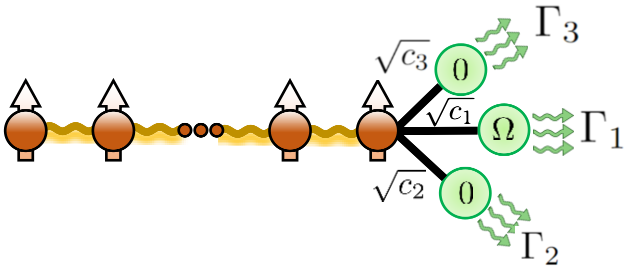
Pseudomodes: from solving the spin-boson model to finding ground states

Neill Lambert



- **N. Lambert, M. Cirio, J. Lin, P. Menczel, P-F. Liang, F. Nori, arXiv:2310.12539 (2023)**
- N. Lambert, S. Ahmed, M. Cirio, F. Nori, Nature Communications 10, 3721 (2019)

Other pseudo-applications of pseudomodes:

- M. Cirio, S. Luo, P. Liang, F. Nori, N. Lambert, PRR (2024) (error mitigation, simulation)
- P. Menczel, K. Funo, M. Cirio, N. Lambert, F. Nori, PRR (2024) (generalized proof, thermodynamics)
- S. Li, N. Lambert, M.Cirio, PRX Quantum (2023) (stochastic)
- M. Cirio, N. Lambert, P-F. Liang, P-C. Kuo, Y-N. Chen, P. Menczel, K. Funo, F. Nori, Phys. Rev. Research (2022) (fermions and Kondo physics)
- M. Cirio, P-C. Kuo, Y-N. Chen, F. Nori, N. Lambert, Phys. Rev. B **105**, 035121 (2022) (fermionic influence functional)

Overview

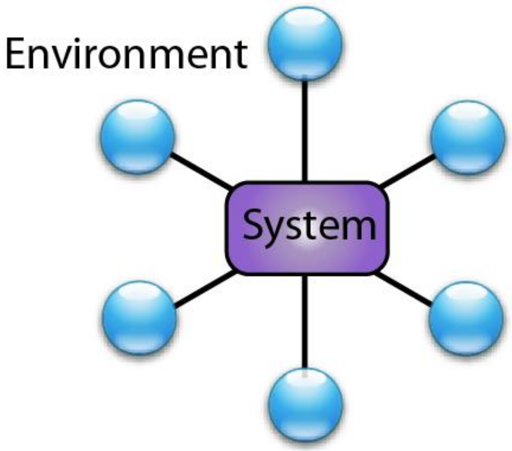
1. **Introduction & open quantum systems**

2. Pseudo-modes for bosonic environments

3. Dissipative state engineering

Introduction

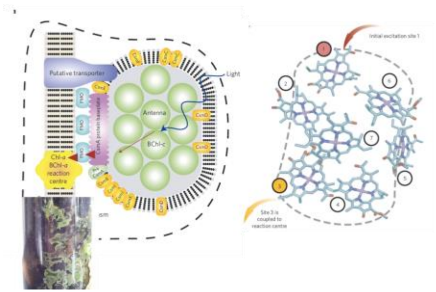
A common approach to understanding noise in quantum systems is a system-bath model. Here the environment is understand as a large continuum of modes, while the system is small and discrete.



The environment is typically composed of infinite degrees of freedom. However, if it is only weakly coupled to the system, one can adopt several perturbative approaches.

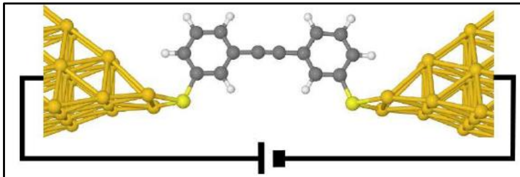
Born-Markov-Secular approximations result in the standard and well known Lindblad master equations.

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



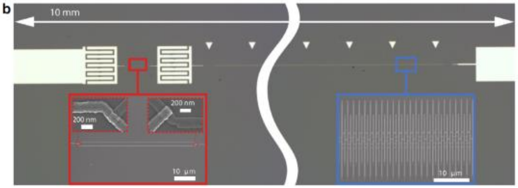
Physical Chemistry: E.g., Energy transfer in photosynthetic complexes:

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.



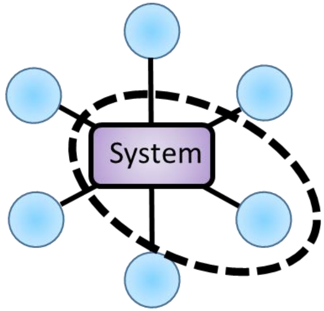
Circuit quantum electro-dynamics (QED):
open transmission lines, SQUID arrays, meta-materials can directly realize engineered quantum environments.

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

Different Strategies to model non-Markovian effects

Physical Approach

Model the most relevant **physical** environmental degrees of freedom

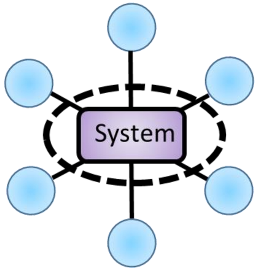


- ✓ Compute both system and bath dynamics

Ex. Polaron transformation, Bath discretizations, Reaction Coordinate...

Effective Approach

Reproduce **the effects** of the environment on the system



- ✓ Minimal knowledge
- ✓ More efficient
- X Only system dynamics

Ex. HEOM, Dissipatons, **Pseudomodes**.

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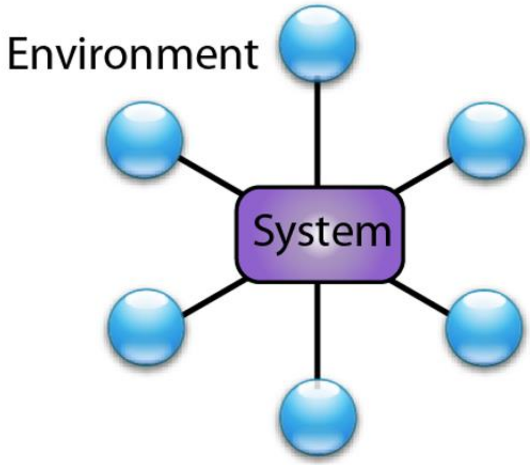
3. Dissipative state engineering

Origin of pseudo-mode concept

A system-environment model can, when the environment is Gaussian, be fully characterized by environment two-time correlation functions; **the Feynman-Vernon influence functional:**

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

Linear



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Linear

$$\boxed{\rho_S(t)} = \mathrm{Tr}_B \left\{ \mathcal{T} e^{-i \int_0^t d\tau \, [\hat{s}(\tau) X(\tau), \cdot]} \rho_S(0) \otimes \rho_B \right\}$$

Gaussian

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Gaussian

$$= F[\hat{s}, \langle X(t) \cdots X(t) \rangle, \rho_S(0)]$$

Wick's theorem

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

$$C(t) = \langle X(t)X(0) \rangle = \frac{1}{\pi}\int_0^\infty d\omega\; J(\omega) \left[\coth\left(\frac{\beta\omega}{2}\right)\cos(\omega t) - i\sin(\omega t)\right]$$

A new approach to the pseudo-mode method

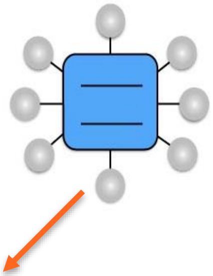
Pseudomodes: We can replace the continous environment with a finite environment with the same correlation functions Garraway (PRB 1997)

Full system-environment model:

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

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

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



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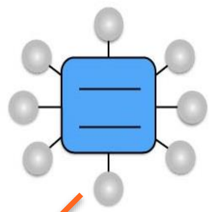

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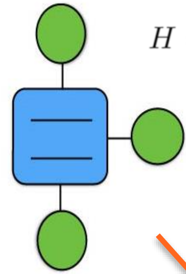
Pseudomodes: Numerically solvable (sometimes)



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

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

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

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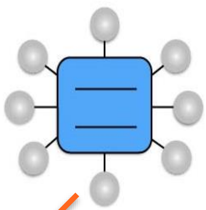

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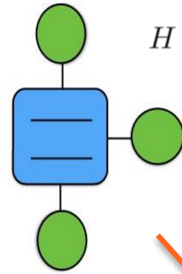

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Our earlier work: Pseudomodes with imaginary parameters are more flexible for this purpose Nat. Comms. 2019, and very powerful for describing non-perturbative baths

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

Overview

1. Introduction & open quantum systems

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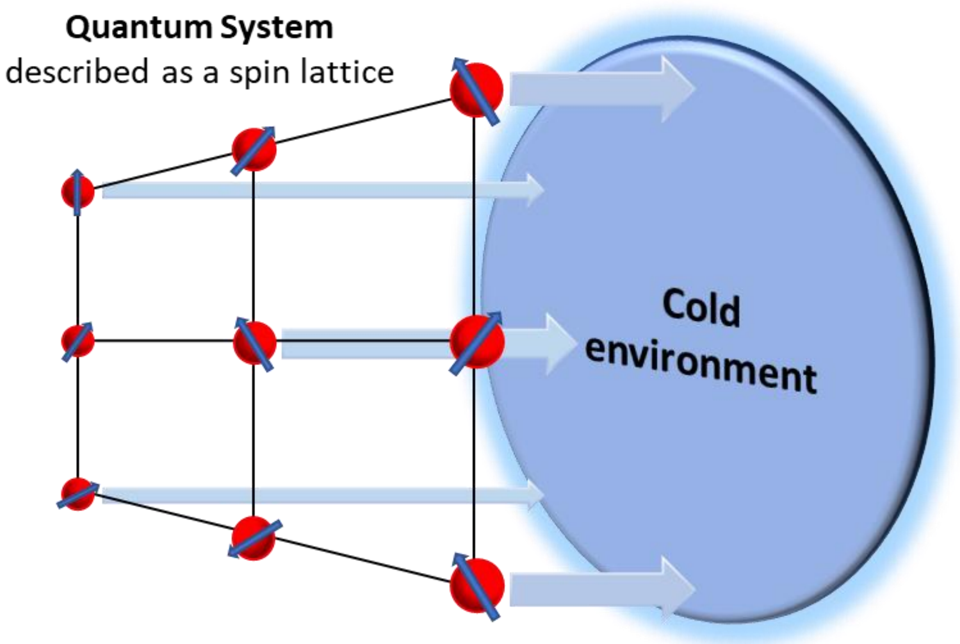
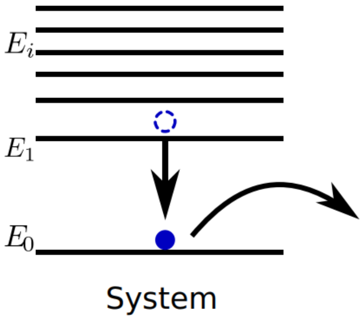
3. **Dissipative state engineering**

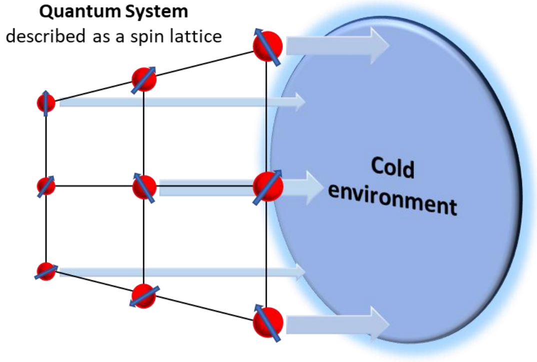
What is 'dissipative state engineering'?

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



Lindblad equations: A useful basis for DSE?

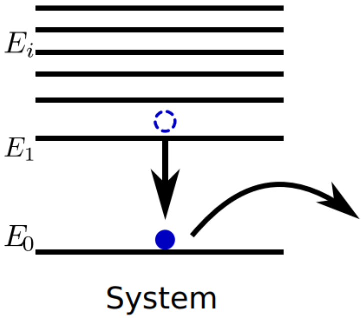


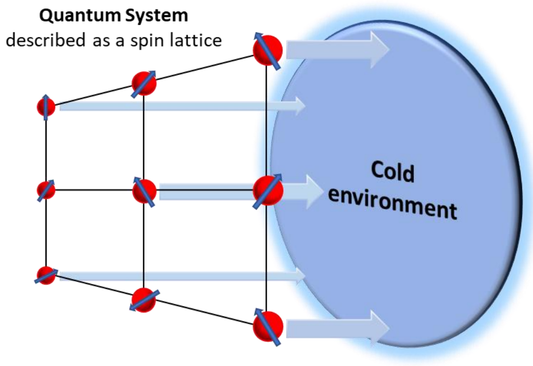


<u>Vestraete, Wolf, Cirac, Nature Physics 2009:</u>
Local (system) measurements/dissipation **for frustration-free Hamiltonians.**

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

Lindblad equations: A useful basis for DSE?





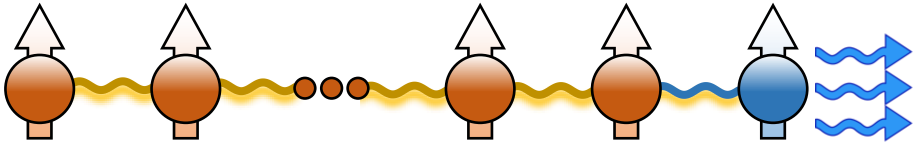
Dissipative state engineering: general case, we already **need to know the eigenstates** to even construct it

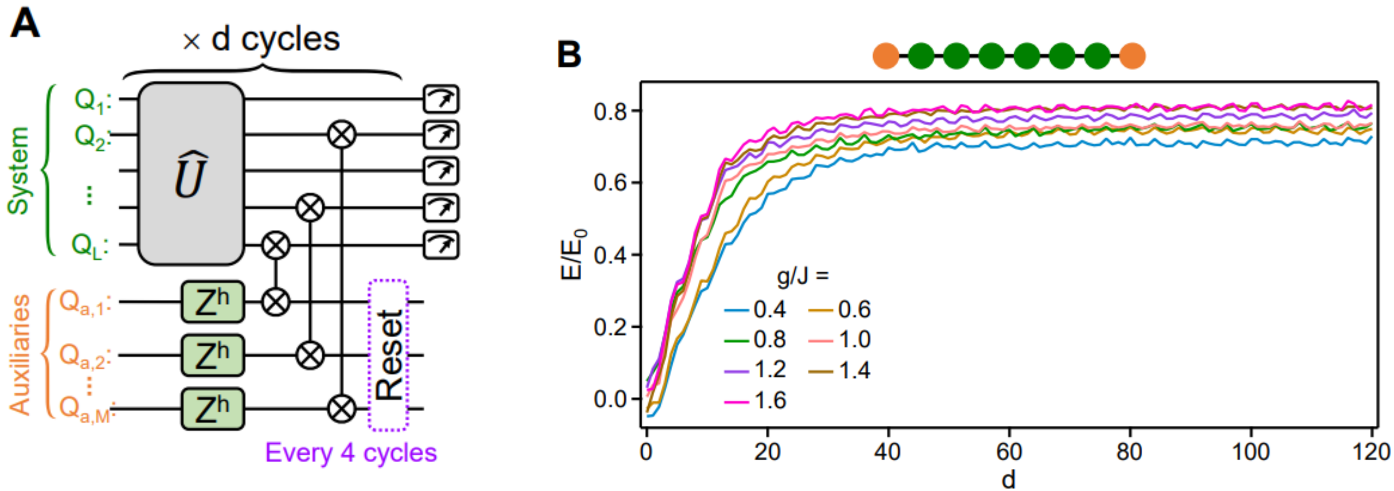
$$\dot{\rho}_s(t) = -i\left[H_s, \rho_s(t)\right] + \sum_{i,j>i} S(\Delta_{j,i}) c_{i,j} L[d_{ij}]\rho_s(t) + \sum_{i,j>i} S(-\Delta_{j,i}) c_{i,j} L[d_{ij}^\dagger]\rho_s(t),$$

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

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)





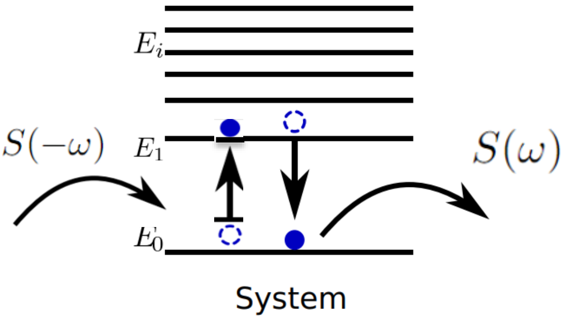
Use of ancilla acts like **structured environment**

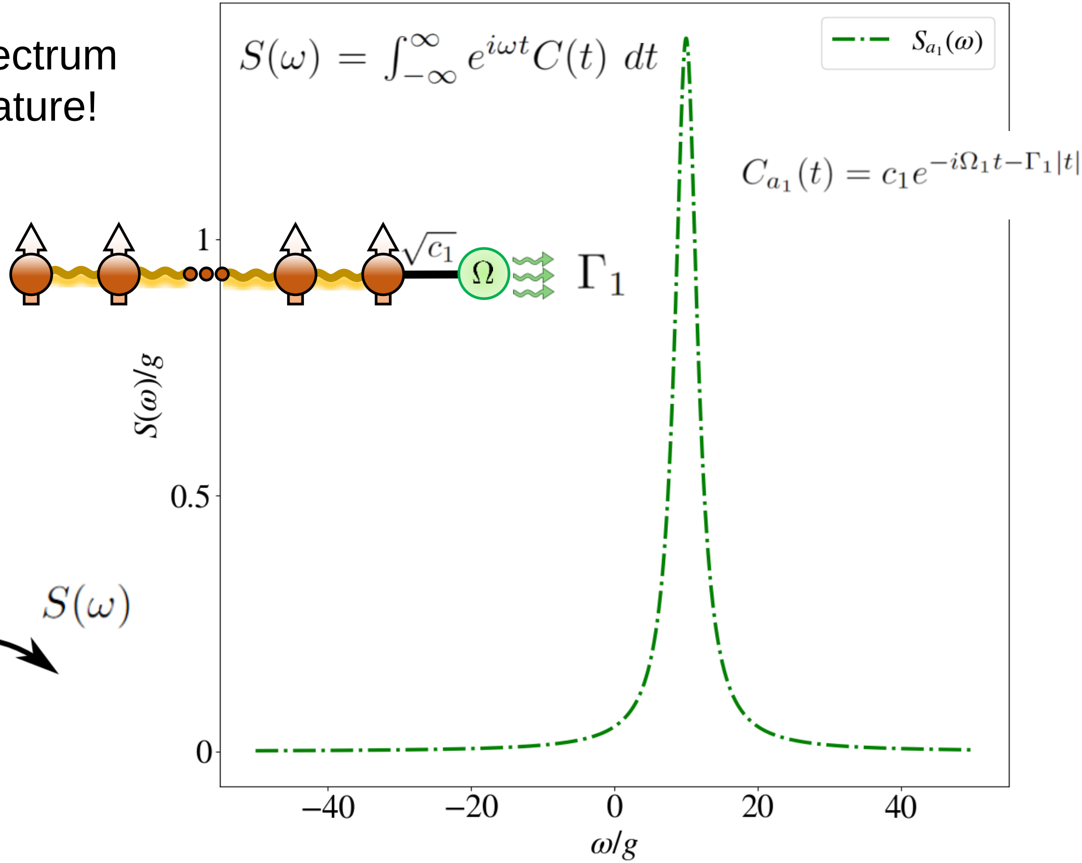
But… not perfect, there is no detailed balance! **Saturates at 90% fidelity even in theoretical simulations**

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!

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





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

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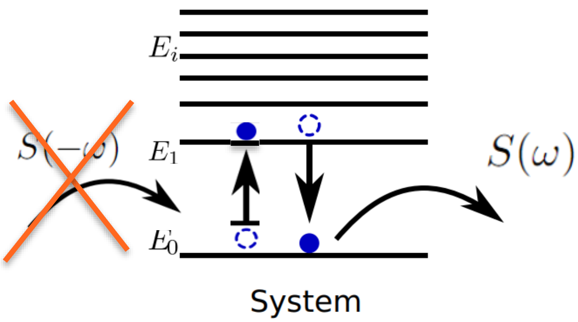
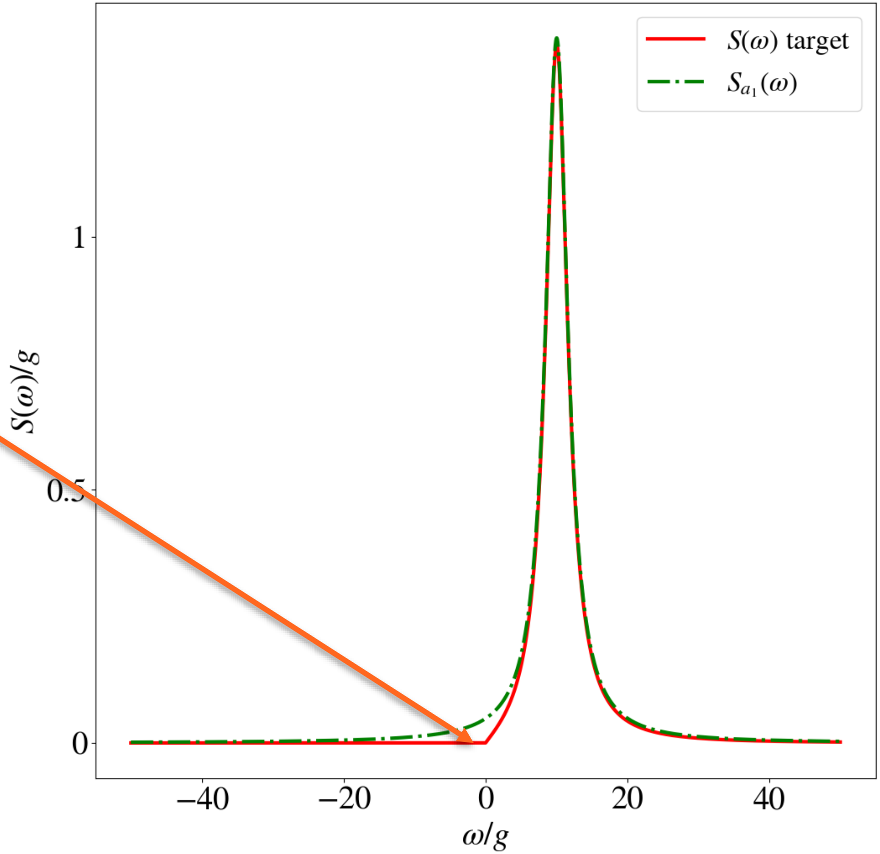
Baths at zero temperature should have zero power spectrum at negative frequencies!





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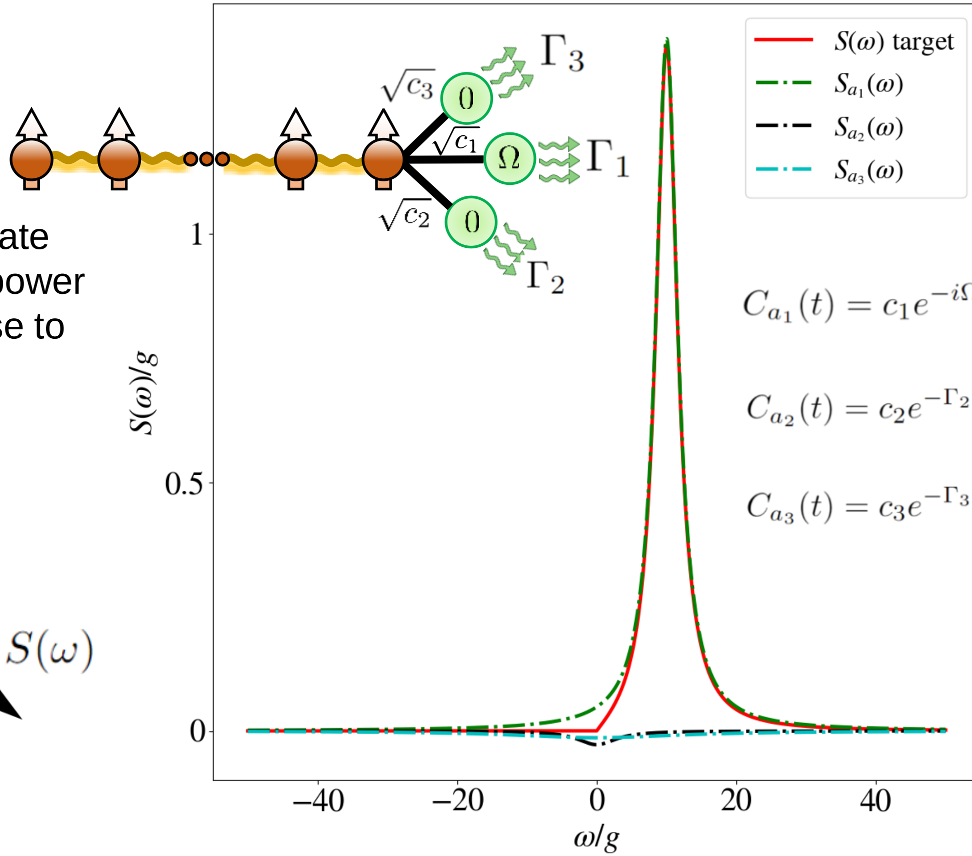
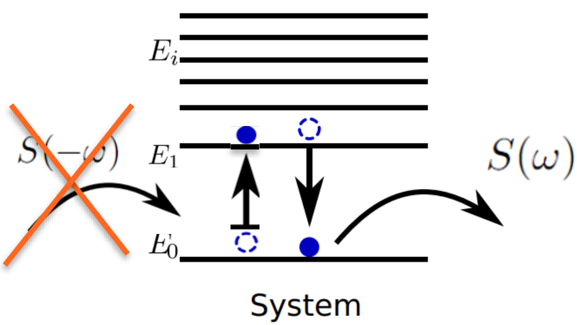
We can add unphysical pseudomodes that compensate and push the total effective power spectrum to be small, or close to zero….



$$C_{a_1}(t) = c_1 e^{-i\Omega_1 t - \Gamma_1 |t|}$$

$$C_{a_2}(t) = c_2 e^{-\Gamma_2 |t|}$$

$$C_{a_3}(t) = c_3 e^{-\Gamma_3 |t|}$$



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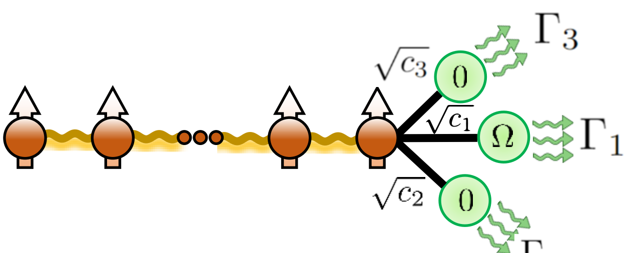

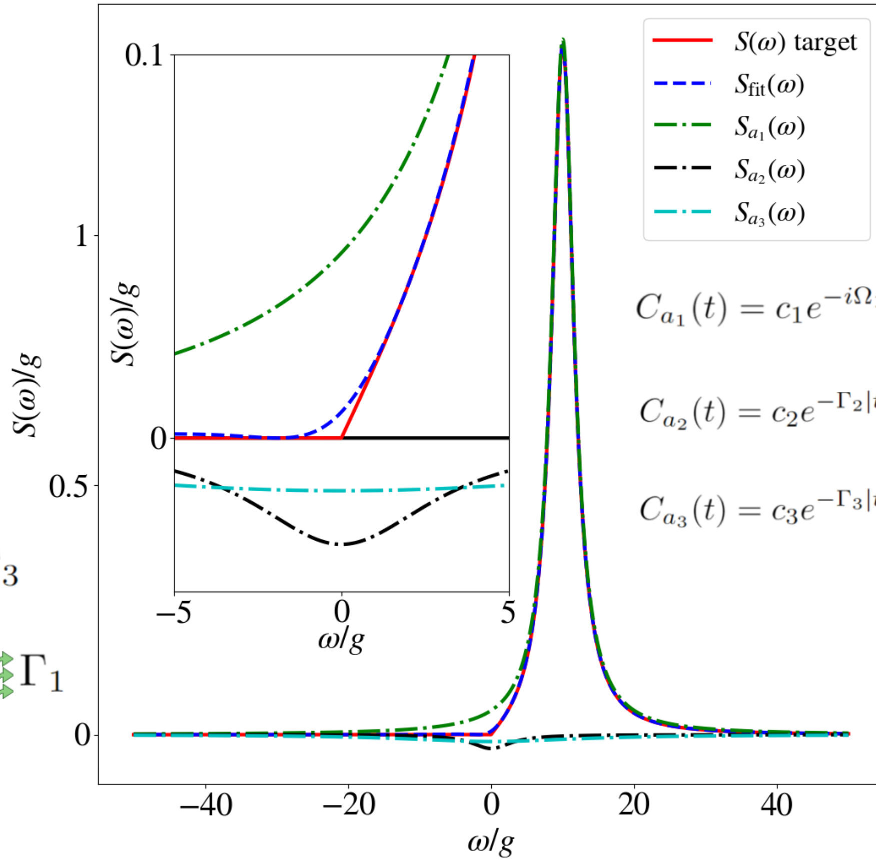

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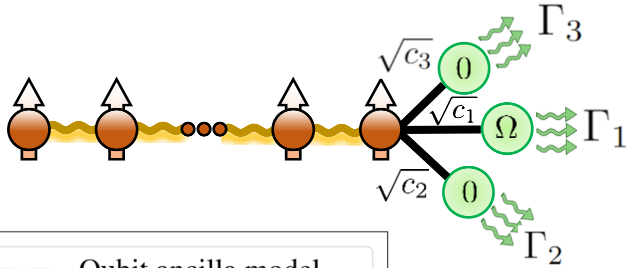
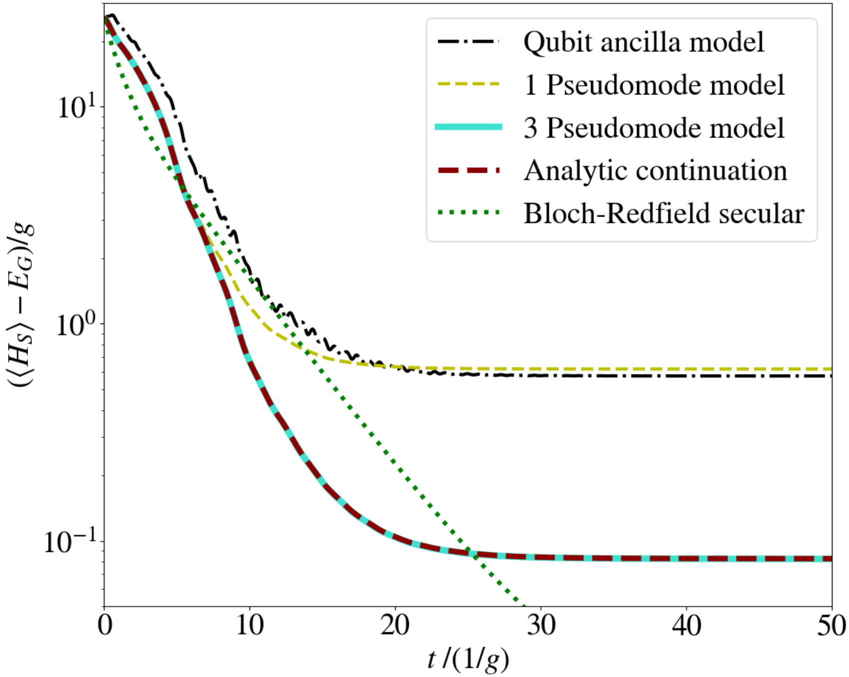
Dissipative state engineering: two additional unphysical ancillas fix detailed balance: 99% ground-state fidelity obtained!

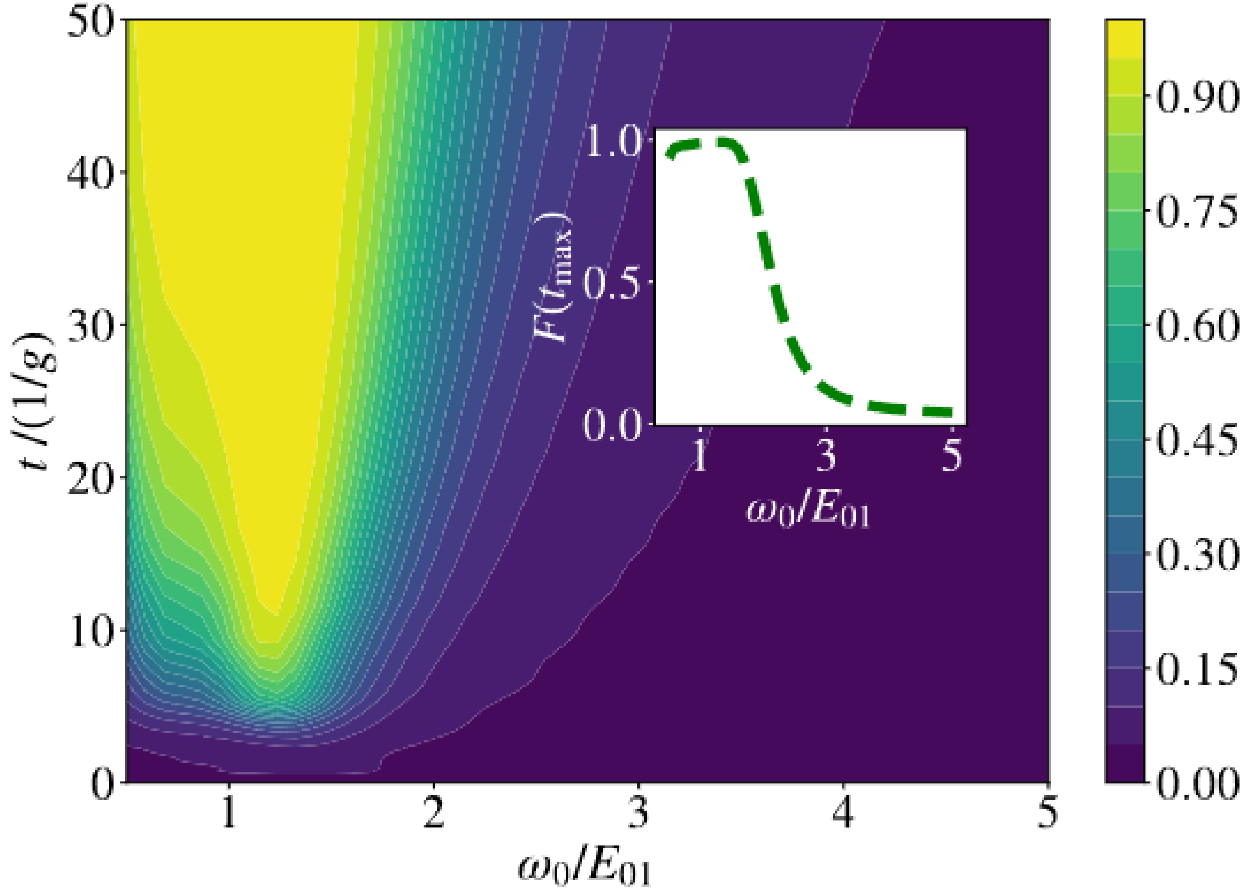




$$H_{\text{sys}} = g\sum_{i=1}^{N}\sigma_z^{(i)} - J\sum_{i=1}^{N-1}\sigma_x^{(i)} \otimes \sigma_x^{(i+1)}$$

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

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



Conclusions

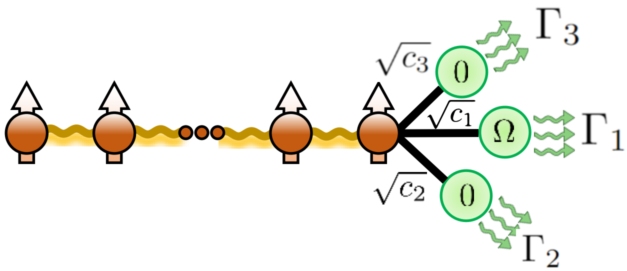
The pseudo-mode method offers a **simple**, approach to modelling non-perturbative and non-Markovian environments

We showed how they can be used as a framework for state engineering in quantum simulation, fixing detailed balance errors of similar ancilla-based schemes

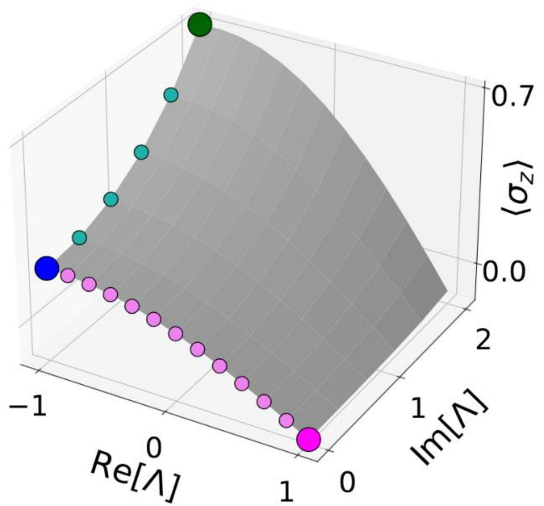
- N. Lambert, **M. Cirio**, J. Lin, **P. Menczel**, P-F., Liang, F. Nori, arXiv:2310.12539 (2023)

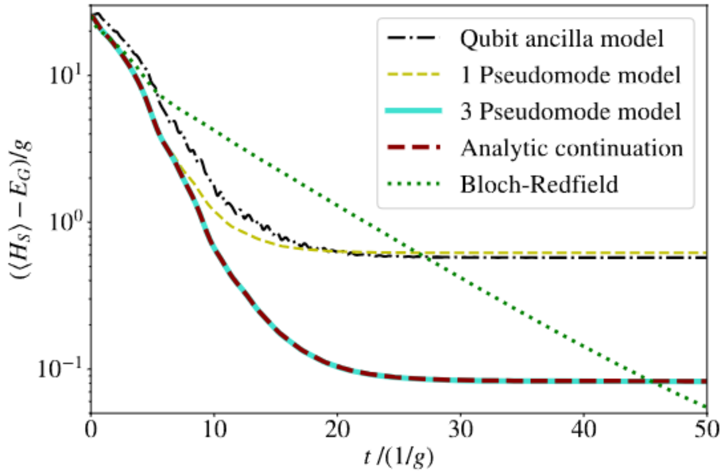
These problems can be implemented digitally with Trotterization + ancillas.
However, unphysical parameters require additional extrapolation step.

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



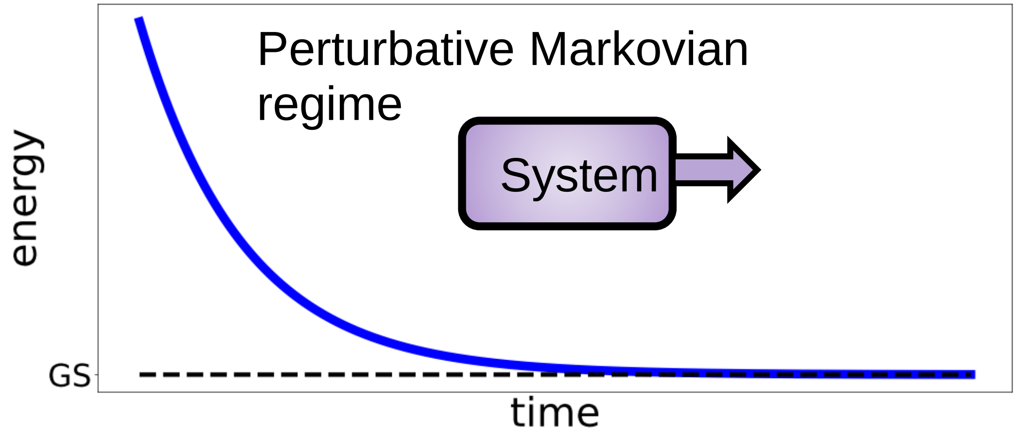
Try extrapolation (analytical continuation) from physical models!

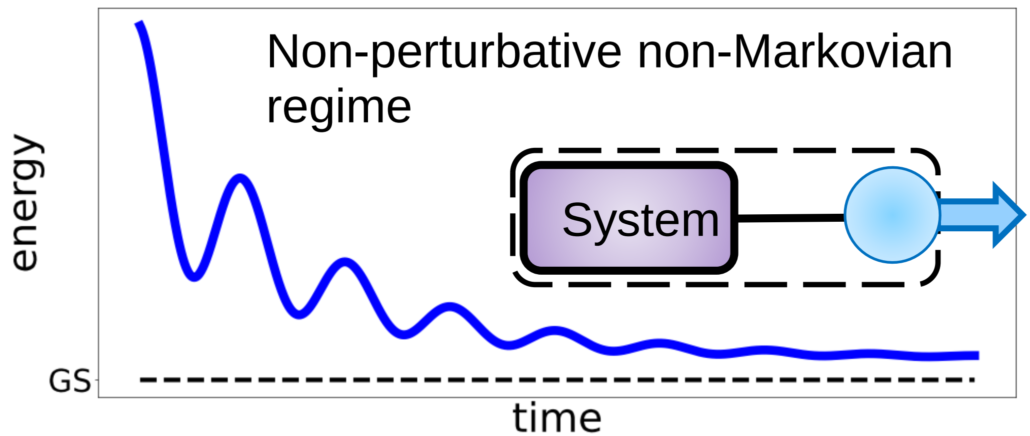




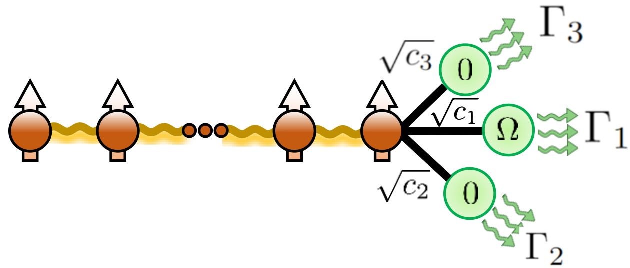
Extrapolated from 9 couplings, 6th order polynomial

Markovian vs. non-Markovian ?





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?

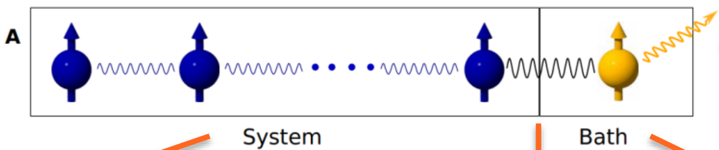
Srednicki hypothesis suggests this might be difficult!

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

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

Turns out, someone tried something very similar already……

Raghunandan *et al., Sci. Adv. (2020)* suggested using a discrete ancilla(s) + local ancilla dissipation

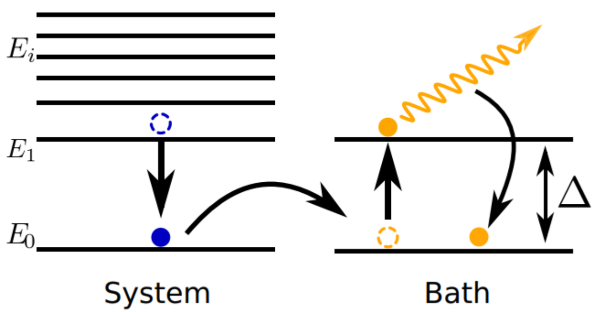


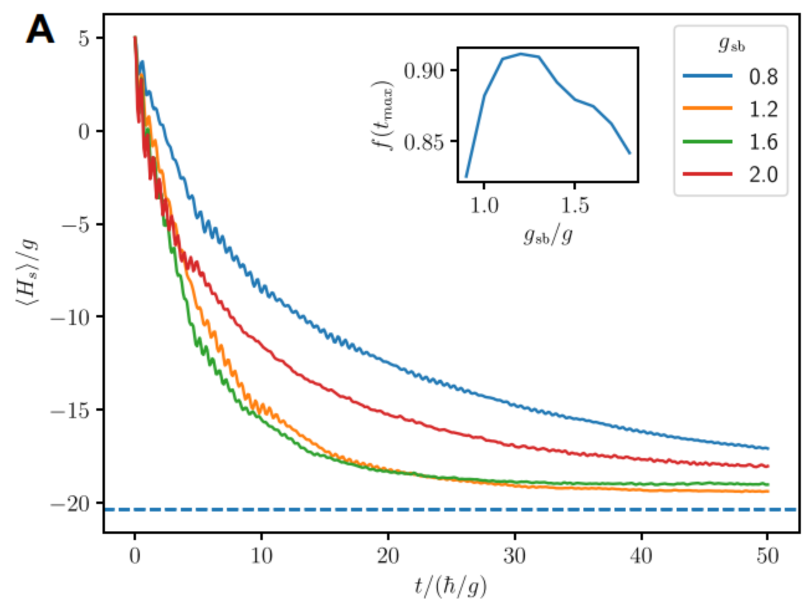
$$\gamma\left(\sigma_-^{(b)}\rho\sigma_+^{(b)} - \frac{1}{2}\left\{\sigma_+^{(b)}\sigma_-^{(b)},\rho\right\}\right)$$

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

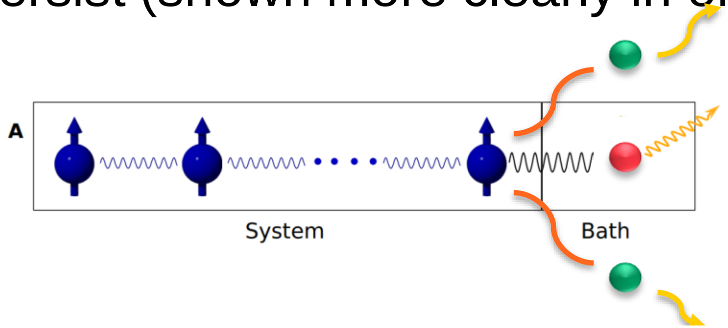
$$H_{\text{int}} = g_{\text{sb}}\sum_{x,y,z} f_i\,\sigma_i^{(N)}\sigma_i^{(b)},$$

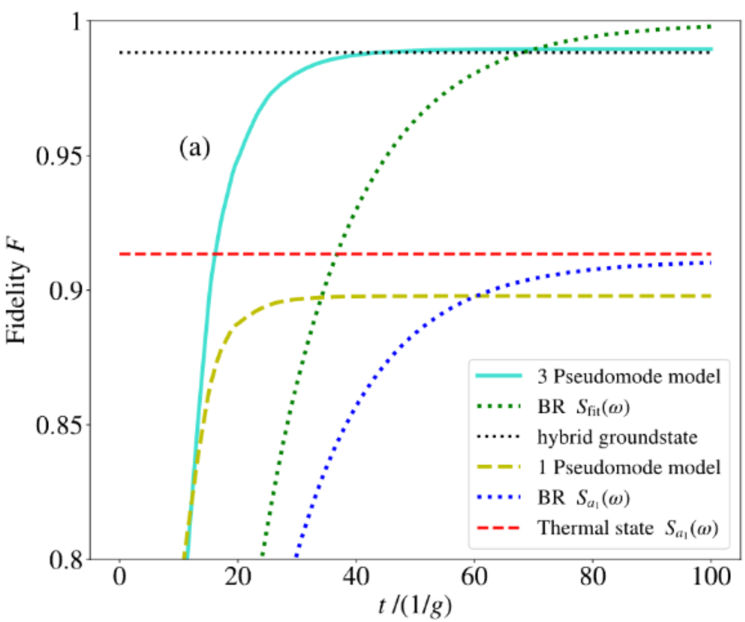
$$H_b = (\Delta/2)\,\sigma_z^{(b)}.$$

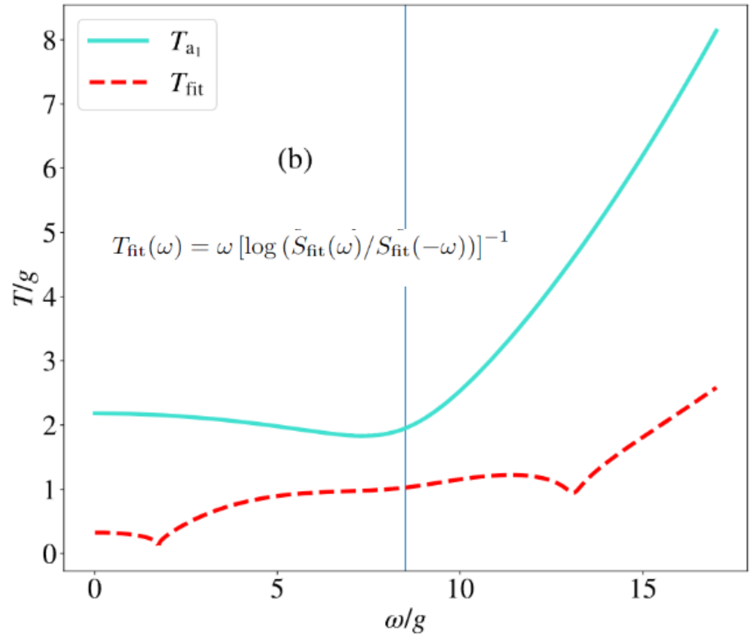




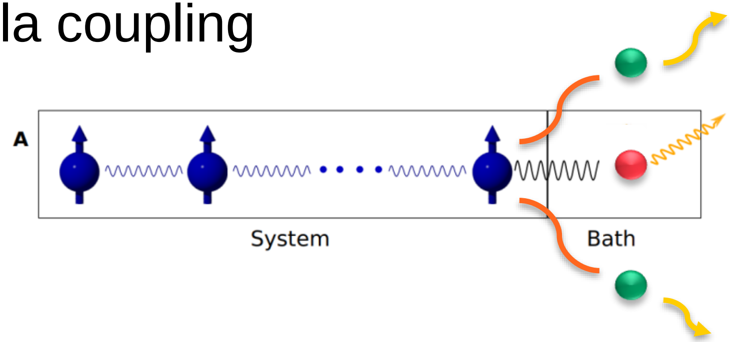
Dissipative state engineering: Hybridization and PM fitting errors still persist (shown more clearly in on-resonance results):

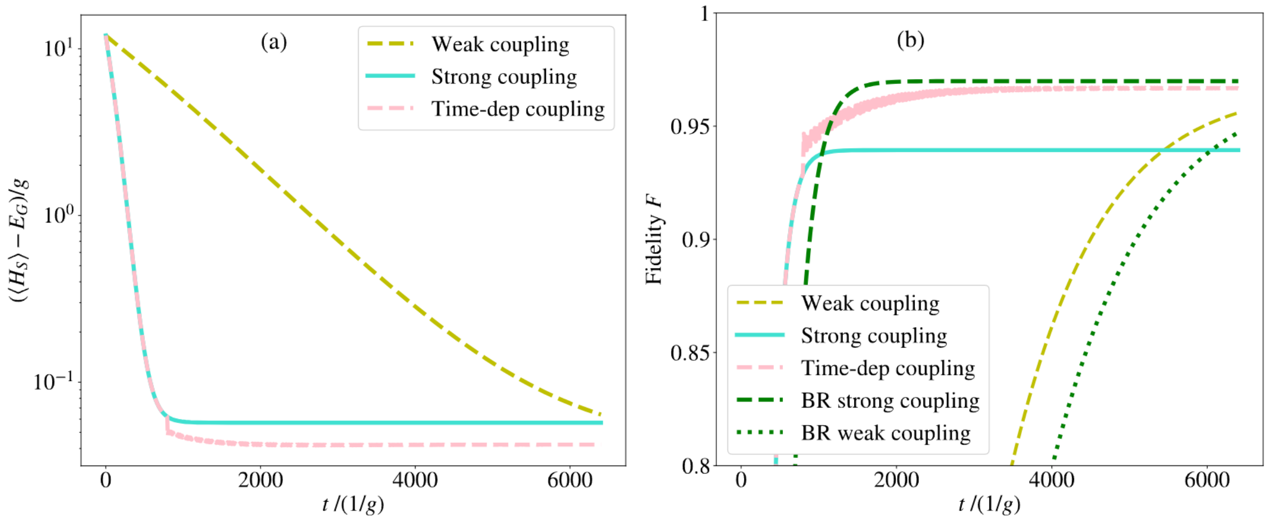




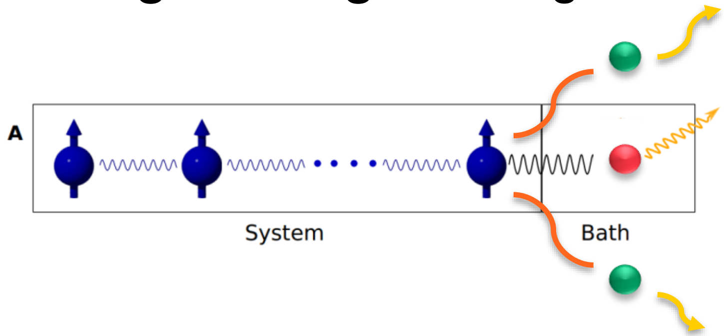


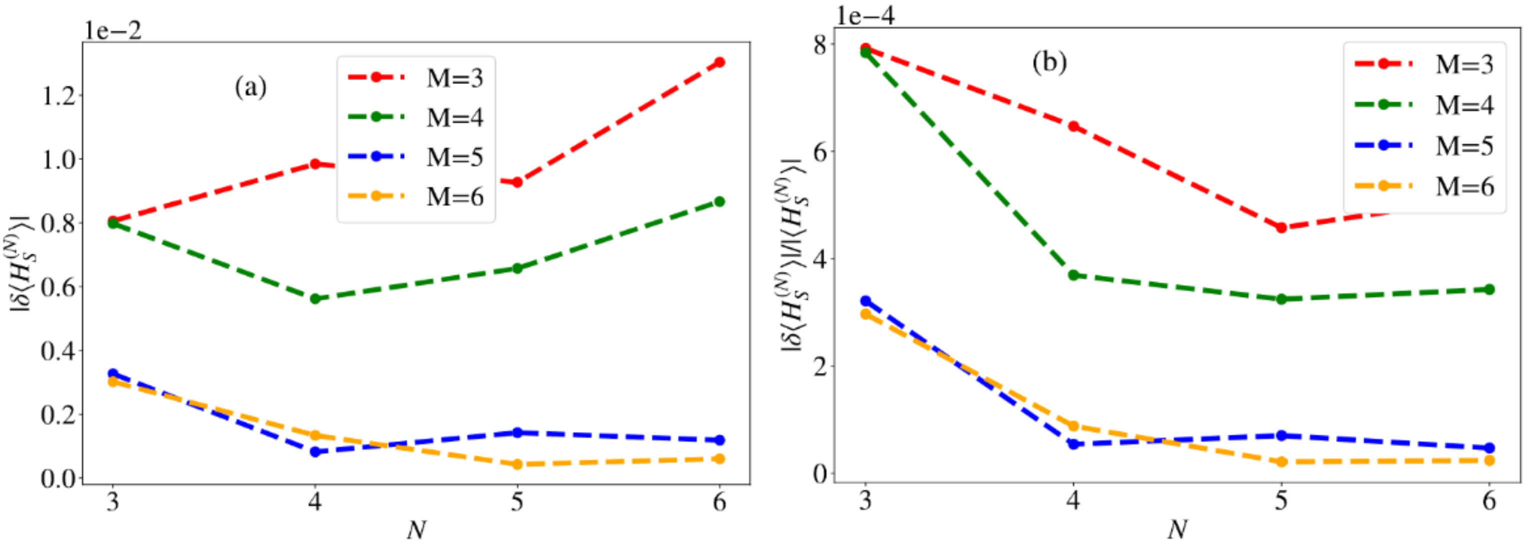
Dissipative state engineering: When gap is small, thermalization slows down. Compensate with time-dependent control of ancilla coupling





Dissipative state engineering: Scaling of extrapolation:





Fermionic baths

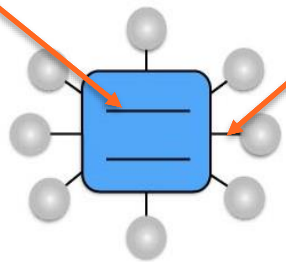
- Generally, we capture the main influence of bath degrees of freedom with a continuum of **fermionic** modes:

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

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?

A new approach to the pseudo-mode method: Fermions

Gaussian environments are fully described by their **correlation functions**

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

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

- We can **replace the continous environment** with a **finite environment** with the **same correlation functions**, and the system should not know the difference.

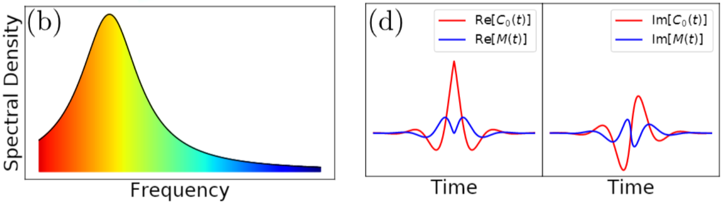
What differs from the bosonic case?

- Correlation functions are split into two:

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

- Parity of initial condition is important (p dependence on initial state above).

Example: Kondo resonance



Two interacting system impurities
in contact with fermionic baths:

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

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

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

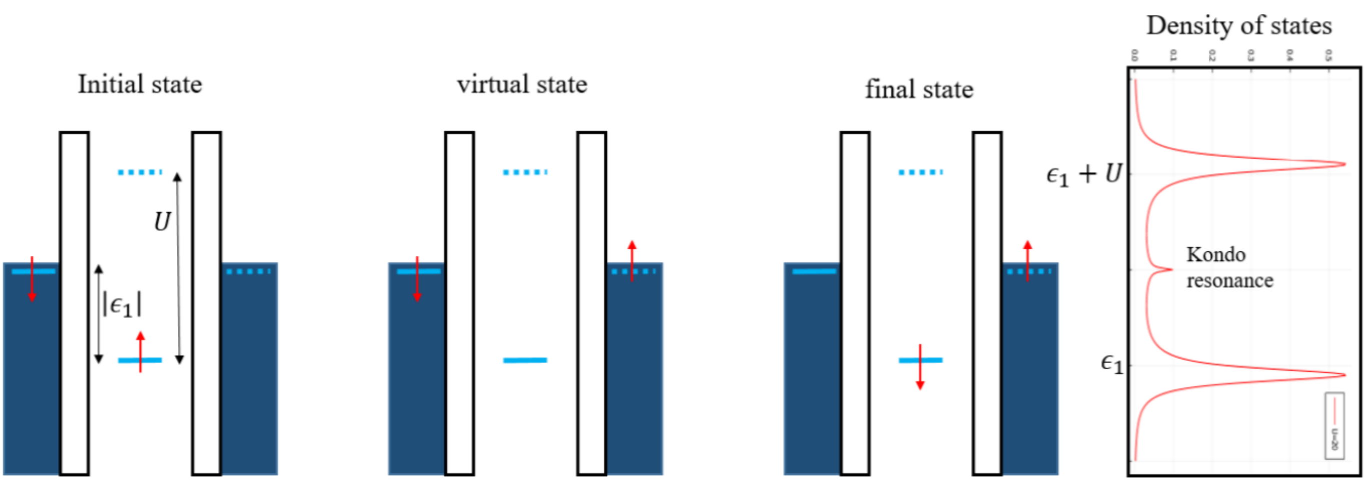
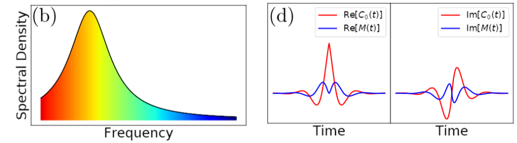


Figure from Po-chen Kuo, PhD Thesis

Example: Kondo resonance



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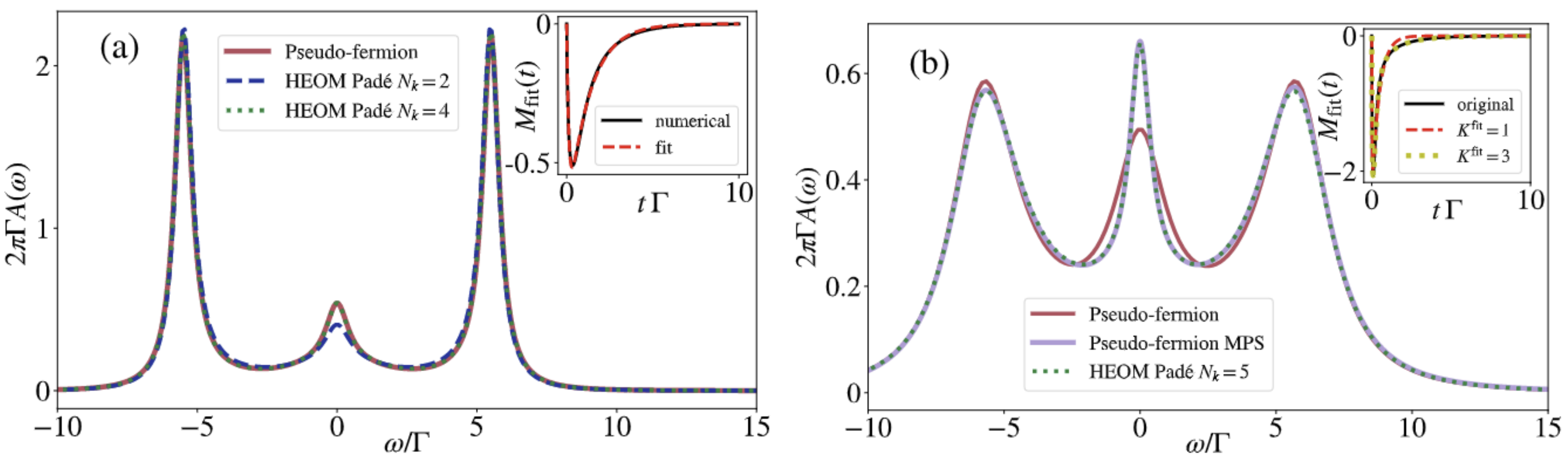

Getting to the scaling limit is hard (as expected), but can be done with MPS, at least for finite temperature