Bath Observables with HOPS

Energy Flow in Strongly Coupled Open Quantum Systems

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- Technical Basics

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- A Little (more) Theory
- Analytic Verification

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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] Rivas, "Strong Coupling Thermodynamics of Open Quantum Systems"; Talkner and Hnggi, "Colloquium: Statistical mechanics and thermodynamics at strong coupling: Quantum and classical".

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

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- 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* $H_{\mathrm{I}}, H_{\mathrm{B}}$

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Is that possible?

Is that possible? Yes.

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Using HOPS :)

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Sneak Peek

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

- more general: $O_\mathrm{S} \otimes (B^a)^\dagger B^b$ with $B = \sum_\lambda g_\lambda a_\lambda$

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

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Using HOPS :)

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

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Standard Model of Open Systems

In the following we will 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

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

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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:

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

with

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

by projecting on coherent bath states.[3]

[3] For details see: Disi, Gisin, and W. T. Strunz, "Non-Markovian quantum state diffusion"

HOPS

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

$$D_\mu^{(n)}(t) \equiv \int_0^t \mathrm{d}s\, G_\mu^{(n)} \mathrm{e}^{-W_\mu^{(n)}(t-s)} \frac{\delta}{\delta\eta_n^*(s)} \tag{5}$$

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

$$\begin{aligned}\dot{\psi}^{\underline{\mathbf{k}}} = &\left[-iH_\mathrm{S}(t) + \mathbf{L}(t)\cdot\boldsymbol{\eta}^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} \underline{\mathbf{k}}_{n,\mu} W_\mu^{(n)}\right]\psi^{\underline{\mathbf{k}}} \\ &+ i\sum_{n=1}^{N}\sum_{\mu=1}^{M_n}\sqrt{G_\mu^{(n)}}\left[\sqrt{\underline{\mathbf{k}}_{n,\mu}} L_n(t)\psi^{\underline{\mathbf{k}}-\underline{\mathbf{e}}_{n,\mu}} + \sqrt{\left(\underline{\mathbf{k}}_{n,\mu}+1\right)} L_n^\dagger(t)\psi^{\underline{\mathbf{k}}+\underline{\mathbf{e}}_{n,\mu}}\right].\end{aligned} \tag{6}$$

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Zero Temperature, One Bath, Linear NMQSD

We want to calculate

$$J = -\frac{\mathrm{d}\left\langle H_{\mathrm{B}}\right\rangle}{\mathrm{d}t} = \left\langle L^\dagger \partial_t B(t) + L \partial_t B^\dagger(t)\right\rangle_{\mathrm{I}}. \tag{7}$$

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...some manipulations ...

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...some manipulations ...

Result (NMQSD)

$$J(t) = -i \mathcal{M}_{\eta^*} \left\langle \psi(\eta, t) \right| L^\dagger \dot{D}_t \left| \psi(\eta^*, t) \right\rangle + \mathrm{c.c.} \tag{8}$$

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

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

Result (HOPS)

$$J(t) = -\sum_\mu \sqrt{G_\mu} W_\mu \mathcal{M}_{\eta^*}\left\langle\psi^{(0)}(\eta,t)\right| L^\dagger \left|\psi^{\mathbf{e}_\mu}(\eta^*,t)\right\rangle + \mathrm{c.c.} \tag{9}$$

Generalizations

Finite Temperature

$$J(t) = J_0(t) + \left[\langle L^\dagger \partial_t \xi(t)\rangle + \text{c.c.}\right] \tag{10}$$

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 $J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(w - \omega_\lambda)$.[4]

- 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 $B = \sum_\lambda g_\lambda a_\lambda$

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

Is this any good?

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Model

$$H = \frac{\Omega}{4}(p^2 + q^2) + \frac{1}{2}q \sum_{\lambda} \left(g_{\lambda}^{*} b_{\lambda} + g_{\lambda} b_{\lambda}^{\dagger} \right) + \sum_{\lambda} \omega_{\lambda} b_{\lambda}^{\dagger} b_{\lambda}, \tag{11}$$

Model

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...leading to ...

$$\dot{q} = \Omega p \tag{12}$$

$$\dot{p} = -\Omega q - \int_0^t \Im[\alpha_0(t-s)] q(s)\, \mathrm{d}s + W(t) \tag{13}$$

$$\dot{b}_\lambda = -i g_\lambda \frac{q}{2} - i\omega_\lambda b_\lambda \tag{14}$$

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

$$\dot{G}(t) = AG(t) - \int_0^t K(t-s)G(s)\,\mathrm{d}s\,, \quad A = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}, \quad K(t) = \begin{pmatrix} 0 & 0 \\ \Im[\alpha_0(t)] & 0 \end{pmatrix}. \tag{15}$$

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Then

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = G(t)\begin{pmatrix} q(0) \\ p(0) \end{pmatrix} + \int_0^t G(t-s)\begin{pmatrix} 0 \\ W(s) \end{pmatrix}\mathrm{d}s\,. \tag{16}$$

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

Result

Solution

$$G(t) = \sum_{l=1}^{N+1} \left[R_l \begin{pmatrix} \tilde{z}_l & \Omega \\ \frac{\tilde{z}_l^2}{\Omega} & \tilde{z}_l \end{pmatrix} \mathrm{e}^{\tilde{z}_l \cdot t} + \text{c.c.} \right] \tag{17}$$

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

Result

Solution

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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

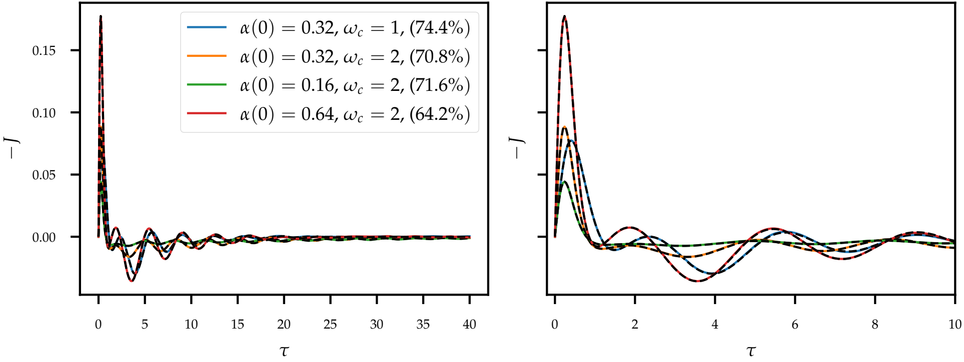
$$
\begin{aligned}
\langle \dot{H}_B \rangle &= \sum_\lambda \omega_\lambda \Big(\Big\langle b_\lambda^\dagger \dot{b}_\lambda \Big\rangle + \text{c.c.} \Big) \\
&= -\frac{1}{2} \Im \Big[\int_0^t \mathrm{d}s \, \langle q(t) q(s) \rangle \, \dot{\alpha}_0(t-s) \Big] \\
&\qquad + \frac{1}{2} G_{12}(t) [\alpha(t) - \alpha_0(t)] - \frac{\Omega}{2} \int_0^t \mathrm{d}s \, G_{11}(s) [\alpha(s) - \alpha_0(s)]
\end{aligned} \tag{18}
$$

- becomes huge sum of exponentials (thanks mathematica)

One Bath, Finite Temperature

Parameters

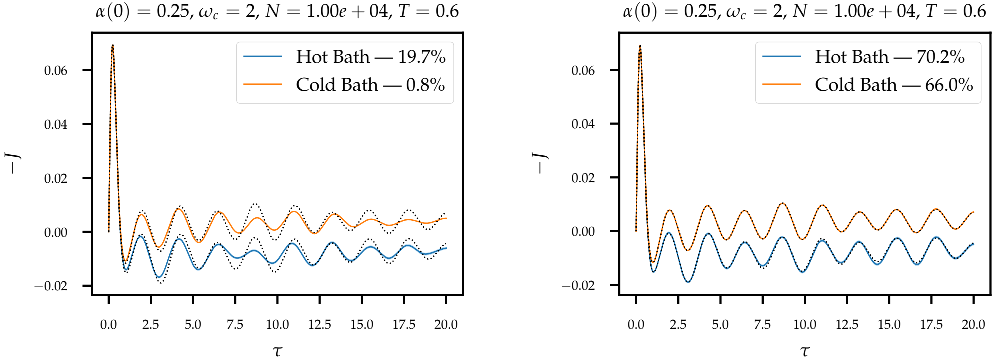
$\Omega = 1$, Ohmic BCF $\frac{\eta}{\pi}(\omega_c/(1+i\omega_c\tau))^2$ with $(\alpha(0) = 0.64,\, \omega_c = 2)$, $N = 10^5$ samples, 15 Hilbert space dimensions, $|\psi(0)\rangle_S = |1\rangle_S$, $T = 1$



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, $|\psi(0)\rangle_S = |0,0\rangle_S$, $T = 0.6$, $\gamma = 0.5$



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One Bath, Zero Temperature

Model: Spin-Boson

$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda,\ |\psi_0\rangle_\mathrm{S} = |\uparrow\rangle \tag{19}$$

One Bath, Zero Temperature

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- how do we check convergence:

One Bath, Zero Temperature

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  - old: difference of results to some “good” configuration

One Bath, Zero Temperature

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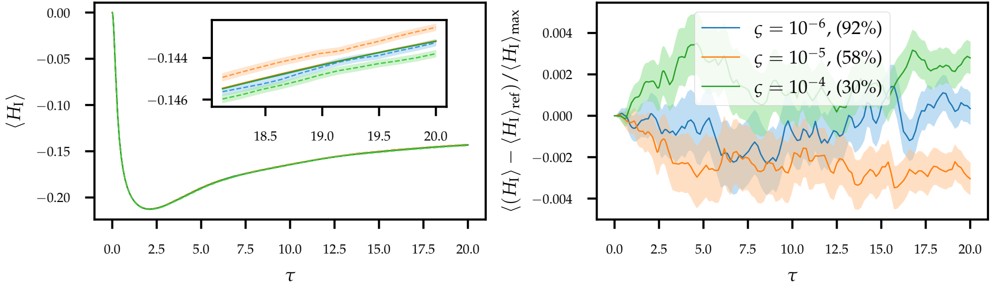
- how do we check convergence:
  - old: difference of results to some “good” configuration
  - new: consistency with energy conservation

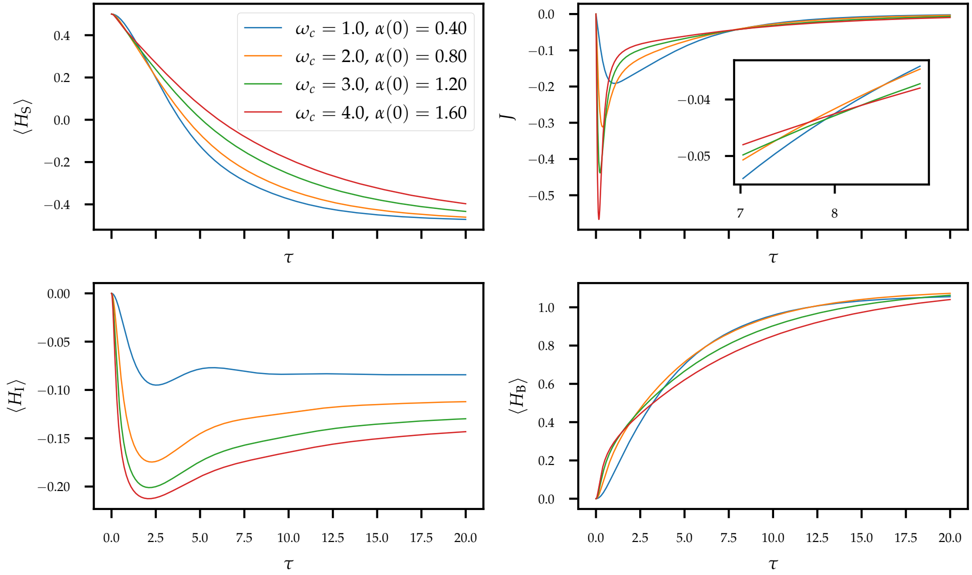
Example: Dependence of Flow on Stochastic Process Sampling



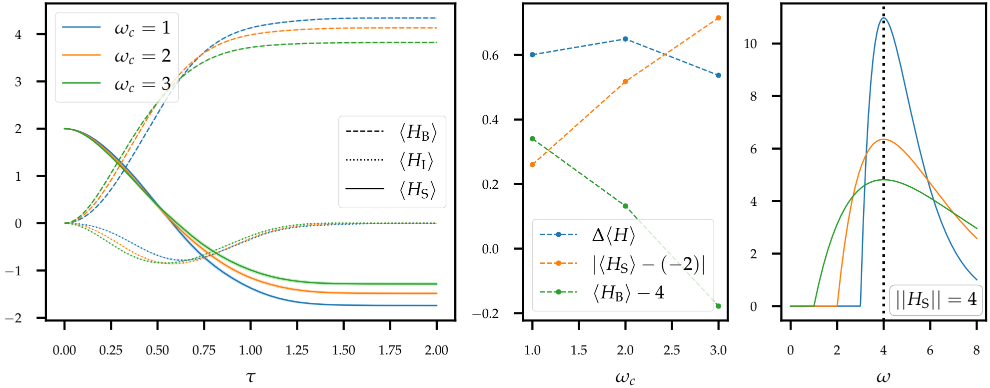
- $\alpha(0) = 1.6$ and $\omega_c = 4 \implies$ stress HOPS through fast decaying BCF
- "perfect" results only with very high accuracy[5] ς
- good qualitative results for less extreme configurations (common theme)

[5]smaller ς is better

Various Cutoff Frequencies

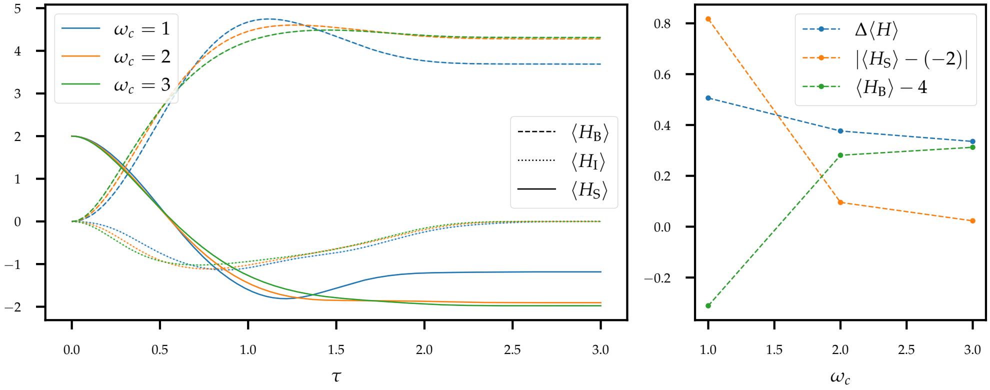


Non-Markovian Dynamics



- 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 :)

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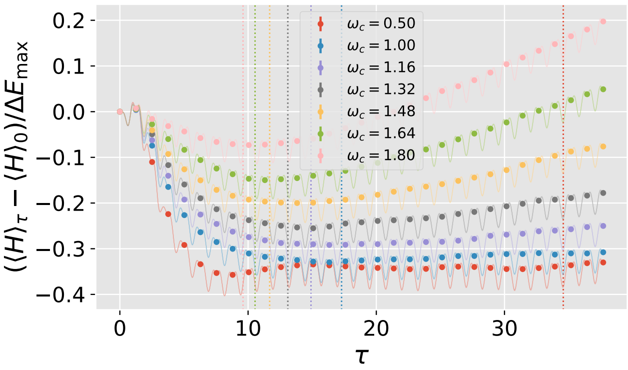
Extracting Energy from One Bath

- same model as above eq. (19), but with $L(\tau) = \sin^2(\frac{\Delta}{2}\tau)\sigma_x$
- how much energy can be *unitarily* extracted? $\implies \Delta E_{\max} = \frac{1}{\beta} S\big(\rho_{\mathrm{S}} \,\big\|\, \rho_{\mathrm{S}}^{\beta}\big)$



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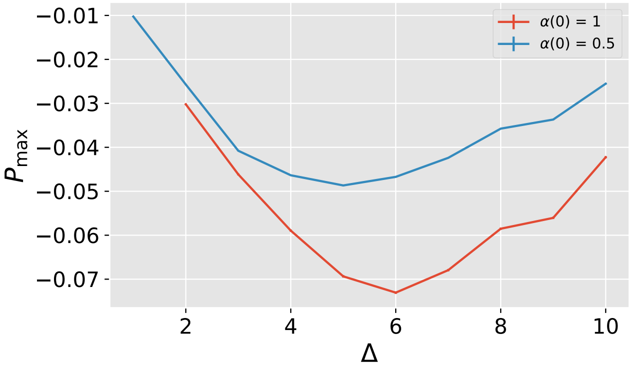

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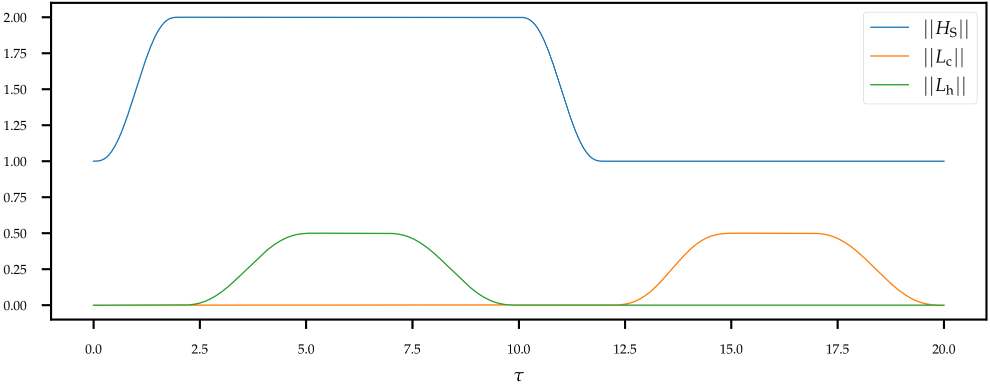
Otto Cycle (proof of concept)

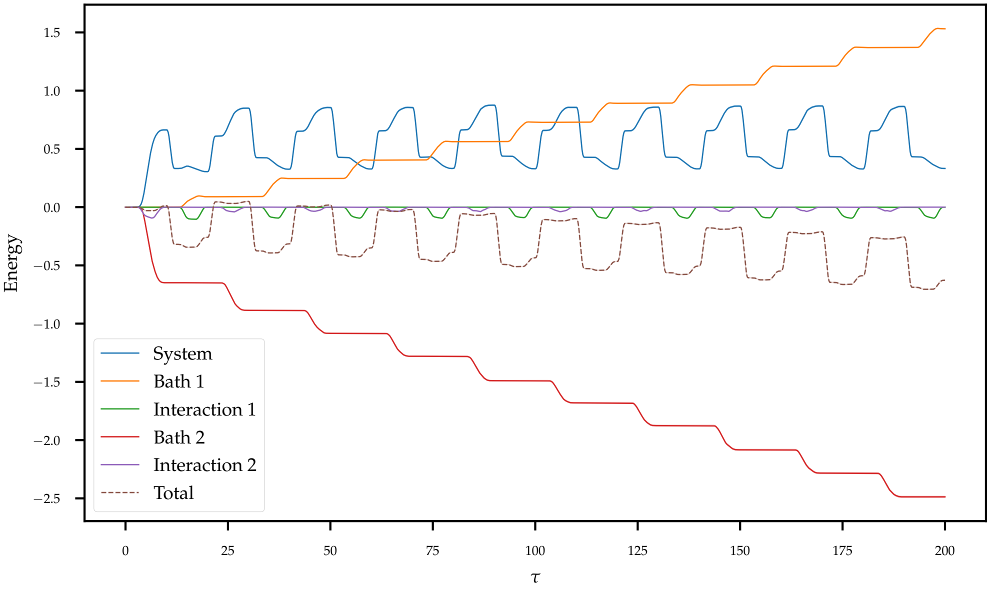
Model

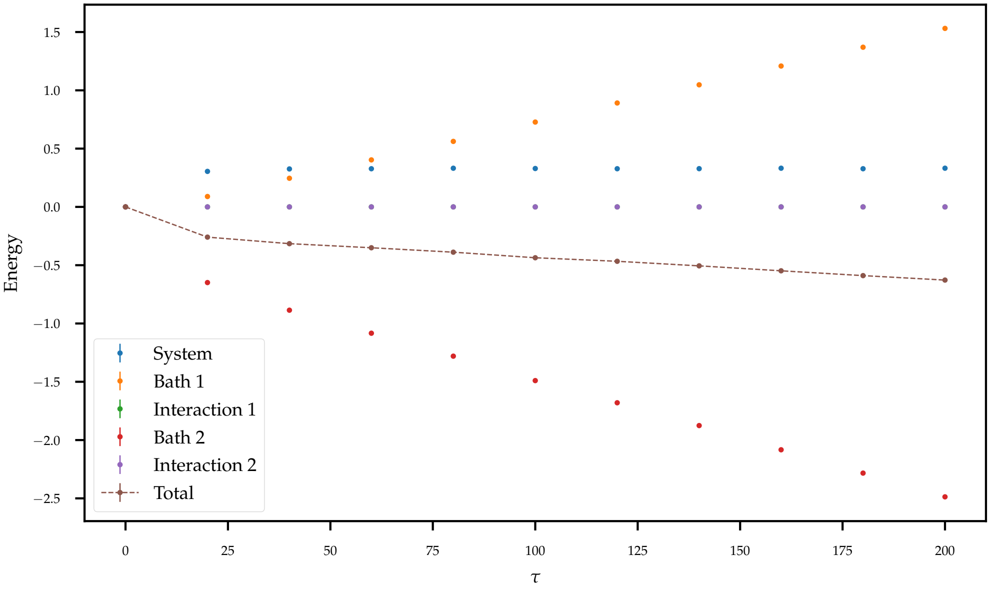
Spin-Boson model with compression of H_S and modulation of L.

- classical toy model of the quantum heat engine community[6]



[6] Geva and Kosloff, "A quantum-mechanical heat engine operating in finite time. A model consisting of spin-1/2 systems as the working fluid".


System
Bath 1
Interaction 1
Bath 2
Interaction 2
Total
Energy
τ
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
25
50
75
100
125
150
175
200


Energy
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1.0
0.5
0.0
−0.5
−1.0
−1.5
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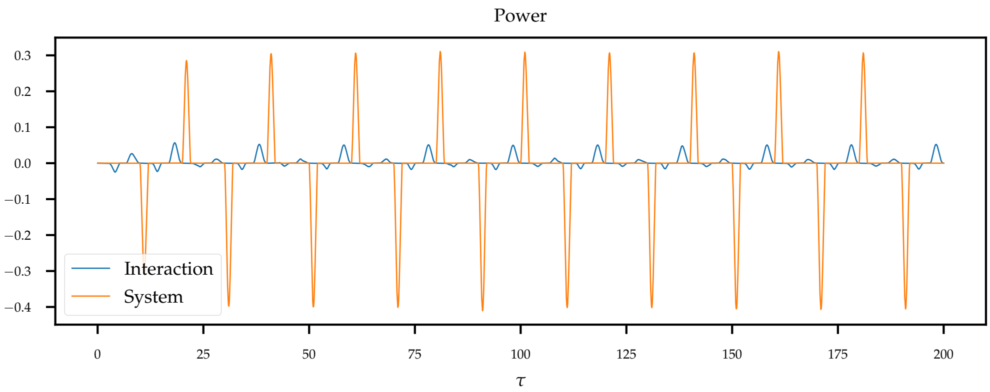
−2.5
System
Bath 1
Interaction 1
Bath 2
Interaction 2
Total



- $\bar{P} = 1.98 \cdot 10^{-3} \pm 2.3 \cdot 10^{-5}$, $\eta \approx 20\%$, $T_c = 1$, $T_h = 20$
- no tuning of parameters, except for resonant coupling
- long bath memory $\omega_c = 1$, but weak coupling

Questions (for the future)

- better performance through "overlapping" phases?
- strong coupling any good?
- non-Markovianity + strong coupling any good?
- what is the optimal efficiency and power? (probably no advantage here)

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- Anti-Zeno Engine

Other Projects

Outlook

Anti-Zeno Engine

Question

Is there a use for non-Markovianity in quantum heat engines?

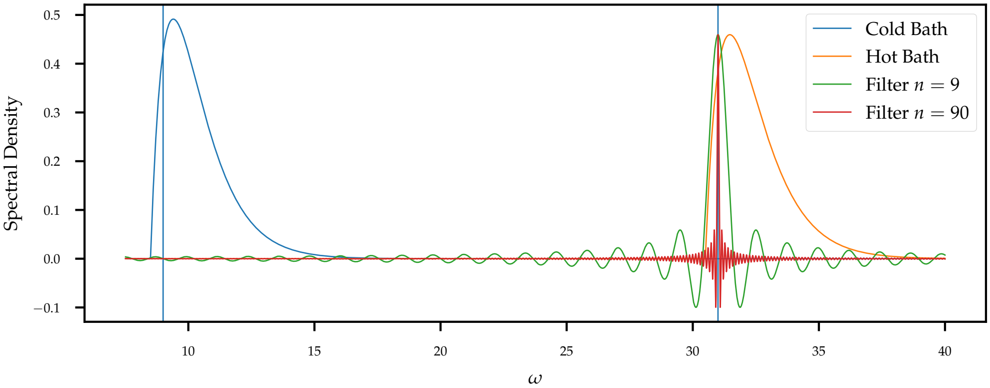
- Mukherjee, Kofman, and Kurizki, "Anti-Zeno quantum advantage in fast-driven heat machines" claims that one can exploit the time-energy uncertainty for quantum advantage[7]

Model

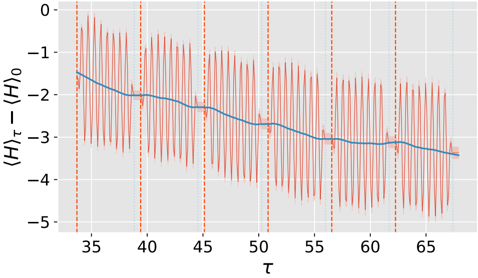
Qubit coupled to two baths of different temperatures (T_c, T_h)

$$H_S = \frac{1}{2}[\omega_0 + \gamma\Delta\sin(\Delta t)]\sigma_z,\ L_{c,h} = \frac{1}{2}\sigma_x \tag{20}$$

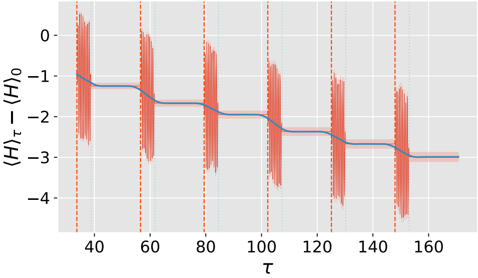
[7] I'd be careful to call this quantum advantage.



- couple for n modulation periods slightly of resonance
- for smaller n the $\sin((\omega - (\omega_0 \pm \Delta))\tau)/((\omega - (\omega_0 \pm \Delta))\tau)$ has a greater overlap $\implies$ controls power output



a) $P = -0.058 \pm 0.014$



b) $P = -0.068 \pm 0.010$

Parameters

$\Delta = 11$, $\gamma = 0.5$, $\alpha(0) = 1.0$, $\omega_0 = 20$, $T_c = 8$, $T_h = 40$

- this is not properly converged yet $\rightarrow$ newer results: no advantage at these temperatures / coupling strengths
- new simulations with temperatures from paper ($\beta_{h(c)} = 0.0005(0.005)$) are promising
  - interesting $\rightarrow$ no good steady state power in this case (insufficient samples?)

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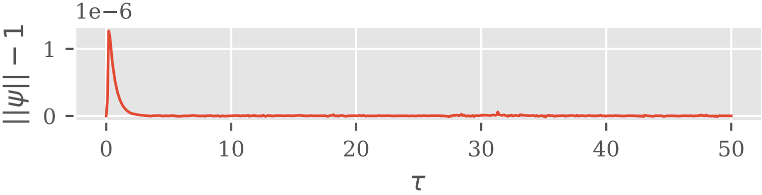
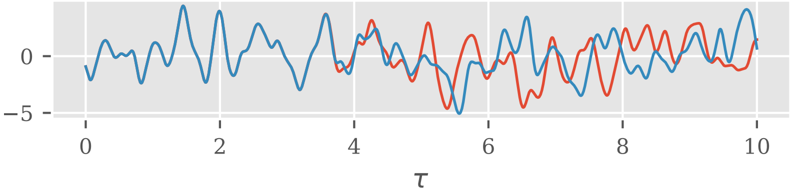
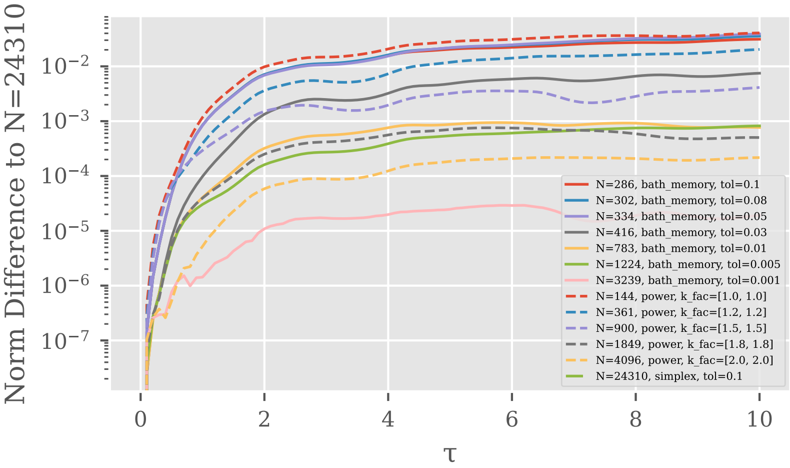
- stabilized normalization in nonlinear HOPS



- stochastic process sampling via Cholesky decomposition



- norm based truncation scheme
  - promising at "friendly" coupling strengths



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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
- ...

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

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Situation (Longer)

Consider an open quantum system

$$H = \underbrace{H_{\mathrm{S}}}_{\text{"small"}} + \underbrace{H_{\mathrm{I}}}_{?} + \underbrace{H_{\mathrm{B}}}_{\text{"big", simple}} \tag{21}$$

with $[H_S, H_B] = 0$.

[8] even in strong coupling equilibrium...

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- no consensus about strong coupling thermodynamics:[10]
- but what is clear: *need to get access to exact dynamics of* $H_{\mathrm{I}}, H_{\mathrm{B}}$

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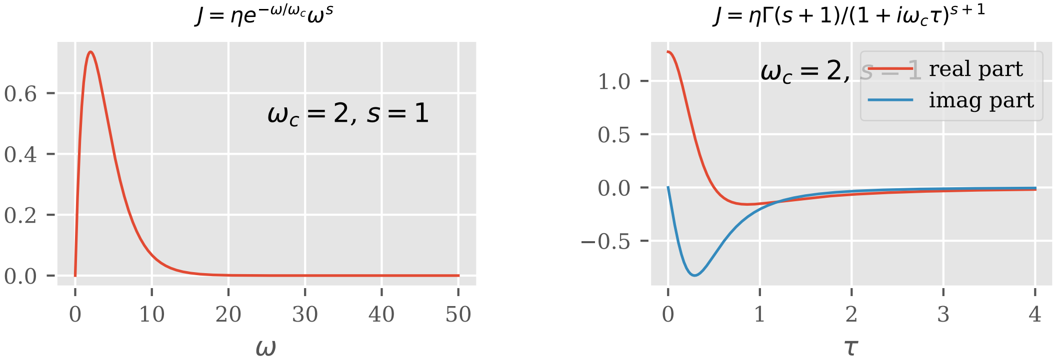
Ohmic SD BCF



$J = \eta e^{-\omega/\omega_c} \omega^s$
$\omega_c = 2,\ s = 1$
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 Klauder and Sudarshan, "Fundamentals of Quantum Optics Benjamin" $\left\{\left|\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots\right\rangle = |\underline{\mathbf{z}}\rangle\right\}$

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

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 $\alpha_n(t-s) = \sum_\lambda \left|g_\lambda^{(n)}\right|^2 \mathrm{e}^{-i\omega_\lambda^{(n)}(t-s)} = \langle B(t)B(s)\rangle_{I,\rho(0)}$ Walter T. Strunz, "Stochastic Schrödinger equation approach to the dynamics of non-Markovian open quantum systems" (fourier transf. of spectral density $J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(\omega - \omega_\lambda)$).

Fock-Space Embedding

As in Gao et al., “Non-Markovian Stochastic Schr\”odinger Equation: Matrix Product State Approach to the Hierarchy of Pure States” we can define

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

where $\left|\underline{\mathbf{k}}\right\rangle = \bigotimes_{n=1}^{N} \bigotimes_{\mu=1}^{N_n} \left|\underline{\mathbf{k}}_{n,\mu}\right\rangle$ are bosonic Fock-states.
Now eq. (6) becomes

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

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

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