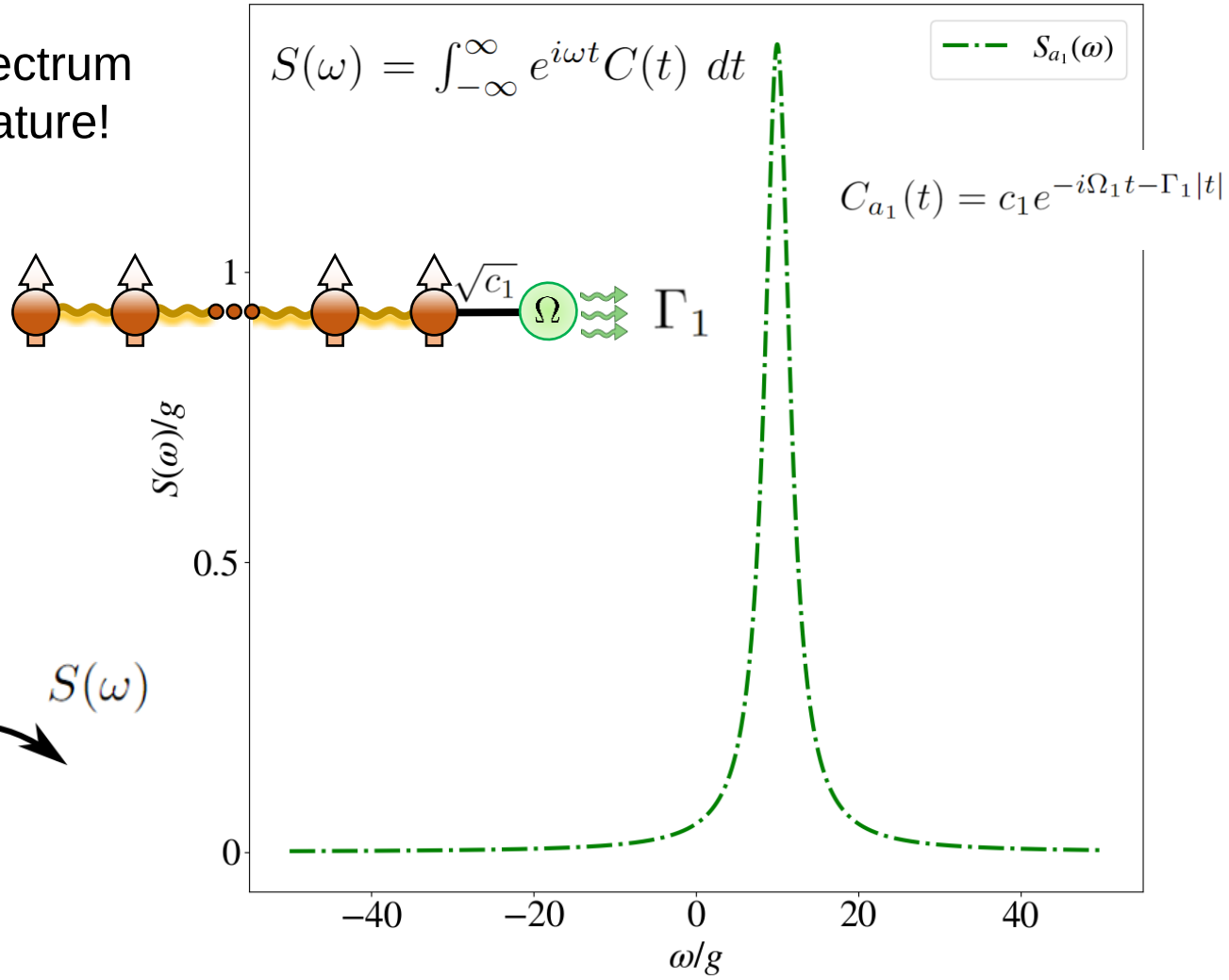
But… not perfect, there is no detailed balance! **Saturates at 90% fidelity even in theoretical simulations**

An ancilla acts like a structured environment with a Lorentzian spectral density, but it also has the wrong detailed balance on its own..

Symmetry of power spectrum determines the temperature!

$$S(\omega) = \exp[\beta\omega]\, S(-\omega)$$



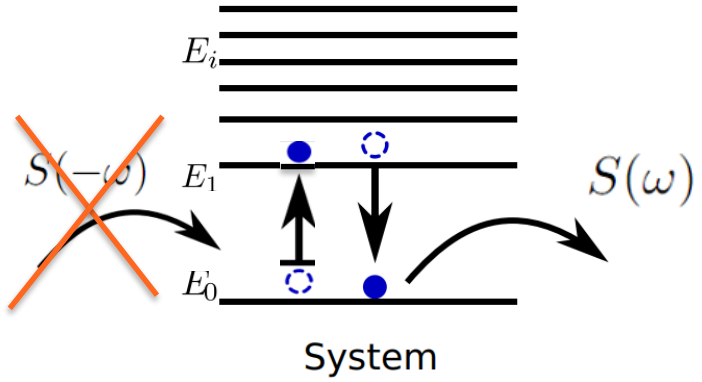


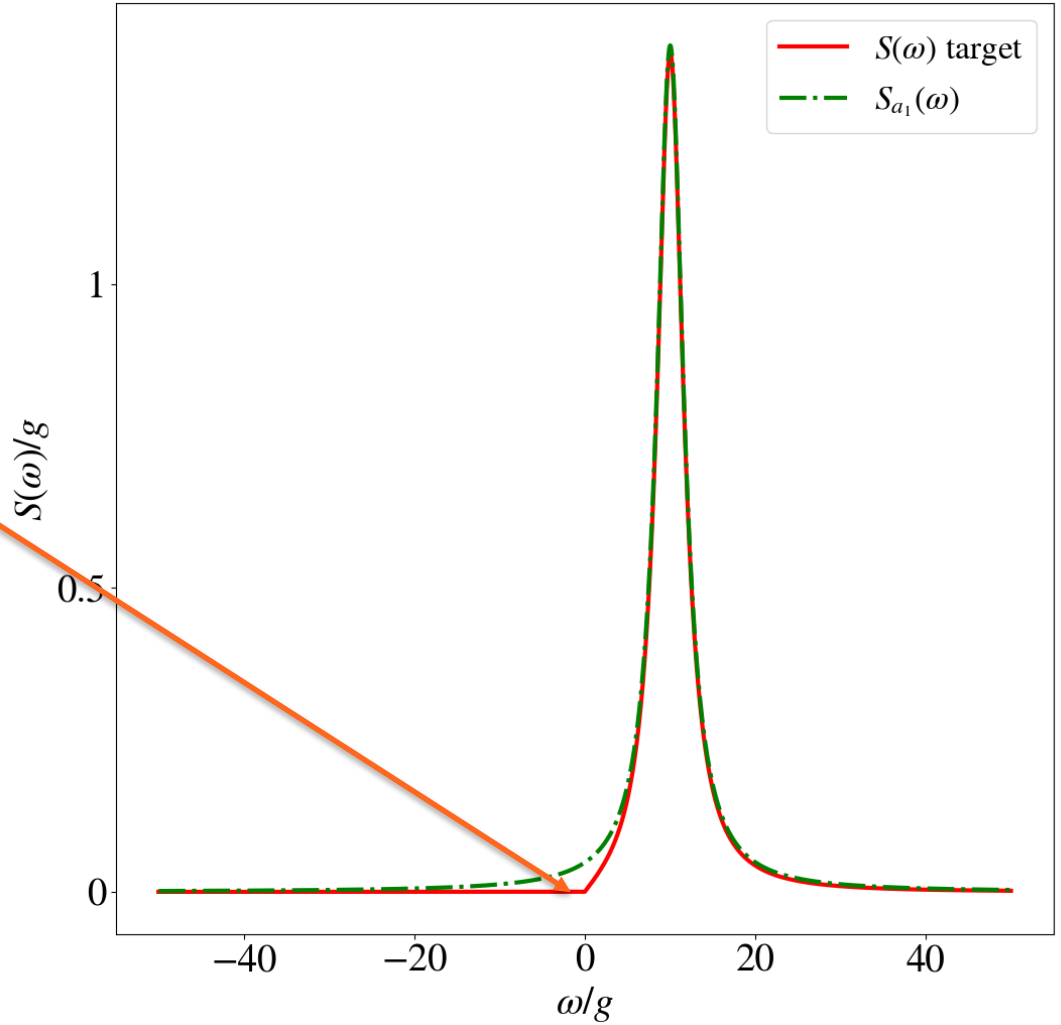
An ancilla acts like a structured environment with a Lorentzian spectral density, but it also has the wrong detailed balance on its own..

$$S(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C(t)\, dt$$

$$S(\omega) = \exp[\beta\omega]\, S(-\omega)$$

Baths at zero temperature should have zero power spectrum at negative frequencies!





The pseudo-mode method

Pseudomodes: We can replace the continous environment with a finite environment with the same correlation functions Garraway (PRB 1997)

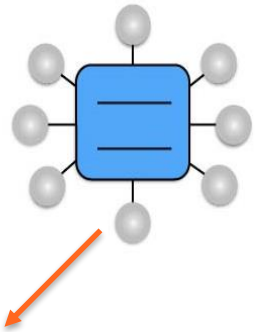
Full system-environment model:

$$H = H_S + \hat{s}X + \sum_k \omega_k a_k^\dagger a_k$$

$$J(\omega) = \pi \sum_k g_k^2 \delta(\omega - \omega_k)$$

$$S(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C(t)\, \hat{dt}$$

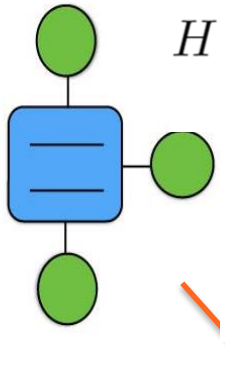
$$C(\tau) = \frac{1}{\pi}\int_0^\infty d\omega J(\omega)\left[\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega\tau) - i\sin(\omega\tau)\right]$$



Pseudomodes: Numerically solvable (sometimes)

$$H = H_{\rm sys} + \sum_r \Omega_r a_r^\dagger a_r + \hat{s}\sum_r \sqrt{c_r}(a_r + a_r^\dagger)$$

$$D_r[\rho] = \Gamma_r(n_r+1)(2a_r\rho a_r^\dagger - a_r^\dagger a_r\rho - \rho a_r^\dagger a_r) + \Gamma_r n_r(2a_r^\dagger \rho a_r - a_r a_r^\dagger \rho - \rho a_r a_r^\dagger)$$



$$C_{\rm PM}(\tau) = \sum_r c_r[(1+n_r)e^{-i\Omega_r\tau - \Gamma_r|\tau|} + n_r e^{i\Omega_r\tau - \Gamma_r|\tau|}]$$

Earlier work: Pseudomodes with imaginary parameters are more flexible for this purpose, **Lambert et al,** Nat. Comms. 2019, **G. Pleasance** PRR (2020), Lin Lin PRA (2024), **P. Menczel, Lambert** PRR 2024. and very powerful for describing non-perturbative baths

Other approaches: Add flexibility through interacting physical PMs....
see works of Mascherpa, Tamascelli, Feist, Arrigoni, **Lin Lin**, and more
(e.g., Mascherpa *et al.*, Phys Rev. A **101**, 052108 (2020))

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$$+\Gamma_r n_r(2a_r^\dagger \rho a_r - a_r a_r^\dagger \rho - \rho a_r a_r^\dagger)$$

$$\sum_r c_r[(1+n_r)e^{-i\Omega_r\tau-\Gamma_r|\tau|} + n_r e^{i\Omega_r\tau-\Gamma_r|\tau|}]$$

``*The simulacrum is never that which conceals the truth--it is the truth which conceals that there is none. The simulacrum is true.*'' – Baudrillard

"When I put it into my mouth the matrix tells my brain that it is juicy and delicious" – Cypher, "The Matrix"

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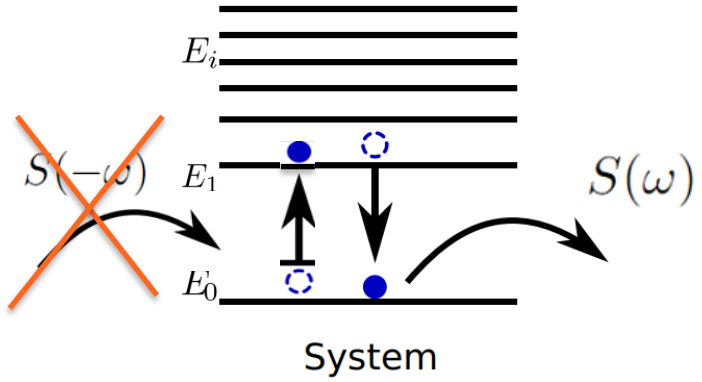
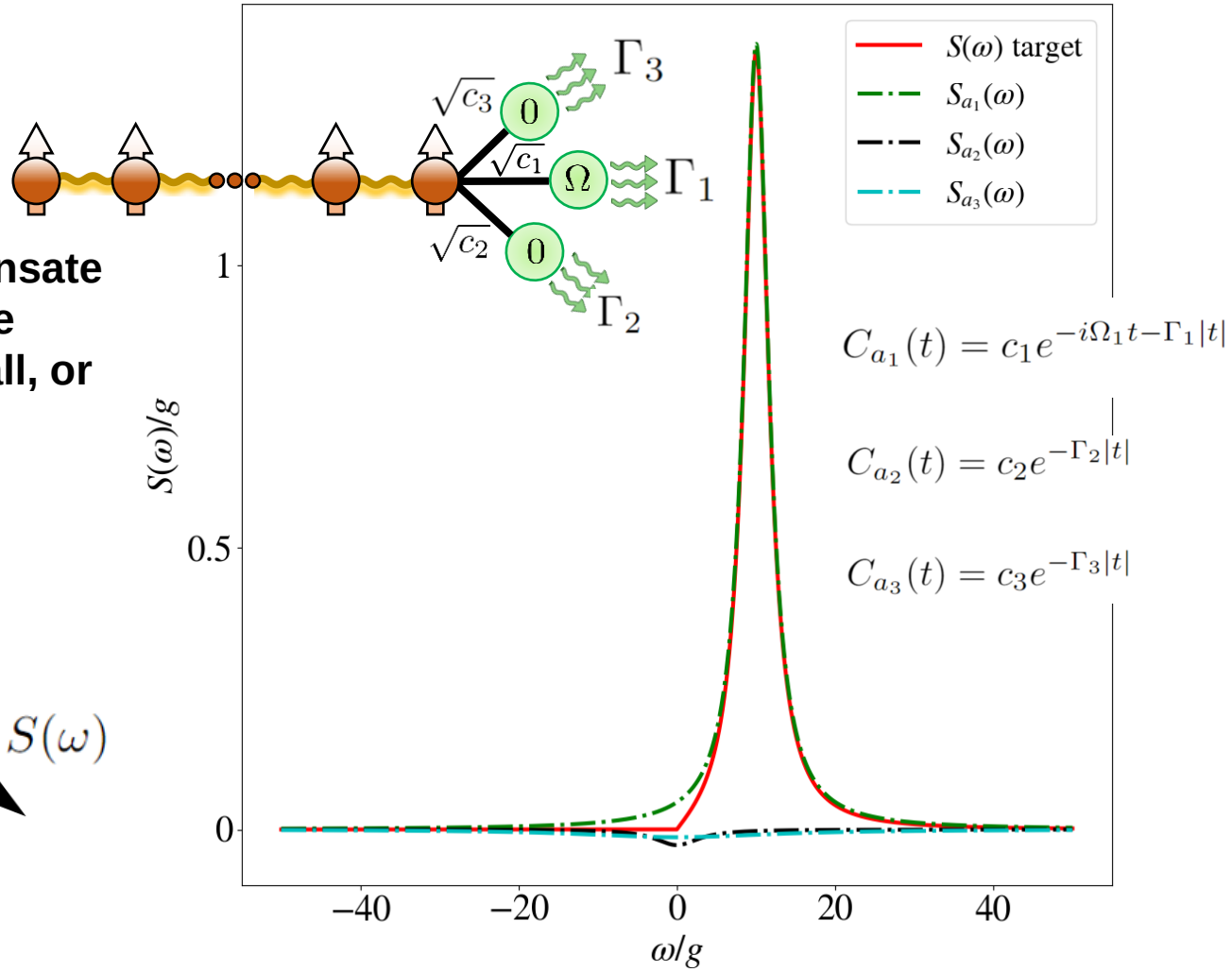
$$S(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C(t)\, dt$$

$$S(\omega) = \exp\left[\beta\omega\right] S(-\omega)$$

We can add **unphysical pseudomodes that compensate and push the total effective power spectrum to be small, or close to zero….**





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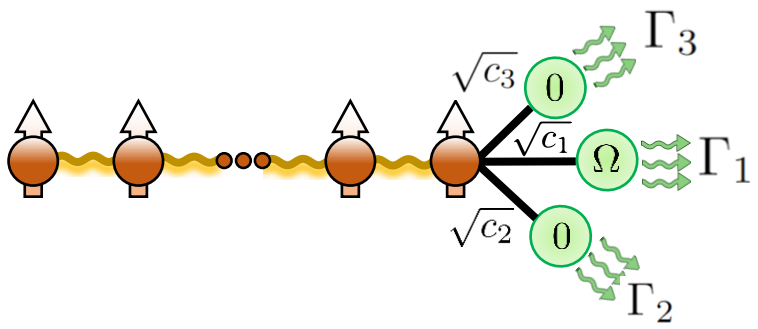
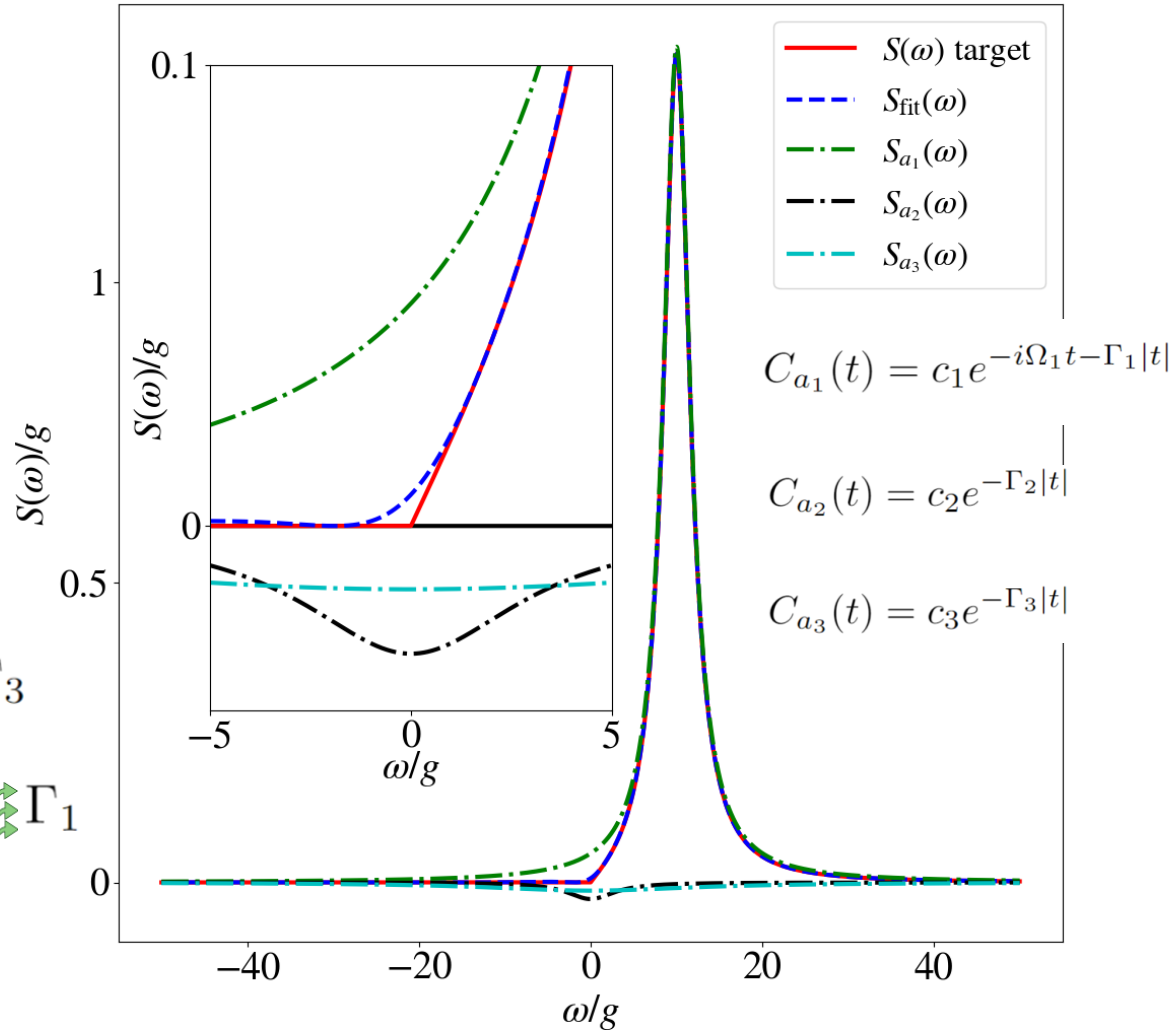
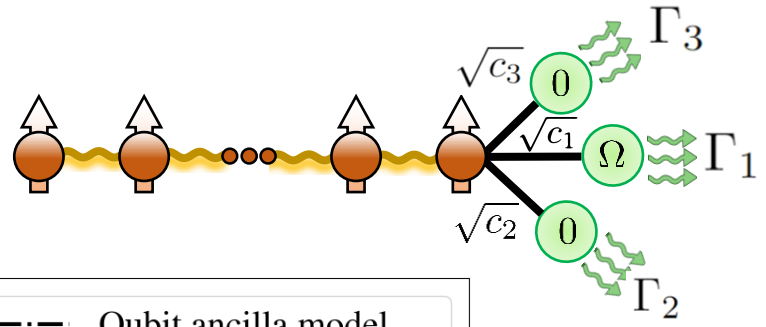
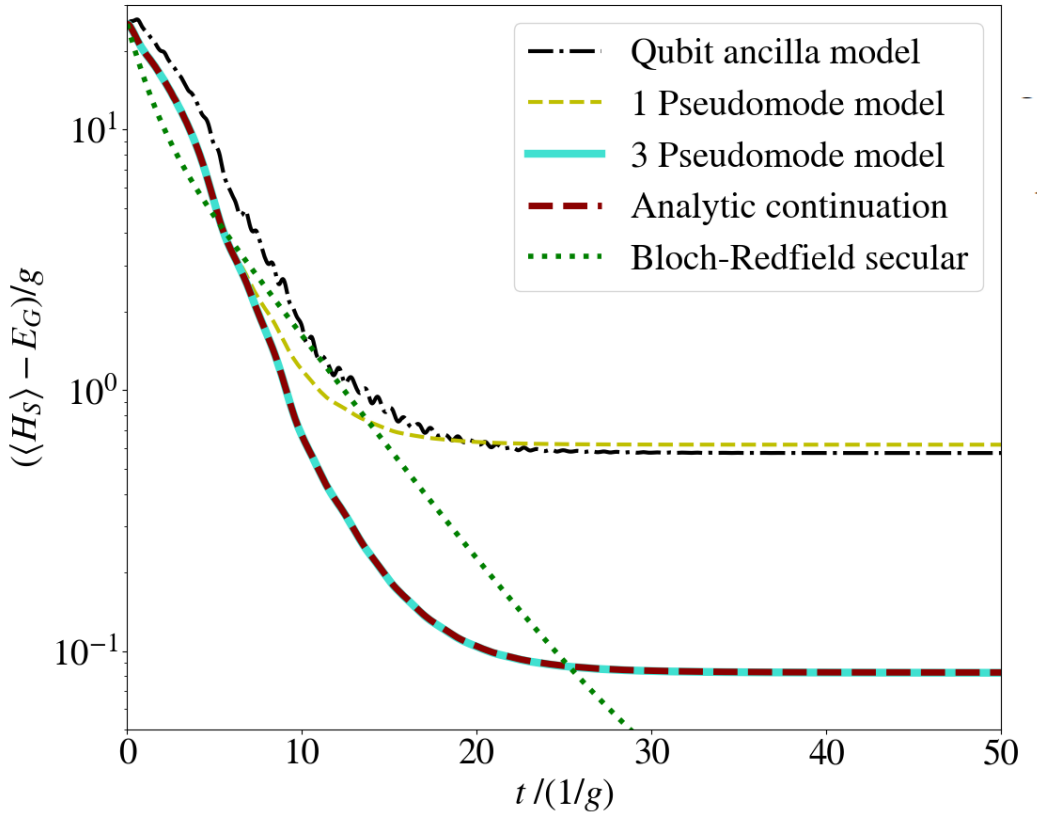




Dissipative state engineering: two additional unphysical ancillas fix detailed balance: 99% ground-state fidelity obtained!



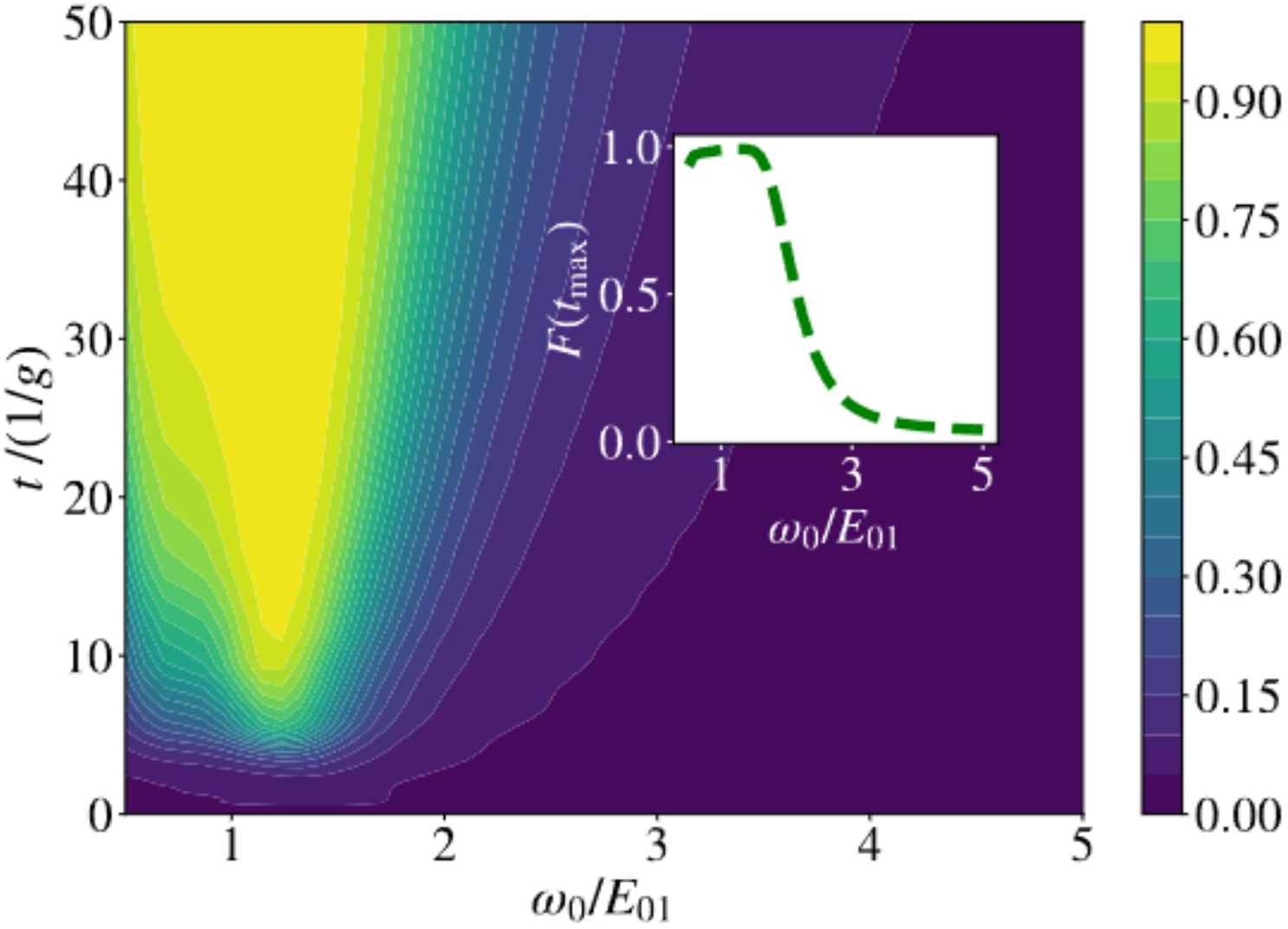


$$H_{\text{sys}} = g\sum_{i=1}^{N}\sigma_z^{(i)} - J\sum_{i=1}^{N-1}\sigma_x^{(i)}\otimes\sigma_x^{(i+1)}$$

$$N = 5,\ J = 5g$$

See Lambert et al., PRR 2024 for more details

Dissipative state engineering: two additional unphysical ancillas fix detailed balance: 99% ground-state fidelity obtained!



Part 3: non-Markovian methods continued, ENR states, optimal control, and other features

- A few more comments on noise with driven systems, HEOM and Bloch-Redfield master equations

- More applications of non-Markovian noise:
  - Dynamical decoupling of noise
  - Extending the HEOM (input output HEOM)
  - Pseudomodes for dissipative state engineering
  - **Fermions**

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- Conclusion and summary

Fermionic baths

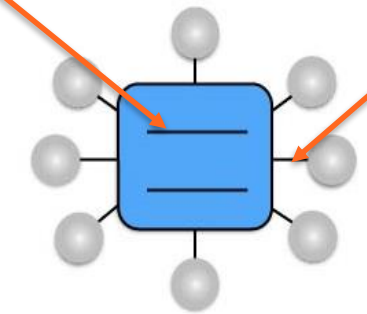
- Generally, we capture the main influence of bath degrees of freedom with a continuum of **fermionic** modes:

$$H = \epsilon s^\dagger s + \sum_k \omega_k c_k^\dagger c_k + \sum_k g_k (s c_k^\dagger - s^\dagger c_k)$$

System energy

Bath mode frequencies

Coupling strengths



$$J(\omega) = \pi \sum_k \frac{g_k^2}{2\omega_k} \delta(\omega - \omega_k)$$

$$B(t) = \sum_k g_k c_k e^{-i\omega_k t}$$

$$\begin{aligned} C^\sigma(t) &= \mathrm{Tr}_E \left[B^\sigma(t_2) B^{\bar{\sigma}}(t_1) \rho_E^{\mathrm{eq}} \right] \\ &= \int_{-\infty}^{\infty} d\omega J(\omega) e^{i\sigma\omega t} [(1-\sigma)/2 + \sigma n_E^{\mathrm{eq}}(\omega)]/\pi \end{aligned}$$

How can we solve dynamics and steady-state for **strong** coupling to such a continuum of modes in a simple and transparent way?

Non-perturbative methods for fermions: HEOM and pseudomodes

Canonical derivation of the fermionic influence superoperator, Mauro Cirio, Po-Chen Kuo, Yueh-Nan Chen, Franco Nori, Neill Lambert, Phys. Rev. B **105**, 035121, (2022), **editor's suggestion**

$$\rho_S(t) = \sum_{p=\pm} \hat{\hat{T}}_S \exp\left\{ \int_0^t dt_2 \int_0^{t_2} dt_1 \hat{\hat{W}}_p(t_2, t_1)[\cdot] \right\} \rho_S^p(0)$$

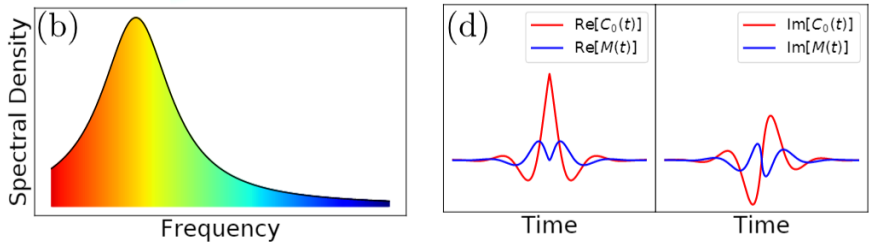
– Again, we can **replace the continous environment** with a **finite environment** with the **same correlation functions**, and the system should not know the difference, or we can derive a fermionic HEOM (solver is in QuTiP)

What differs from the bosonic case?

– Correlation functions are split into two:

$$\begin{aligned} C^\sigma(t) &= \mathrm{Tr}_E \left[B^\sigma(t_2) B^{\bar{\sigma}}(t_1) \rho_E^{\mathrm{eq}} \right] \\ &= \int_{-\infty}^{\infty} d\omega J(\omega) e^{i\sigma\omega t} [(1-\sigma)/2 + \sigma n_E^{\mathrm{eq}}(\omega)]/\pi \end{aligned}$$

Example: Kondo resonance



Two interacting system impurities
in contact with fermionic baths:

$$J_L(\omega) = \frac{\Gamma W^2}{(\omega-\mu)^2 + W^2}$$

$$\begin{aligned} H_S &= \epsilon\left(s_\uparrow^\dagger s_\uparrow + s_\downarrow^\dagger s_\downarrow\right) + U s_\uparrow^\dagger s_\uparrow s_\downarrow^\dagger s_\downarrow \\ H_E + H_I &= \sum_{k,\nu} c_{k,\nu}^\dagger c_{k,\nu} + \sum_\nu s_\nu B_\nu^\dagger + B_\nu s_\nu^\dagger \end{aligned}$$

$$A_\nu(\omega) = \frac{1}{2\pi}\int dt e^{i\omega t}\langle\{s_\nu(t), s_\nu^\dagger(0)\}\rangle.$$

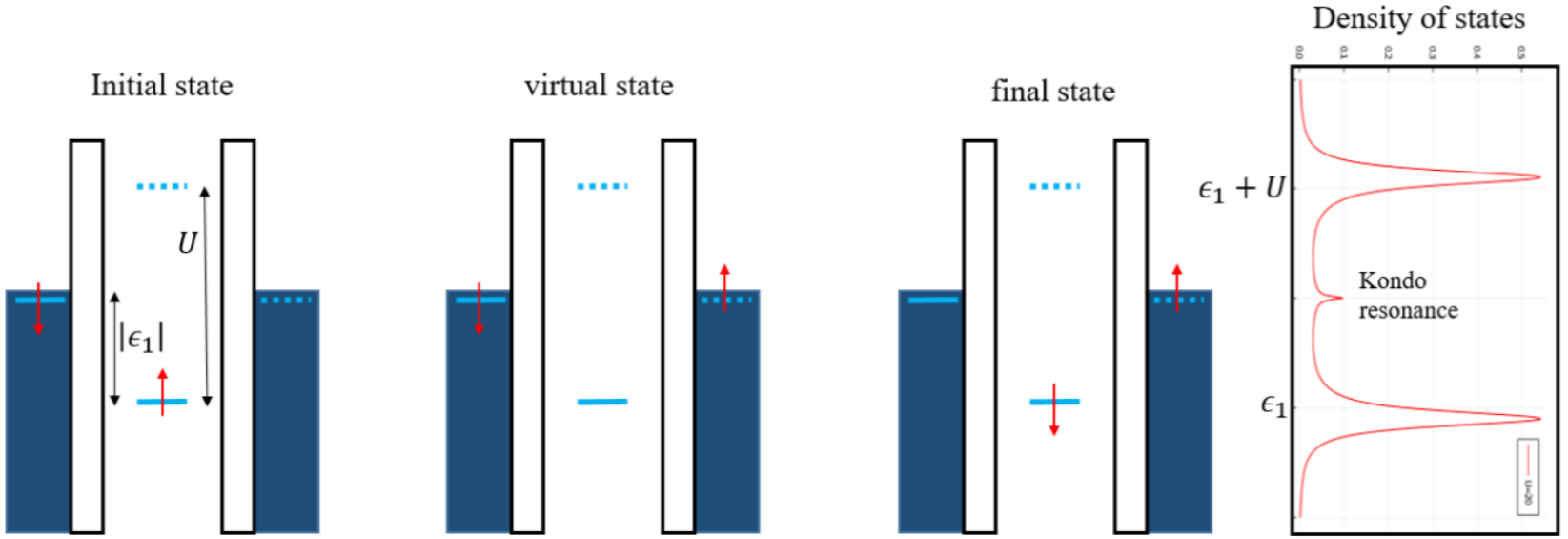
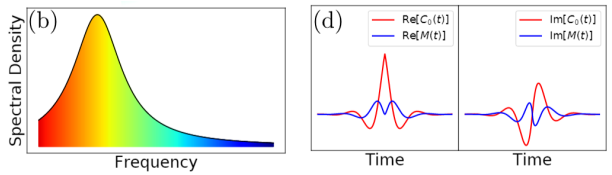


Figure from Po-chen Kuo, PhD Thesis

Example: Kondo resonance



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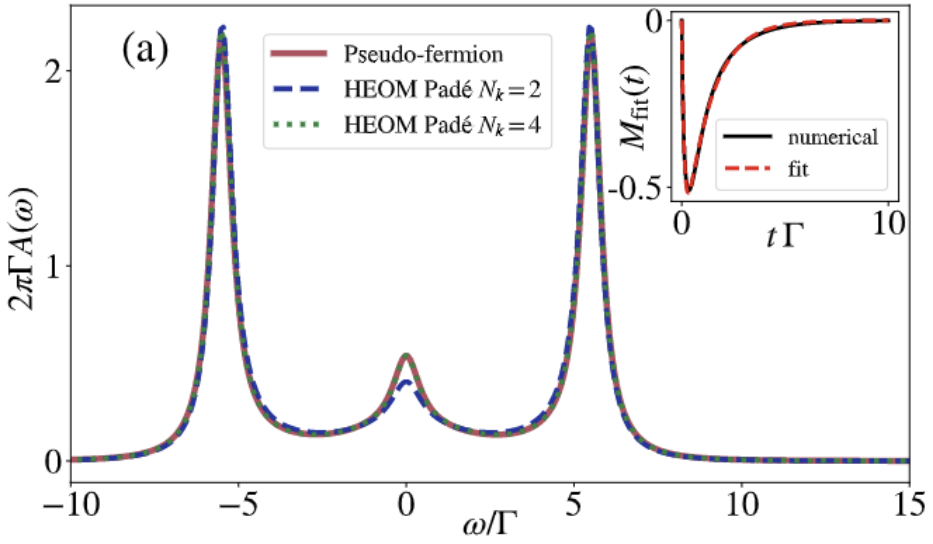
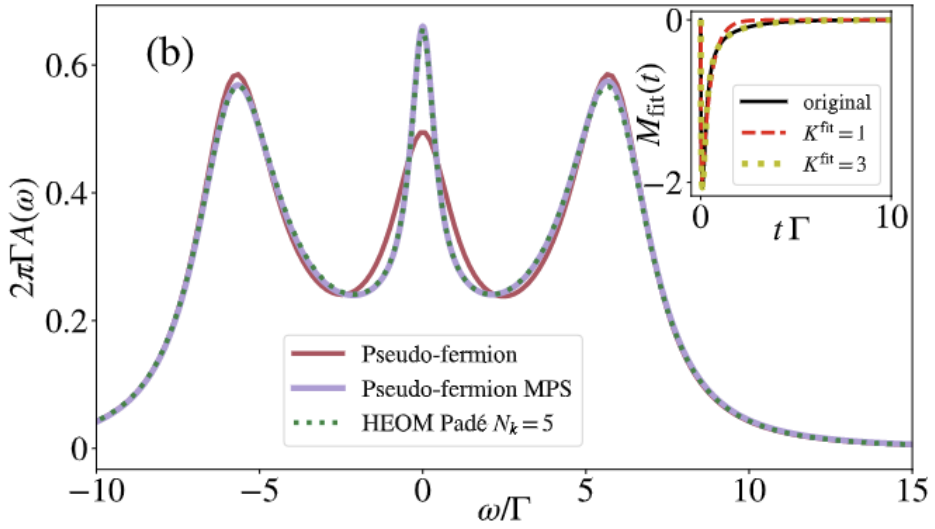




Getting to the scaling limit is hard (as expected), but can be done with MPS, at least for finite temperature

Part 3: non-Markovian methods continued, ENR states, optimal control, and other features

- A few more comments on noise with driven systems, HEOM and Bloch-Redfield master equations

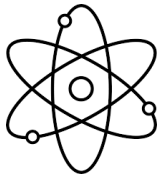
- More applications of non-Markovian noise:
  - Dynamical decoupling of noise
  - Extending the HEOM (input output HEOM)
  - Pseudomodes for dissipative state engineering
  - Fermions

- Hidden QuTiP features that might be useful for you
  - **ENR states**
  - Optimal control libraries

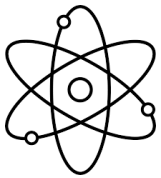
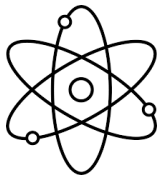
- Conclusion and summary

ENR: Excitation number restricted states

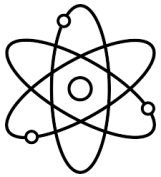
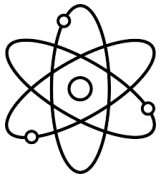
When we create composite quantum systems, we inevitable have an exponential growth in the number of states



$$\psi = \alpha|0\rangle + \beta|1\rangle$$

$$\psi = \gamma|00\rangle + \epsilon|01\rangle + \zeta|10\rangle + \eta|11\rangle$$

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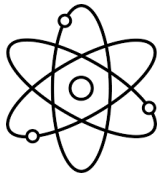
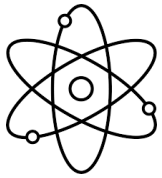


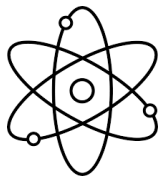
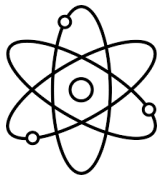
N atoms require 2^N parameters.

ENR: Excitation number restricted states

ENR states are an approximation to the full state space of composite systems which discard states that have total excitation number than a given cut-off



$$\psi = \alpha|0\rangle + \beta|1\rangle$$

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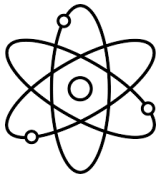
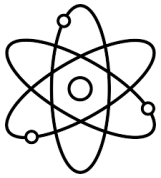

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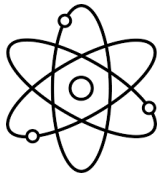


N atoms with cut-off K, # of states is….

ENR: Excitation number restricted states

Consider the standard Jaynes-Cummings model, where the Hamiltonian naturally splits into subspaces with # excitation Number conserved

Normal construction:

```
N_cut = 2

psi0 = qt.basis(2, 0) & qt.basis(N_cut, 0)
sz = qt.sigmaz() & qt.qeye(N_cut)
sm = qt.sigmam() & qt.qeye(N_cut)
a = qt.qeye(2) & qt.destroy(N_cut)

H_JC = (
    0.5 * eps * sz + omega_c * a.dag() * a +
    g * (a * sm.dag() + a.dag() * sm)
)
print(psi0)
print(H_JC)
```

```
Quantum object: dims=[[2, 2], [1, 1]], shape=(4, 1), type='ket', dtype=Dense
Qobj data =
[[1.]
 [0.]
 [0.]
 [0.]]
Quantum object: dims=[[2, 2], [2, 2]], shape=(4, 4), type='oper', dtype=CSR, isherm=True
Qobj data =
[[ 3.14159265  0.          0.          0.62831853]
 [ 0.          9.42477796  0.          0.        ]
 [ 0.          0.         -3.14159265  0.        ]
 [ 0.62831853  0.          0.          3.14159265]]
```

ENR state construction (uses custom functions)

```
N_exc = 1
dims = [2, N_cut]

psi0 = qt.enr_fock(dims, N_exc, [0, 0])
sm, a = qt.enr_destroy(dims, N_exc)
sz = 2 * sm.dag() * sm - 1

H_enr = (
    0.5 * eps * sz + omega_c * a.dag() * a +
    g * (sm.dag() * a  + a.dag() * sm)
)
print(psi0)
print(H_enr)
```

```
Quantum object: dims=[[2, 2], [1, 1]], shape=(3, 1), type='ket', dtype=Dense
Qobj data =
[[1.]
 [0.]
 [0.]]
Quantum object: dims=[[2, 2], [2, 2]], shape=(3, 3), type='oper', dtype=CSR, isherm=True
Qobj data =
[[-3.14159265  0.          0.        ]
 [ 0.          3.14159265  0.62831853]
 [ 0.          0.62831853  3.14159265]]
```

ENR: Excitation number restricted states

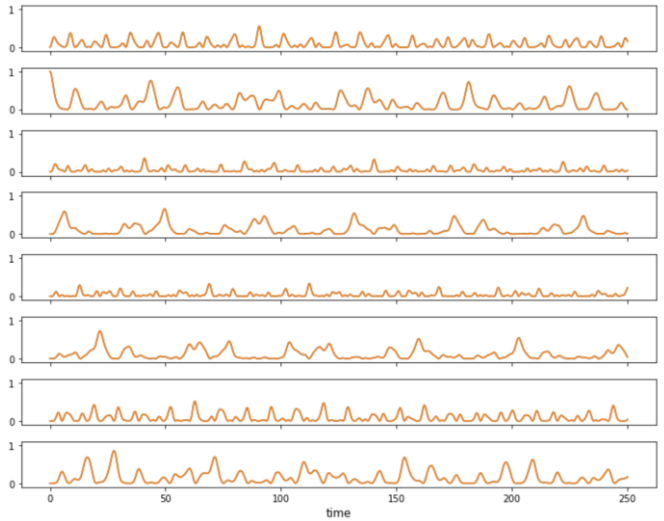
Two quick examples of when this is useful: JC Chain, many coupled sites, with coupling that conserves excitation number

```
H0 = sum([aa.dag() * aa for aa in a]) + sum([s.dag() * s for s in sm])

# atom-cavity couplings
Hint_ac = 0
for n in range(N):
    Hint_ac += 0.5 * (a[n].dag() * sm[n] + sm[n].dag() * a[n])

# coupling beetween cavities
Hint_cc = 0
for n in range(N-1):
    Hint_cc += 0.9 * (a[n].dag() * a[n+1] + a[n+1].dag() * a[n])

H = H0 + Hint_ac + Hint_cc
```




```
#This is the normal QuTip solution, without using ENR states
%time result1, H1, L1 = solve(d, psi0)
```

```
Wall time: 34.1 s
```

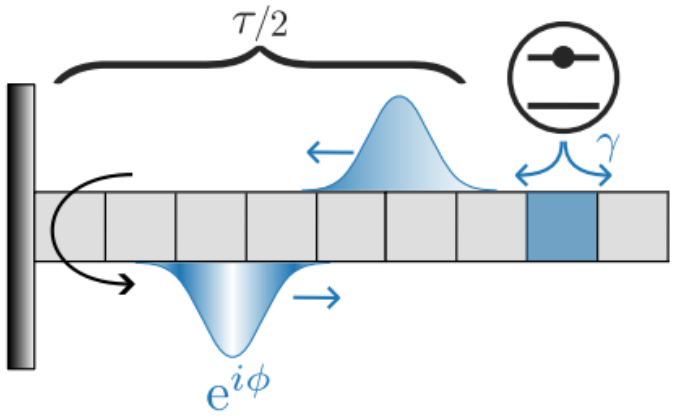
```
#This is the solution using the ENR states/operators

%time result2, H2, L2 = solve(d, psi0)
```

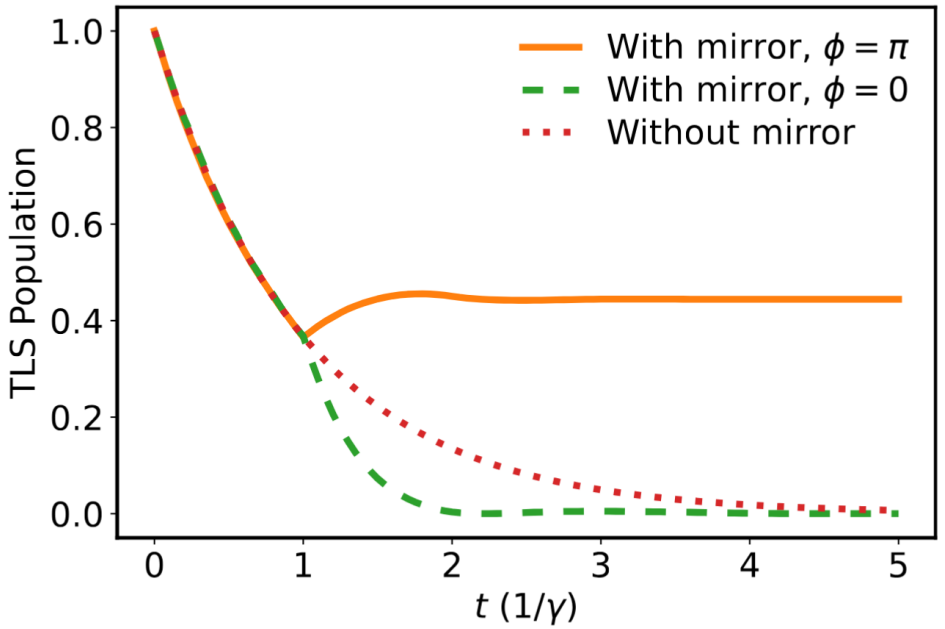
```
Wall time: 432 ms
```

ENR: Excitation number restricted states

Two quick examples of when this is useful: collision model of photons propagating in a waveguide



$$H = \frac{\epsilon}{2}\sigma_z + \sum_{\alpha\in\{L,R\}}\sum_{k=0}^{N-1}\omega_k b^\dagger_{k,\alpha}b_{k,\alpha} + \sqrt{\frac{2\pi}{L_0}}\sum_{\alpha\in\{L,R\}}\sum_{k=0}^{N-1}\kappa_\alpha(\omega_k)\left[\sigma_+ b_{k,\alpha} + \text{H.c.}\right]$$



[Figure from](#) Bundgaard-Nielsen et al., [arXiv:2412.13332](#)

N = 21 waveguide modes, difficult without ENR states! (see our qutip 5 paper for implementation details)

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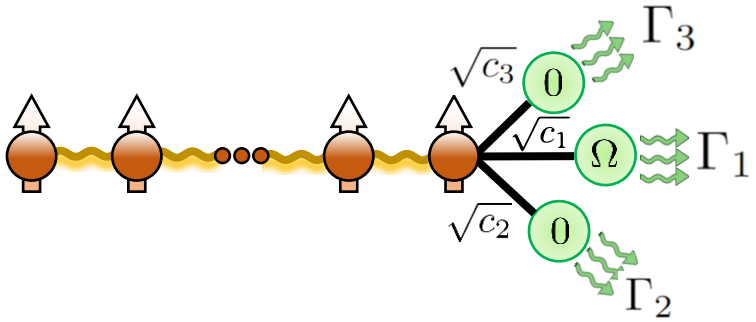
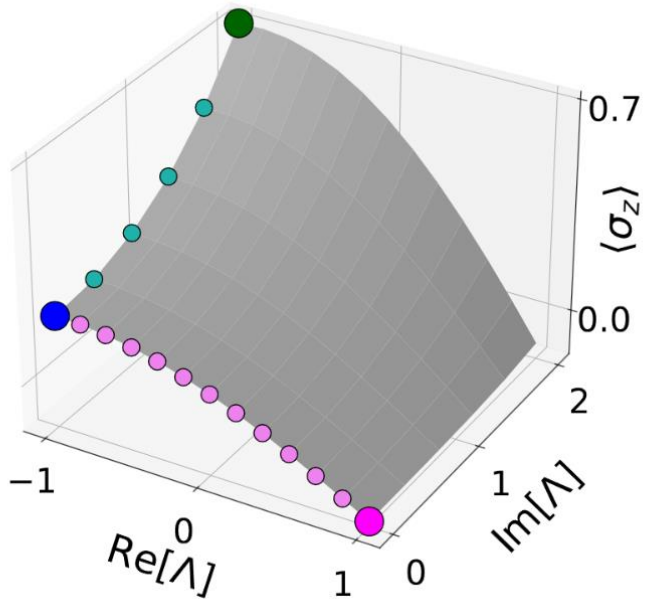
Conclusions and summary

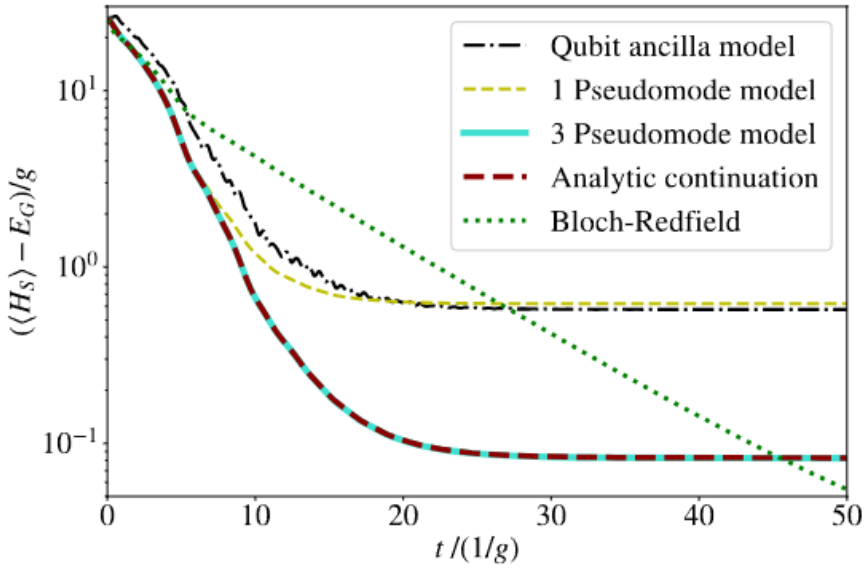
- Open – source software is important and fun.
  - Will it help get you a job? Yes, but probably in industry!
  - How to do it? Just contribute! Put your code on github, keep it upto date, contribute it to an existing library (Julia, python, etc)
- **Non-Markovian solvers and methods have uses in many topics!**
- But… the field is running out of acronyms, and many similar methods are being developed.
- As a user, how can we know what is best for certain problems, and whether we are using it correctly?

Unphysical couplings can’t be realized directly….
How can this be done in a quantum simulation?



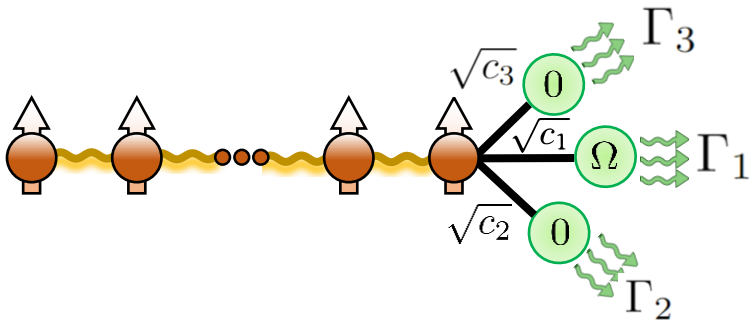
Try extrapolation (analytical continuation) from physical models!





Extrapolated from 9 couplings, 6th order polynomial

Limitations of this approach:



- Extrapolation amplifies measurement error exponentially: need to keep order of fitting polynomial small

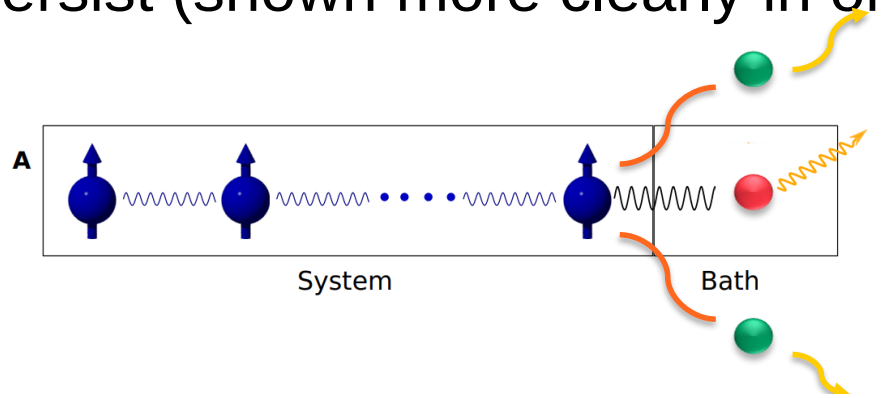
- Can any set of ancillas with local couplings connect any arbitrary Hamiltonian to the ground-state?

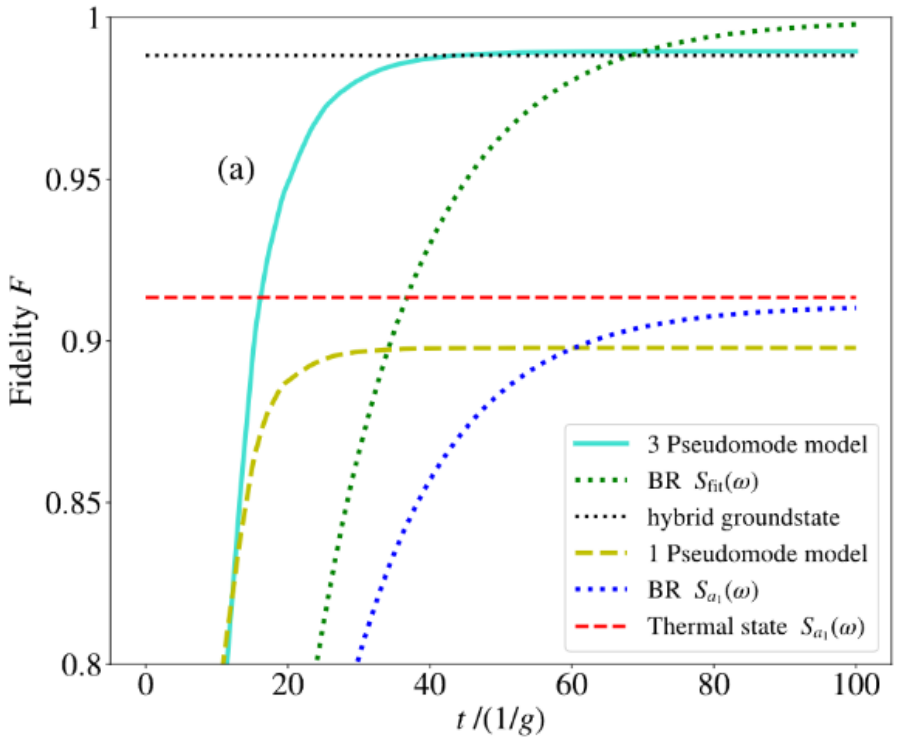
  Srednicki hypothesis suggests this might be difficult!

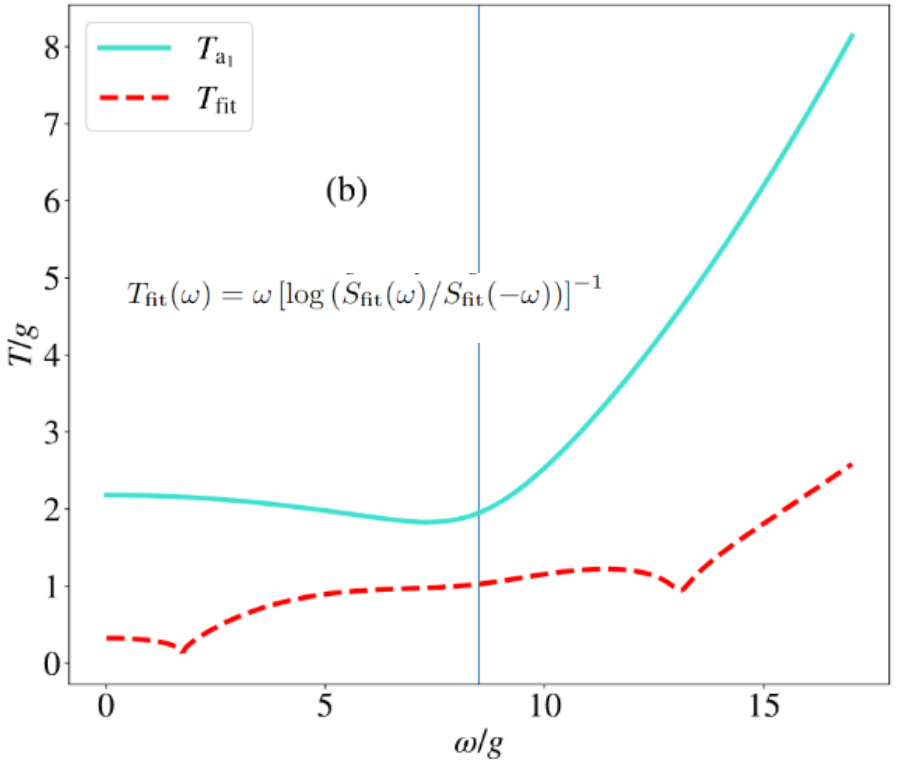
$$\dot{\rho}_s(t) \;=\; -i\,[H_{\rm s},\rho_s(t)] + \sum_{i,j>i} S(\Delta_{j,i})c_{i,j}L[d_{ij}]\rho_s(t) + \sum_{i,j>i} S(-\Delta_{j,i})c_{i,j}L[d_{ij}^\dagger]\rho_s(t),$$

$$c_{i,j} = |\,\langle\psi_i|\,Q\,|\psi_j\rangle\,|^2 \propto \Omega(E)^{-1/2},$$

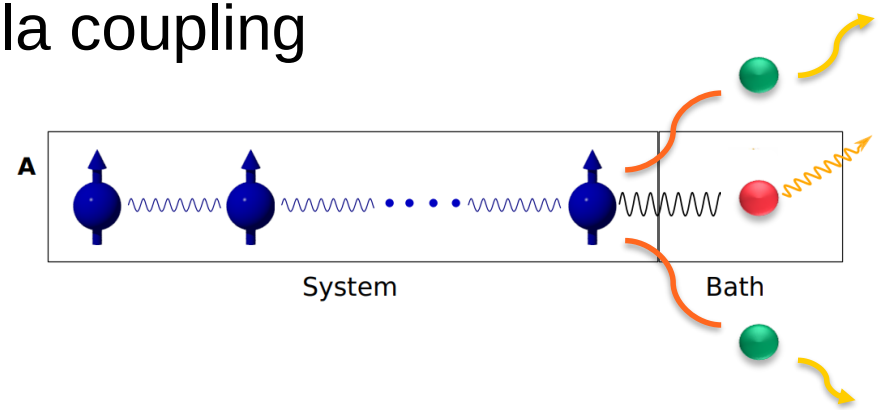
Dissipative state engineering: Hybridization and PM fitting errors still persist (shown more clearly in on-resonance results):

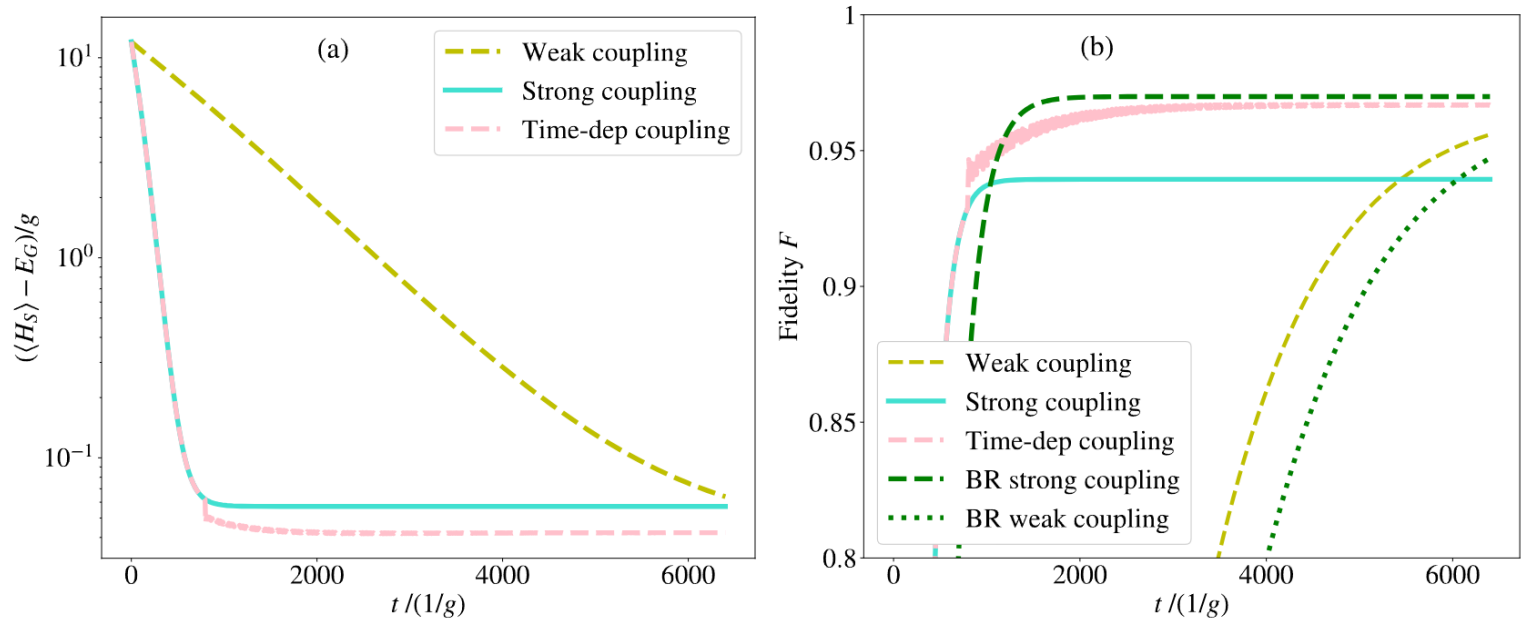






Dissipative state engineering: When gap is small, thermalization slows down. Compensate with time-dependent control of ancilla coupling





Dissipative state engineering: Scaling of extrapolation: