Bath Observables with HOPS

Energy Flow in Strongly Coupled Open Quantum Systems

Valentin Boettcher, Richard Hartmann, Konstantin Beyer, Walter Strunz

Institute for Theoretical Physics, Dresden, Germany

17.08.2022

TECHNISCHE UNIVERSITÄT DRESDEN

Situation

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{1}$$

with $[H_S, H_B] = 0$.

[1] 1, 2.

Situation

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{1}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_{\mathrm{I}} \approx 0$ thermodynamics of open systems are somewhat understood[1]

[1] 1, 2.

Situation

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{1}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_{\mathrm{I}} \approx 0$ thermodynamics of open systems are somewhat understood[1]
- strong coupling: $\langle H_{\mathrm{I}} \rangle \sim \langle H_{\mathrm{S}} \rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?

[1] 1, 2.

Situation

Consider an open quantum system

$$H = \underbrace{H_\mathrm{S}}_{\text{"small"}} + \underbrace{H_\mathrm{I}}_{?} + \underbrace{H_\mathrm{B}}_{\text{"big", simple}} \tag{1}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_\mathrm{I} \approx 0$ thermodynamics of open systems are somewhat understood[1]
- strong coupling: $\langle H_\mathrm{I}\rangle \sim \langle H_\mathrm{S}\rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?
- but what is clear: *need to get access to exact dynamics of* $H_\mathrm{I}, H_\mathrm{B}$

[1] 1, 2.

Is that possible?

Is that possible? Yes.

Is that possible? Yes.
Using HOPS :)

Is that possible? Yes.
Using HOPS :)

Sneak Peek

We will be able to calculate $\frac{\mathrm{d}\langle H_{\mathrm{B}}\rangle}{\mathrm{d}t}$ (and $\langle H_{\mathrm{I}}\rangle$).

- and still more general observables (omitted)

Is that possible? Yes.
Using HOPS :)

Sneak Peek

We will be able to calculate $\frac{\mathrm{d}\langle H_{\mathrm{B}}\rangle}{\mathrm{d}t}$ (and $\langle H_{\mathrm{I}}\rangle$).

- and still more general observables (omitted)

- won't call this *heat-flow* because it isn't *the* thermodynamic heat flow

Is that possible? Yes. Using HOPS :)

Sneak Peek

We will be able to calculate $\frac{\mathrm{d}\langle H_{\mathrm{B}}\rangle}{\mathrm{d}t}$ (and $\langle H_{\mathrm{I}}\rangle$).

- and still more general observables (omitted)

- won't call this *heat-flow* because it isn't *the* thermodynamic heat flow
- nevertheless: may be interesting *qualitative* measure for energy flow

Standard Model of Open Systems

In the following we will work with models of the form[2]

$$H = H_{\mathrm{S}}(t) + \sum_{n=1}^{N} \left[H_{\mathrm{B}}^{(n)} + \left(L_n^\dagger(t) B_n + \mathrm{h.c.} \right) \right], \tag{2}$$

where

- H_{S} is the System Hamiltonian
- $H_B^{(n)} = \sum_\lambda \omega_\lambda^{(n)} a_\lambda^{(n),\dagger} a_\lambda^{(n)}$
- $B_n = \sum_\lambda g_\lambda^{(n)} a_\lambda^{(n)}$.

[2] Sometimes this is called the "Standard Model of Open Systems".

What remains of the Bath?

Bath Correlation Function

$$\alpha(t-s) = \langle B(t)B(s)\rangle \left(\stackrel{T=0}{=} \sum_{\lambda} |g_{\lambda}|^2 \, \mathrm{e}^{-i\omega_{\lambda}(t-s)} \right) = \frac{1}{\pi} \int J(\omega) \, \mathrm{e}^{-i\omega t} \, \mathrm{d}\omega$$

What remains of the Bath?

Bath Correlation Function

$$\alpha(t-s) = \langle B(t)B(s)\rangle \left(\stackrel{T=0}{=} \sum_\lambda |g_\lambda|^2 \, \mathrm{e}^{-i\omega_\lambda(t-s)} \right) = \frac{1}{\pi} \int J(\omega)\, \mathrm{e}^{-i\omega t}\, \mathrm{d}\omega$$

Spectral Density

$$J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(\omega - \omega_\lambda)$$

- in thermodynamic limit $\rightarrow$ smooth function
- here usually: Ohmic SD $J(\omega) = \eta\omega\, \mathrm{e}^{-\omega/\omega_c}$ (think phonons)

NMQSD (Zero Temperature)

Open system dynamics formulated as a *stochastic* differential equation:

$$\partial_t |\psi_t(\boldsymbol{\eta}_t^*)\rangle = -iH(t) |\psi_t(\boldsymbol{\eta}_t^*)\rangle + \mathbf{L} \cdot \boldsymbol{\eta}_t^* |\psi_t(\boldsymbol{\eta}_t^*)\rangle - \sum_{n=1}^{N} L_n^\dagger(t) \int_0^t \mathrm{d}s \, \alpha_n(t-s) \frac{\delta |\psi_t(\boldsymbol{\eta}_t^*)\rangle}{\delta \eta_n^*(s)}, \quad (3)$$

with

$$\mathcal{M}(\eta_n(t)) = 0, \quad \mathcal{M}(\eta_n(t)\eta_m(s)) = 0, \quad \mathcal{M}(\eta_n(t)\eta_m(s)^*) = \delta_{nm}\alpha_n(t-s), \quad (4)$$

by projecting on coherent bath states.[3]
System state can be recovered by averaging over η

$$\rho_\mathrm{S}(t) = \mathrm{tr}_\mathrm{B}\left[|\psi(t)\rangle\langle\psi(t)|\right] = \mathcal{M}_{\boldsymbol{\eta}_t^*}[|\psi_t(\boldsymbol{\eta}_t)\rangle\langle\psi_t(\boldsymbol{\eta}_t^*)|]. \quad (5)$$

[3] For details see: [3]

HOPS

Using $\alpha_n(\tau) = \sum_{\mu}^{M_n} G_{\mu}^{(n)}\, \mathrm{e}^{-W_{\mu}^{(n)}\tau}$ we define

$$D_{\mu}^{(n)}(t) \equiv \int_0^t \mathrm{d}s\, G_{\mu}^{(n)}\, \mathrm{e}^{-W_{\mu}^{(n)}(t-s)}\, \frac{\delta}{\delta \eta_n^*(s)} \tag{6}$$

and $D^{\underline{\mathbf{k}}} \equiv \prod_{n=1}^{N} \prod_{\mu=1}^{M_n} \sqrt{\frac{\underline{\mathbf{k}}_{n,\mu}!}{\left(G_{\mu}^{(n)}\right)^{\underline{\mathbf{k}}_{n,\mu}}}} \frac{1}{i^{\underline{\mathbf{k}}_{n,\mu}}} \left(D_{\mu}^{(n)}\right)^{\underline{\mathbf{k}}_{n,\mu}}$, $\psi_t^{\underline{\mathbf{k}}} \equiv D^{\underline{\mathbf{k}}}\psi_t$ we find

$$\begin{aligned} \dot{\psi}_t^{\underline{\mathbf{k}}} = {} & \left[-iH_{\mathrm{S}}(t) + \mathbf{L}(t)\cdot \boldsymbol{\eta}_t^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} \underline{\mathbf{k}}_{n,\mu} W_{\mu}^{(n)}\right]\psi_t^{\underline{\mathbf{k}}} \\ & + i \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} \sqrt{G_{\mu}^{(n)}} \left[\sqrt{\underline{\mathbf{k}}_{n,\mu}} L_n(t) \psi_t^{\underline{\mathbf{k}}-\underline{\mathbf{e}}_{n,\mu}} + \sqrt{\left(\underline{\mathbf{k}}_{n,\mu}+1\right)} L_n^{\dagger}(t) \psi_t^{\underline{\mathbf{k}}+\underline{\mathbf{e}}_{n,\mu}}\right]. \end{aligned} \tag{7}$$

Zero Temperature, One Bath, Linear NMQSD

We want to calculate

$$J = -\frac{\mathrm{d}\left\langle H_{\mathrm{B}}\right\rangle}{\mathrm{d}t} = \left\langle L^\dagger \partial_t B(t) + L\partial_t B^\dagger(t)\right\rangle_{\mathrm{I}}. \tag{8}$$

Zero Temperature, One Bath, Linear NMQSD

We want to calculate

$$J = -\frac{\mathrm{d}\left\langle H_{\mathrm{B}}\right\rangle}{\mathrm{d}t} = \left\langle L^\dagger \partial_t B(t) + L \partial_t B^\dagger(t)\right\rangle_{\mathrm{I}}. \tag{8}$$

...some manipulations ...

Zero Temperature, One Bath, Linear NMQSD

We want to calculate

$$J = -\frac{\mathrm{d}\langle H_{\mathrm{B}}\rangle}{\mathrm{d}t} = \left\langle L^\dagger \partial_t B(t) + L \partial_t B^\dagger(t) \right\rangle_{\mathrm{I}}. \tag{8}$$

...some manipulations ...

Result (NMQSD)

$$J(t) = -i\mathcal{M}_{\eta^*} \langle\psi(\eta, t)| L^\dagger \dot{D}_t |\psi(\eta^*, t)\rangle + \mathrm{c.c.} \tag{9}$$

with $\dot{D}_t = \int_0^t \mathrm{d}s\, \dot{\alpha}(t-s) \frac{\delta}{\delta\eta_s^*}$.

Zero Temperature, One Bath, Linear NMQSD

We want to calculate

$$J = -\frac{\mathrm{d}\langle H_\mathrm{B}\rangle}{\mathrm{d}t} = \left\langle L^\dagger \partial_t B(t) + L \partial_t B^\dagger(t)\right\rangle_\mathrm{I}. \tag{8}$$

...some manipulations ...

Result (NMQSD)

$$J(t) = -i\mathcal{M}_{\eta^*}\langle\psi(\eta,t)|\, L^\dagger \dot{D}_t \,|\psi(\eta^*,t)\rangle + \mathrm{c.c.} \tag{9}$$

with $\dot{D}_t = \int_0^t \mathrm{d}s\,\dot{\alpha}(t-s)\frac{\delta}{\delta\eta^*_s}$.

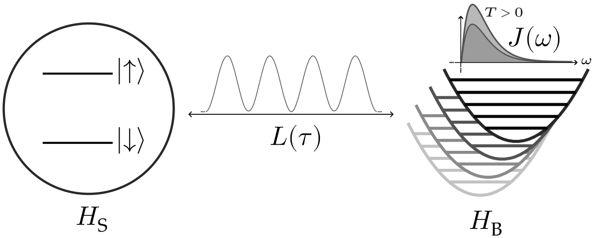
Result (HOPS)

$$J(t) = -\sum_\mu \sqrt{G_\mu} W_\mu \mathcal{M}_{\eta^*}\left\langle\psi^{(0)}(\eta,t)\right|\, L^\dagger \,|\psi^{\mathbf{e}_\mu}(\eta^*,t)\rangle + \mathrm{c.c.} \tag{10}$$

Generalizations

- finite temperatures
- nonlinear NMQSD/HOPS
- multiple baths straight forward
- interaction energy: “removing the dot”...
- general “collective” bath observables $O_{\mathrm{S}} \otimes (B^a)^\dagger B^b$ with $B = \sum_\lambda g_\lambda a_\lambda$

Model

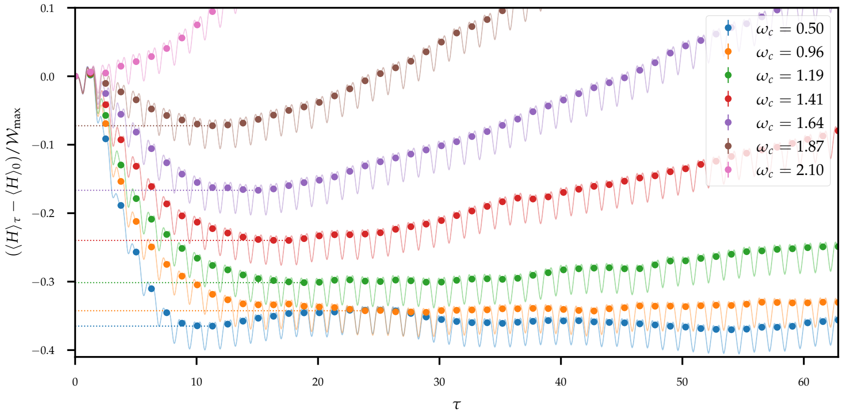


$$H = \frac{1}{2}\sigma_z + \frac{f(\tau)}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda,\ |\psi_0\rangle_{\mathrm{S}} = |\downarrow\rangle \tag{11}$$

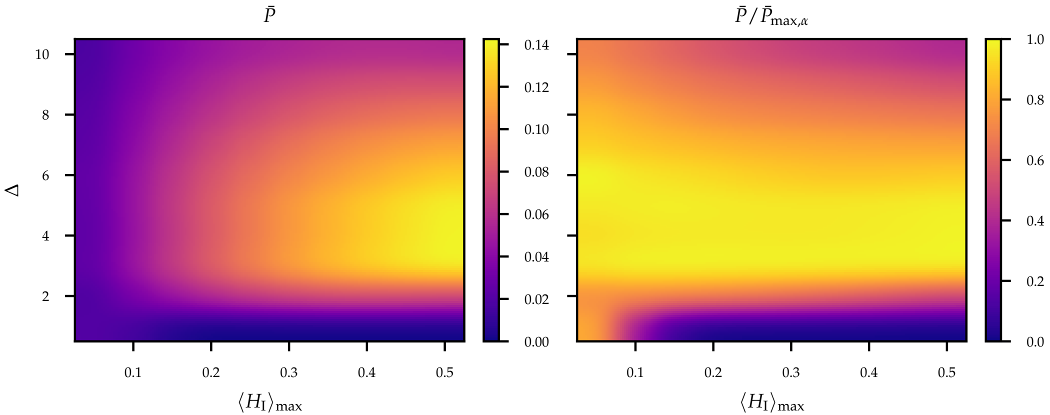
- $f(\tau) = \sin^2(\frac{\Delta}{2}\tau)$
- initial state of total system: $\rho_0 = |\downarrow\rangle\langle\downarrow| \otimes \frac{\mathrm{e}^{-\beta H_{\mathrm{B}}}}{Z}$
- Shifted SD for resonance

Extracting Energy from One Bath

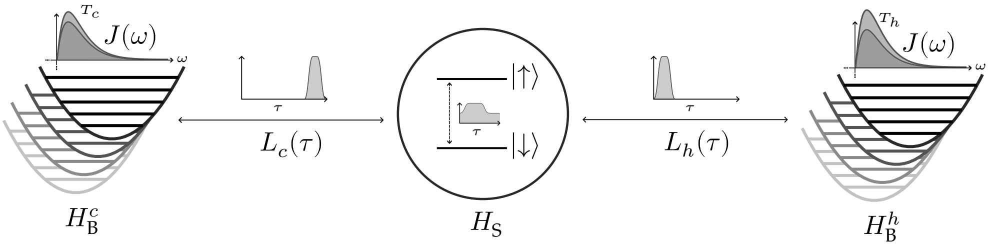
- how much energy can be *unitarily* extracted? $\implies \mathcal{W}_{\max} = \frac{1}{\beta} S\left(\rho_{\mathrm{S}} \,\middle\|\, \rho_{\mathrm{S}}^{\beta}\right)$



Speed Limit


$\bar{P}$
$\bar{P}/\bar{P}_{\max,\alpha}$
Δ
10
8
6
4
2
0.1
0.2
0.3
0.4
0.5
$\langle H_I \rangle_{\max}$
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1.0
0.8
0.6
0.4
0.2
0.0

Quantum Otto Cycle



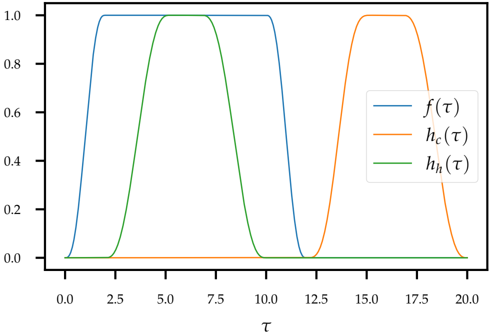
Model

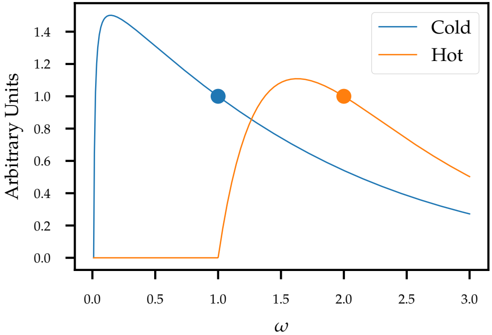
Spin-Boson model with compression of H_{S} and modulation of L.

- classical toy model of the quantum heat engine community[4]

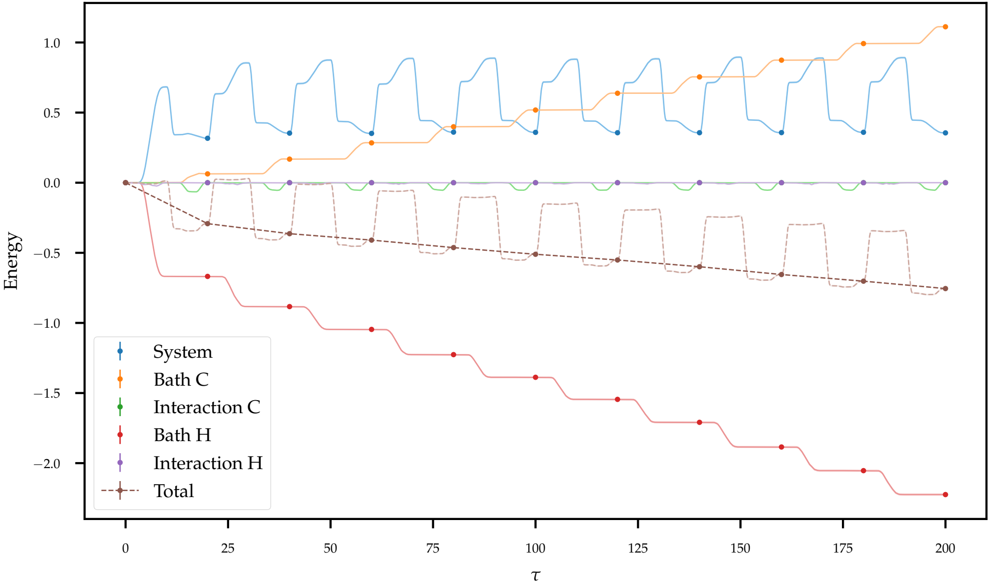
[4] 4.

Modulation and Spectral Densities

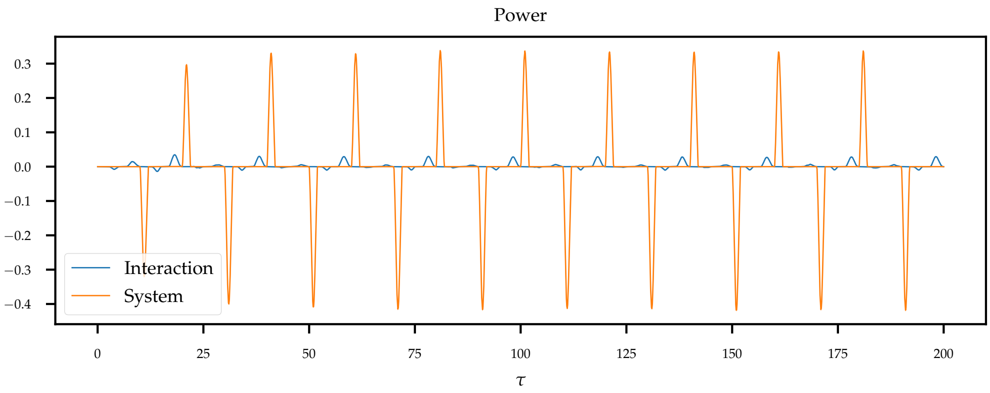




Full Energy Overview

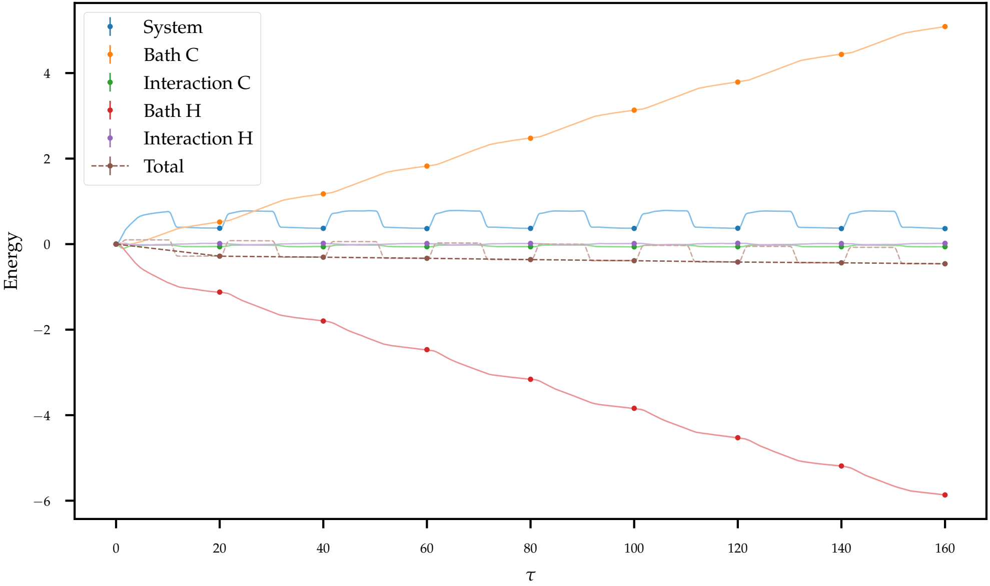


Power Contributions



- $\bar{P} = .0025$, $\eta \approx 29\%$, $T_c = 1$, $T_h = 20$
- no tuning of parameters, except for resonant coupling
- long bath memory $\omega_c = 1$, but weak-ish coupling

Continuously Coupled Version



Current Work

- better performance through "overlapping" and shifting strokes?
- stronger coupling any good?
- non-Markovianity + strong coupling any good?
- what is the optimal efficiency and power?

On the “To Do” List

- verify/falsify weak coupling results in the literature (engines)
- three-level systems: there is an experimental paper ;)
- parameter scan of two qubit model
- filter modes
- ...

Lessons Learned

- careful convergence checks pay off
- surveying literature is important
- properly documenting observations is a great help and should be done as early as possible
- applications should be carefully chosen to answer interesting questions
- numerics are helpful, but physical insights are important
- comparison with some experiments would have been nice

References I

[1] Á. Rivas, "Strong Coupling Thermodynamics of Open Quantum Systems", arXiv, 10.1103/PhysRevLett.124.160601 (2019) (cit. on pp. 4–7, 54–60, 62).

[2] P. Talkner and P. Hnggi, "Colloquium: Statistical mechanics and thermodynamics at strong coupling: Quantum and classical", Rev. Mod. Phys. **92**, 041002 (2020) (cit. on pp. 4–7, 54–60, 62).

[3] L. Disi, N. Gisin, and W. T. Strunz, "Non-Markovian quantum state diffusion", Phys. Rev. A **58**, 1699–1712 (1998) (cit. on p. 18).

[4] E. Geva and R. Kosloff, "A quantum-mechanical heat engine operating in finite time. A model consisting of spin-1/2 systems as the working fluid", J. Chem. Phys. **96**, 3054–3067 (1992) (cit. on p. 32).

[5] T. Motz, M. Wiedmann, J. T. Stockburger, and J. Ankerhold, "Rectification of heat currents across nonlinear quantum chains: a versatile approach beyond weak thermal contact", New J. Phys. **20**, 113020 (2018) (cit. on p. 62).

References II

[6] M. Wiedmann, J. T. Stockburger, and J. Ankerhold, “Non-Markovian dynamics of a quantum heat engine: out-of-equilibrium operation and thermal coupling control”, New J. Phys. **22**, 033007 (2020) (cit. on p. 62).

[7] J. Senior, A. Gubaydullin, B. Karimi, J. T. Peltonen, J. Ankerhold, and J. P. Pekola, “Heat rectification via a superconducting artificial atom - Communications Physics”, Commun. Phys. **3**, 1–5 (2020) (cit. on p. 62).

[8] A. Kato and Y. Tanimura, “Quantum heat transport of a two-qubit system: Interplay between system-bath coherence and qubit-qubit coherence”, J. Chem. Phys. **143**, 064107 (2015) (cit. on p. 62).

[9] A. Kato and Y. Tanimura, “Quantum heat current under non-perturbative and non-Markovian conditions: Applications to heat machines”, J. Chem. Phys. **145**, 224105 (2016) (cit. on p. 62).

[10] P. Strasberg and A. Winter, “First and Second Law of Quantum Thermodynamics: A Consistent Derivation Based on a Microscopic Definition of Entropy”, PRX Quantum **2**, 030202 (2021) (cit. on p. 62).

References III

[11] P. Talkner and P. Hnggi, “Open system trajectories specify fluctuating work but not heat”, Phys. Rev. E **94**, 022143 (2016) (cit. on p. 62).

[12] M. L. Bera, M. Lewenstein, and M. N. Bera, “Attaining Carnot efficiency with quantum and nanoscale heat engines - npj Quantum Information”, npj Quantum Inf. **7**, 1–7 (2021) (cit. on p. 62).

[13] M. L. Bera, S. Juli-Farr, M. Lewenstein, and M. N. Bera, “Quantum Heat Engines with Carnot Efficiency at Maximum Power”, arXiv (2021) (cit. on p. 62).

[14] M. Esposito, M. A. Ochoa, and M. Galperin, “Nature of heat in strongly coupled open quantum systems”, Phys. Rev. B **92**, 235440 (2015) (cit. on p. 62).

[15] J. Klauder and E. Sudarshan, “Fundamentals of quantum optics benjamin”, Inc., New York (1968) (cit. on p. 64).

[16] W. T. Strunz, “Stochastic schrödinger equation approach to the dynamics of non-markovian open quantum systems”, (Fachbereich Physik der Universität Essen, 2001) (cit. on p. 64).

References IV

[17] X. Gao, J. Ren, A. Eisfeld, and Z. Shuai, "Non-Markovian Stochastic Schr\"odinger Equation: Matrix Product State Approach to the Hierarchy of Pure States", arXiv (2021) (cit. on pp. 65–67).

Model

$$H = \frac{\Omega}{4}(p^2 + q^2) + \frac{1}{2}q\sum_{\lambda}\left(g_{\lambda}^{*}b_{\lambda} + g_{\lambda}b_{\lambda}^{\dagger}\right) + \sum_{\lambda}\omega_{\lambda}b_{\lambda}^{\dagger}b_{\lambda}, \quad (12)$$

Model

$$H = \frac{\Omega}{4}(p^2 + q^2) + \frac{1}{2} q \sum_\lambda \left(g_\lambda^* b_\lambda + g_\lambda b_\lambda^\dagger \right) + \sum_\lambda \omega_\lambda b_\lambda^\dagger b_\lambda, \tag{12}$$

...leading to ...

$$\dot{q} = \Omega p \tag{13}$$

$$\dot{p} = -\Omega q - \int_0^t \Im[\alpha_0(t-s)] q(s) \, \mathrm{d}s + W(t) \tag{14}$$

$$\dot{b}_\lambda = -i g_\lambda \frac{q}{2} - i\omega_\lambda b_\lambda \tag{15}$$

with the operator noise $W(t) = -\sum_\lambda \left(g_\lambda^* b_\lambda(0) \, \mathrm{e}^{-i\omega_\lambda t} + g_\lambda b_\lambda^\dagger(0) \, \mathrm{e}^{i\omega_\lambda t} \right)$,
$\langle W(t) W(s) \rangle = \alpha(t-s)$ and $\alpha_0 \equiv \alpha\big|_{T=0}$.

Solution through a matrix $G(t)$ with $G(0) = \mathbb{1}$ and

$$\dot{G}(t) = AG(t) - \int_0^t K(t-s)G(s)\,\mathrm{d}s\,, \quad A = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}, \quad K(t) = \begin{pmatrix} 0 & 0 \\ \Im[\alpha_0(t)] & 0 \end{pmatrix}. \quad (16)$$

Solution through a matrix $G(t)$ with $G(0) = \mathbb{1}$ and

$$\dot{G}(t) = AG(t) - \int_0^t K(t-s)G(s)\,\mathrm{d}s\,, \quad A = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}, \quad K(t) = \begin{pmatrix} 0 & 0 \\ \Im[\alpha_0(t)] & 0 \end{pmatrix}. \tag{16}$$

Then

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = G(t)\begin{pmatrix} q(0) \\ p(0) \end{pmatrix} + \int_0^t G(t-s)\begin{pmatrix} 0 \\ W(s) \end{pmatrix}\mathrm{d}s\,. \tag{17}$$

- “exact” solution via laplace transform and BCF expansion + residue theorem

Result

Solution

$$G(t) = \sum_{l=1}^{N+1} \left[R_l \begin{pmatrix} \tilde{z}_l & \Omega \\ \frac{\tilde{z}_l^2}{\Omega} & \tilde{z}_l \end{pmatrix} \mathrm{e}^{\tilde{z}_l \cdot t} + \text{c.c.} \right] \tag{18}$$

with $R_l = f_0(\tilde{z}_l)/p'(\tilde{z}_l)$, f_0, p polynomials, $\tilde{z}_l$ roots of p.

Result

Solution

$$G(t) = \sum_{l=1}^{N+1} \left[R_l \begin{pmatrix} \tilde{z}_l & \Omega \\ \frac{\tilde{z}_l^2}{\Omega} & \tilde{z}_l \end{pmatrix} \mathrm{e}^{\tilde{z}_l \cdot t} + \text{c.c.} \right] \tag{18}$$

with $R_l = f_0(\tilde{z}_l)/p'(\tilde{z}_l)$, f_0, p polynomials, $\tilde{z}_l$ roots of p.

- note: G doesn't depend on temperature
- solution very sensitive to precision of the fits and roots

Bath Energy Derivative

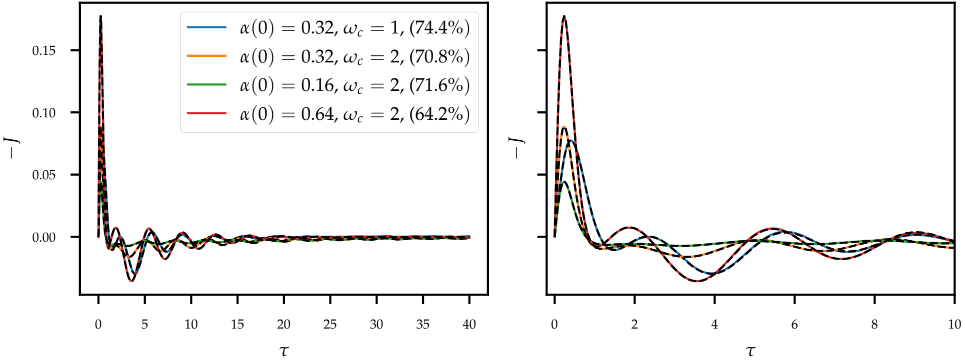
$$
\begin{aligned}
\langle \dot{H}_B \rangle &= \sum_\lambda \omega_\lambda \Big(\Big\langle b_\lambda^\dagger \dot{b}_\lambda \Big\rangle + \text{c.c.} \Big) \\
&= -\frac{1}{2} \Im \Bigg[\int_0^t \mathrm{d}s \, \langle q(t) q(s) \rangle \, \dot{\alpha}_0(t-s) \Bigg] \\
&\qquad + \frac{1}{2} G_{12}(t) [\alpha(t) - \alpha_0(t)] - \frac{\Omega}{2} \int_0^t \mathrm{d}s \, G_{11}(s) [\alpha(s) - \alpha_0(s)]
\end{aligned}
\tag{19}
$$

- becomes huge sum of exponentials (thanks Mathematica)

One Bath, Finite Temperature

Parameters

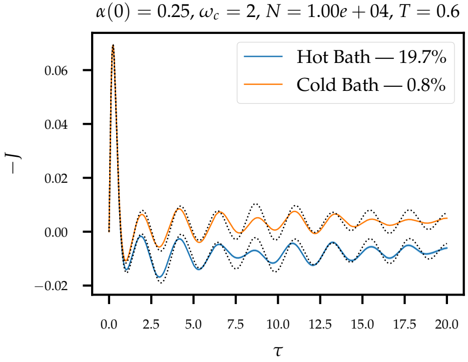
$\Omega = 1$, Ohmic BCF $\frac{\eta}{\pi}(\omega_c/(1+i\omega_c\tau))^2$ with $(\alpha(0) = 0.64,\, \omega_c = 2)$, $N = 10^5$ samples, 15 Hilbert space dimensions, $|\psi(0)\rangle_S = |1\rangle_S$, $T = 1$

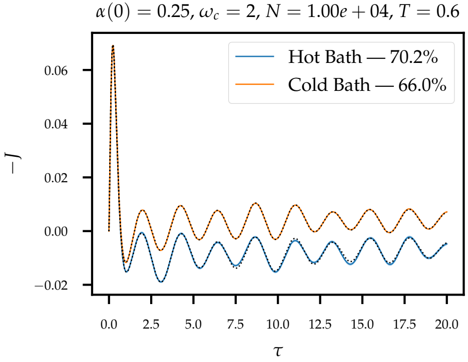


Two Baths, Finite Temperature (Gradient)

Parameters

$\Omega = \Lambda = 1$, symmetric Ohmic BCFs with $(\alpha(0) = 0.25,\ \omega_c = 2)$, $N = 10^4$ samples, 9 Hilbert space dimensions, $|\psi(0)\rangle_S = |0, 0\rangle_S$, $T = 0.6$, $\gamma = 0.5$





Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

[5] even in strong coupling equilibrium...

[6] 1, 2.

Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_{\mathrm{I}} \approx 0$ thermodynamics[5] of open systems are somewhat understood[6]

[5] even in strong coupling equilibrium...
[6] 1, 2.

Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_\mathrm{S}}_{\text{"small"}} + \underbrace{H_\mathrm{I}}_{?} + \underbrace{H_\mathrm{B}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_\mathrm{I} \approx 0$ thermodynamics[5] of open systems are somewhat understood[6]
- strong coupling: $\langle H_\mathrm{I} \rangle \sim \langle H_\mathrm{S} \rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?

[5] even in strong coupling equilibrium…
[6] 1, 2.

Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_{\mathrm{I}} \approx 0$ thermodynamics[5] of open systems are somewhat understood[6]
- strong coupling: $\langle H_{\mathrm{I}} \rangle \sim \langle H_{\mathrm{S}} \rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?
- we do quantum mechanics $\implies$ can't separate bath and system

[5] even in strong coupling equilibrium...
[6] 1, 2.

Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_\mathrm{S}}_{\text{"small"}} + \underbrace{H_\mathrm{I}}_{?} + \underbrace{H_\mathrm{B}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_\mathrm{I} \approx 0$ thermodynamics[5] of open systems are somewhat understood[6]
- strong coupling: $\langle H_\mathrm{I}\rangle \sim \langle H_\mathrm{S}\rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?
- we do quantum mechanics $\implies$ can't separate bath and system, especially not dynamics!

[5] even in strong coupling equilibrium…
[6] 1, 2.

Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_{\mathrm{I}} \approx 0$ thermodynamics[5] of open systems are somewhat understood[6]
- strong coupling: $\langle H_{\mathrm{I}} \rangle \sim \langle H_{\mathrm{S}} \rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?
- we do quantum mechanics $\implies$ can't separate bath and system, especially not dynamics!
- no consensus about strong coupling thermodynamics:

[5] even in strong coupling equilibrium...
[6] 1, 2.

Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{20}$$

with $[H_S, H_B] = 0$.

- weak coupling $H_{\mathrm{I}} \approx 0$ thermodynamics[5] of open systems are somewhat understood[6]
- strong coupling: $\langle H_{\mathrm{I}} \rangle \sim \langle H_{\mathrm{S}} \rangle \implies$ we can't neglect the interaction $\implies$ thermodynamics?
- we do quantum mechanics $\implies$ can't separate bath and system, especially not dynamics!
- no consensus about strong coupling thermodynamics:
- but what is clear: *need to get access to exact dynamics of* $H_{\mathrm{I}}, H_{\mathrm{B}}$

---

[5] even in strong coupling equilibrium…
[6] 1, 2.

Generalizations

Finite Temperature

$$J(t) = J_0(t) + \left[\langle L^\dagger \partial_t \xi(t)\rangle + \text{c.c.}\right] \tag{21}$$

with $\mathcal{M}(\xi(t)) = 0 = \mathcal{M}(\xi(t)\xi(s))$, $\mathcal{M}\left(\xi(t)\xi^*(s)\right) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega \bar{n}(\beta\omega) J(\omega) e^{-\mathrm{i}\omega(t-s)}$ and $J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(w - \omega_\lambda)$.[7]

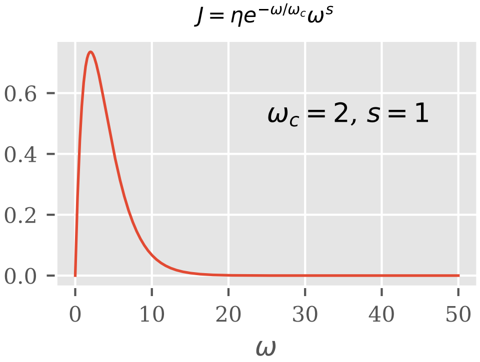
- finite temperatures
- nonlinear NMQSD/HOPS
- multiple baths straight forward
- interaction energy: "removing the dot"...
- general "collective" bath observables $O_\mathrm{S} \otimes (B^a)^\dagger B^b$ with $B = \sum_\lambda g_\lambda a_\lambda$

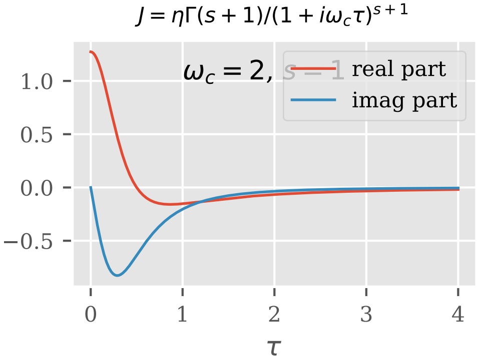
[7] $\partial_t \xi(t)$ exists if correlation function is smooth

More Papers on Thermo

[1, 2, 5–14]

Ohmic SD BCF


$J = \eta e^{-\omega/\omega_c}\omega^s$
$\omega_c = 2,\ s = 1$
0.0
0.2
0.4
0.6
0
10
20
30
40
50
ω


$J = \eta\Gamma(s+1)/(1+i\omega_c\tau)^{s+1}$
$\omega_c = 2,\ s = 1$
real part
imag part
−0.5
0.0
0.5
1.0
0
1
2
3
4
τ

NMQSD (Zero Temperature)

Expanding in a Bargmann (unnormalized) coherent state basis [15] $\{|\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots\rangle = |\underline{\mathbf{z}}\rangle\}$

$$|\psi(t)\rangle = \int \prod_{n=1}^{N} \left(\frac{\mathrm{d}\mathbf{z}^{(n)}}{\pi^{N_n}} \, \mathrm{e}^{-|\mathbf{z}|^2} \right) |\psi(t, \underline{\mathbf{z}}^*)\rangle \, |\underline{\mathbf{z}}\rangle \,, \tag{22}$$

we obtain

$$\partial_t \psi_t(\boldsymbol{\eta}_t^*) = -iH\psi_t(\boldsymbol{\eta}_t^*) + \mathbf{L} \cdot \boldsymbol{\eta}_t^* \psi_t(\boldsymbol{\eta}_t^*) - \sum_{n=1}^{N} L_n^\dagger \int_0^t \mathrm{d}s \, \alpha_n(t-s) \frac{\delta \psi_t(\boldsymbol{\eta}_t^*)}{\delta \eta_n^*(s)}, \tag{23}$$

with

$$\mathcal{M}(\eta_n^*(t)) = 0, \quad \mathcal{M}(\eta_n(t)\eta_m(s)) = 0, \quad \mathcal{M}(\eta_n(t)\eta_m(s)^*) = \delta_{nm}\alpha_n(t-s), \tag{24}$$

where $\alpha_n(t-s) = \sum_\lambda \left|g_\lambda^{(n)}\right|^2 \mathrm{e}^{-i\omega_\lambda^{(n)}(t-s)} = \langle B(t)B(s)\rangle_{I,\rho(0)}$ [16] (fourier transf. of spectral density $J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(\omega - \omega_\lambda)$).

Fock-Space Embedding

As in Ref. [17] we can define

$$|\Psi\rangle = \sum_{\underline{\mathbf{k}}} \left|\psi^{\underline{\mathbf{k}}}\right\rangle \otimes |\underline{\mathbf{k}}\rangle \tag{25}$$

where $|\underline{\mathbf{k}}\rangle = \bigotimes_{n=1}^{N} \bigotimes_{\mu=1}^{N_n} \left|\underline{\mathbf{k}}_{n,\mu}\right\rangle$ are bosonic Fock-states.
Now eq. (7) becomes

$$\partial_t |\Psi\rangle = \left[-iH_{\mathrm{S}} + \mathbf{L}\cdot\boldsymbol{\eta}^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} b_{n,\mu}^\dagger b_{n,\mu} W_\mu^{(n)} + i\sum_{n=1}^{N}\sum_{\mu=1}^{M_n} \sqrt{G_{n,\mu}}\left(b_{n,\mu}^\dagger L_n + b_{n,\mu} L_n^\dagger\right)\right] |\Psi\rangle \,. \tag{26}$$

Fock-Space Embedding

As in Ref. [17] we can define

$$|\Psi\rangle = \sum_{\underline{\mathbf{k}}} \left|\psi^{\underline{\mathbf{k}}}\right\rangle \otimes |\underline{\mathbf{k}}\rangle \tag{25}$$

where $|\underline{\mathbf{k}}\rangle = \bigotimes_{n=1}^{N} \bigotimes_{\mu=1}^{N_n} \left|\underline{\mathbf{k}}_{n,\mu}\right\rangle$ are bosonic Fock-states.
Now eq. (7) becomes

$$\partial_t |\Psi\rangle = \left[-iH_{\mathrm{S}} + \mathbf{L}\cdot\boldsymbol{\eta}^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} b_{n,\mu}^\dagger b_{n,\mu} W_\mu^{(n)} + i\sum_{n=1}^{N}\sum_{\mu=1}^{M_n}\sqrt{G_{n,\mu}}\left(b_{n,\mu}^\dagger L_n + b_{n,\mu} L_n^\dagger\right)\right]|\Psi\rangle\,. \tag{26}$$

$\implies$ possible to derive an upper bound for the norm of $\left|\psi^{\underline{\mathbf{k}}}\right\rangle$

Fock-Space Embedding

As in Ref. [17] we can define

$$|\Psi\rangle = \sum_{\underline{\mathbf{k}}} \left|\psi^{\underline{\mathbf{k}}}\right\rangle \otimes |\underline{\mathbf{k}}\rangle \tag{25}$$

where $|\underline{\mathbf{k}}\rangle = \bigotimes_{n=1}^{N} \bigotimes_{\mu=1}^{N_n} \left|\underline{\mathbf{k}}_{n,\mu}\right\rangle$ are bosonic Fock-states.
Now eq. (7) becomes

$$\partial_t |\Psi\rangle = \left[-iH_\mathrm{S} + \mathbf{L}\cdot\boldsymbol{\eta}^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} b_{n,\mu}^\dagger b_{n,\mu} W_\mu^{(n)} + i\sum_{n=1}^{N}\sum_{\mu=1}^{M_n} \sqrt{G_{n,\mu}}\left(b_{n,\mu}^\dagger L_n + b_{n,\mu} L_n^\dagger\right)\right]|\Psi\rangle\,. \tag{26}$$

$\implies$ possible to derive an upper bound for the norm of $\left|\psi^{\underline{\mathbf{k}}}\right\rangle$ $\implies$ new truncation scheme

Multiple Baths

- theory generalizes easily to N baths
- generalized our HOPS code to N baths
- solving a model with two coupled HOs is now possible

$$H = \sum_{i\in\{1,2\}} \left[H_O^{(i)} + q_i B^{(i)} + H_B^{(i)}\right] + \frac{\gamma}{4}(q_1 - q_2)^2, \tag{27}$$

where $H_O^{(i)} = \frac{\Omega_i}{4}(p_i^2 + q_i^2)$, $B^{(i)} = \sum_\lambda \left(g_\lambda^{(i),*} b_\lambda^{(i)} + g_\lambda^{(i)} b_\lambda^{(i),\dagger}\right)$ and $H_B^{(i)} = \sum_\lambda \omega_\lambda b_\lambda^{(i),\dagger} b_\lambda^{(i)}$.

One Bath

Other Projects

One Bath, Zero Temperature

Model: Spin-Boson

$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda,\ |\psi_0\rangle_\mathrm{S} = |\uparrow\rangle \tag{28}$$

- how do we check convergence:

One Bath, Zero Temperature

Model: Spin-Boson

$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_{\lambda}\left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_{\lambda}\omega_\lambda a_\lambda^\dagger a_\lambda,\ |\psi_0\rangle_{\mathrm{S}} = |\uparrow\rangle \tag{28}$$

- how do we check convergence:

One Bath, Zero Temperature

Model: Spin-Boson

$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda,\ |\psi_0\rangle_{\mathrm{S}} = |\uparrow\rangle \tag{28}$$

- how do we check convergence:
  - old: difference of results to some “good” configuration

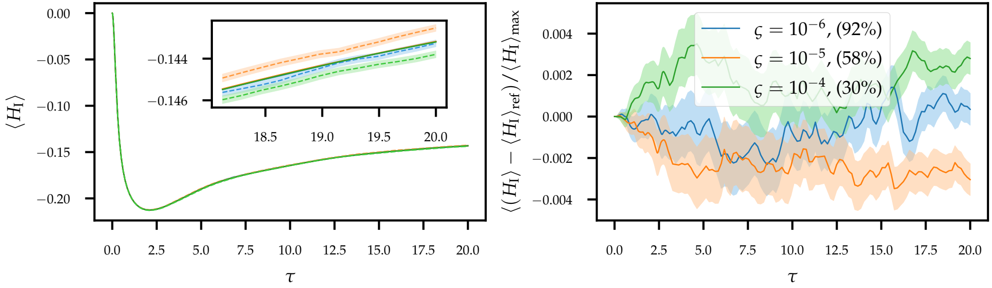
One Bath, Zero Temperature

Model: Spin-Boson

$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda,\ |\psi_0\rangle_{\mathrm{S}} = |\uparrow\rangle \tag{28}$$

- how do we check convergence:
  - old: difference of results to some “good” configuration
  - new: consistency with energy conservation

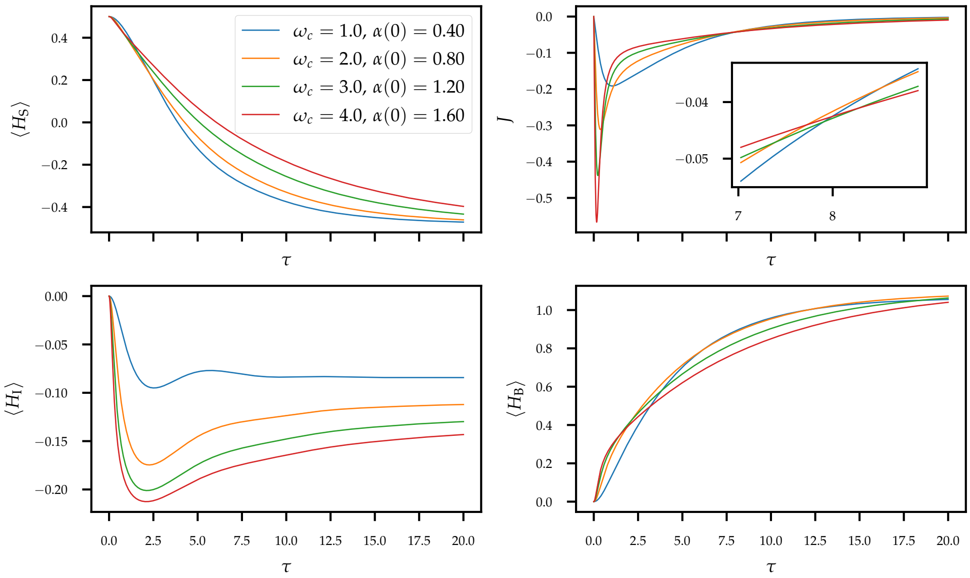
Example: Dependence of the Interaction Energy on Stochastic Process Sampling



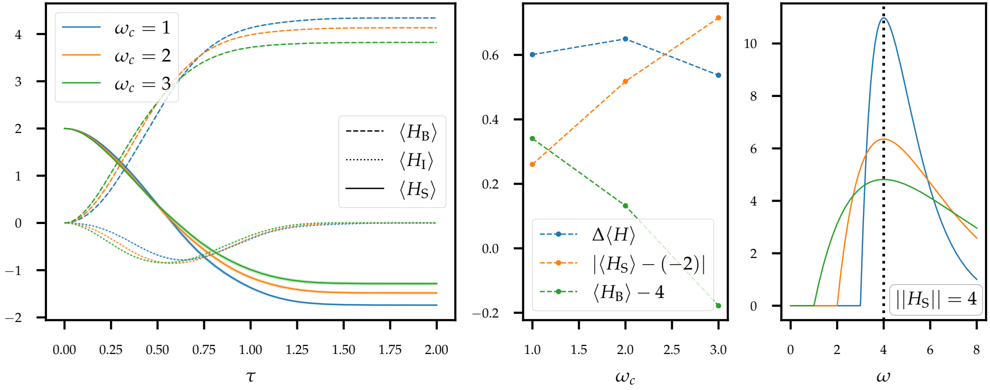
- $\alpha(0) = 1.6$ and $\omega_c = 4 \implies$ stress HOPS through fast decaying BCF
- "perfect" results only with very high accuracy[8] ς
- good qualitative results for less extreme configurations (common theme)

[8] smaller ς is better

Various Cutoff Frequencies

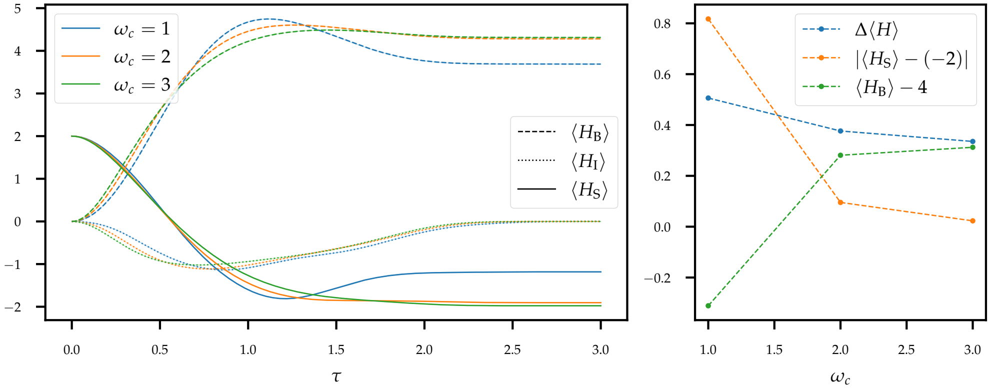


Non-Markovian Dynamics



- interaction strengths chosen for approx. same interaction energy

Non-Markovian Dynamics



- interaction strengths chosen for approx. same interaction energy
- timing important for energy transfer "performance"

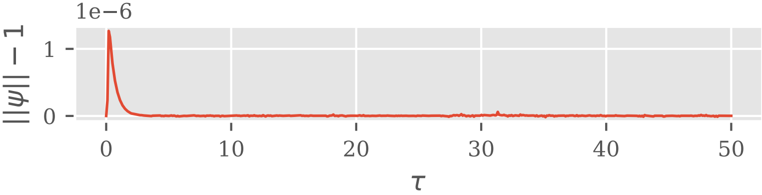
Beware :)

The following is WIP and has not been written up properly yet.

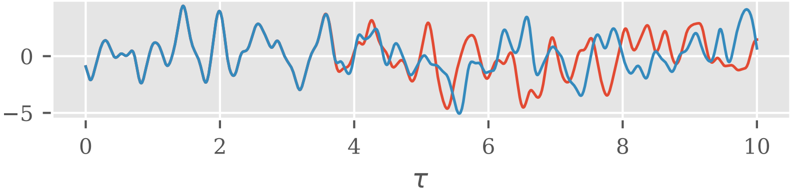
One Bath

Other Projects

- stabilized normalization in nonlinear HOPS



- stochastic process sampling via Cholesky decomposition



- norm based truncation scheme
  - promising at “friendly” coupling strengths