Bath Observables with HOPS

Energy Flow in Strongly Coupled Open Quantum Systems

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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] 1, 2.

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

[1] 1, 2.

Is that possible?

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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 $\langle H_\mathrm{I}\rangle$).

- and still more general observables (omitted)

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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

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

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

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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:

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

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]
System state can be recovered by averaging over η

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

[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

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

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...some manipulations ...

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

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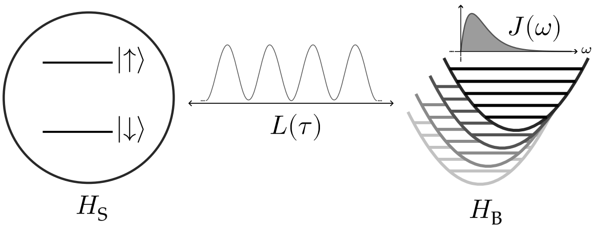
Result (HOPS)

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

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

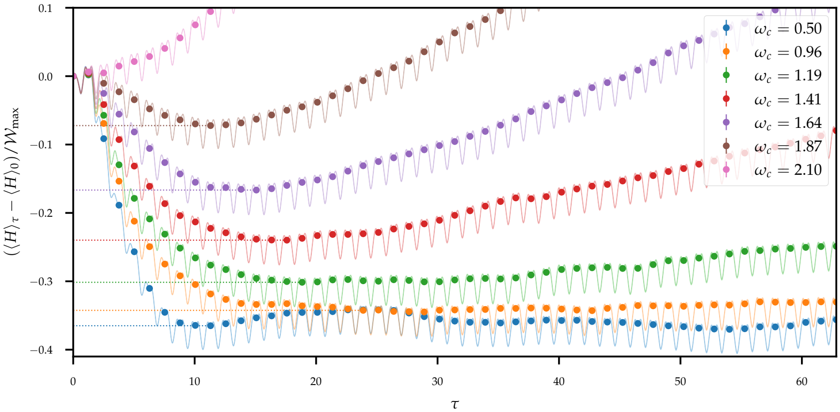


$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda, \; |\psi_0\rangle_{\mathrm{S}} = |\downarrow\rangle \tag{11}$$

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

Extracting Energy from One Bath

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



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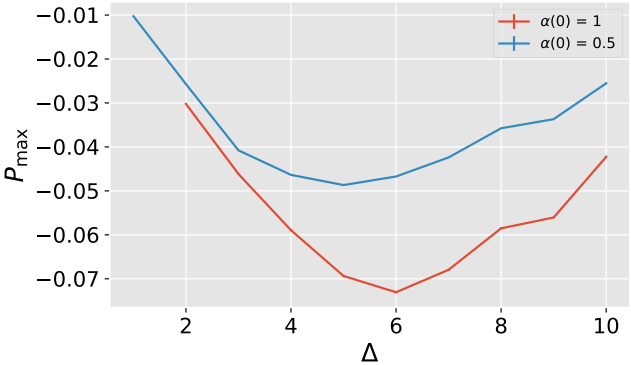
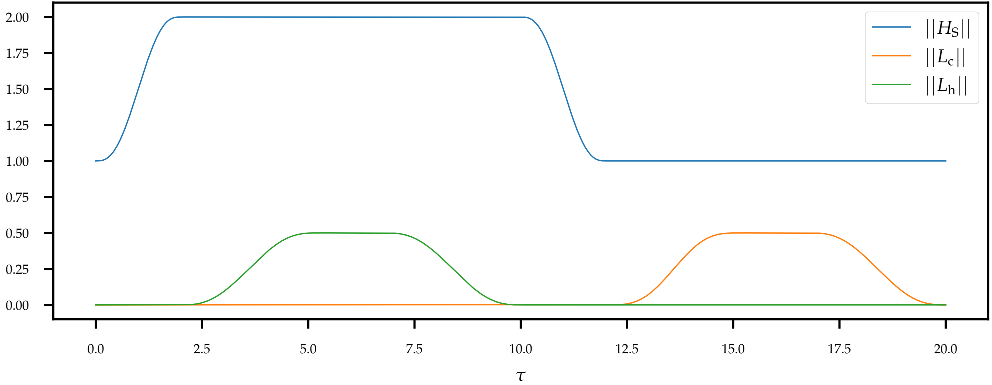


Otto Cycle (proof of concept)

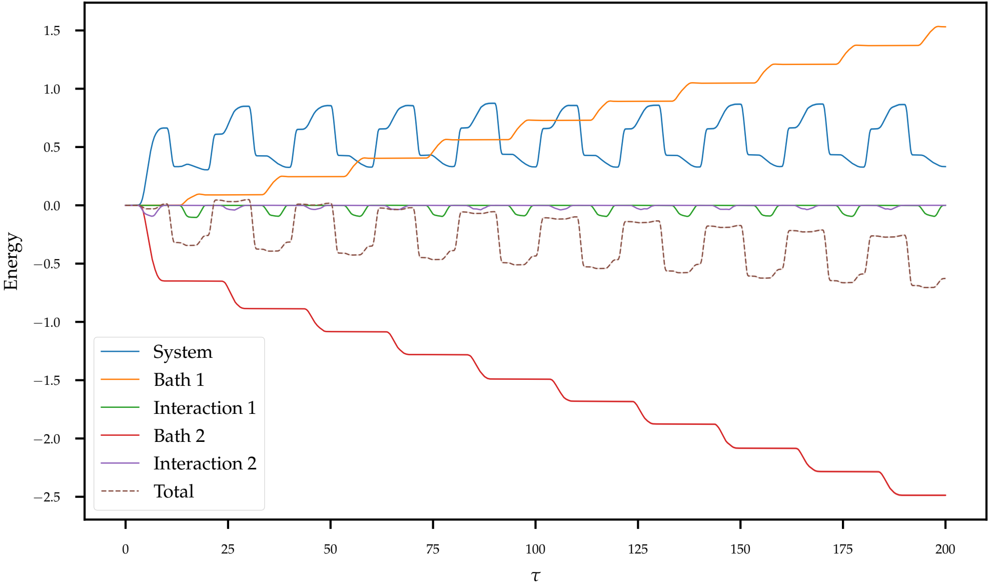
Model

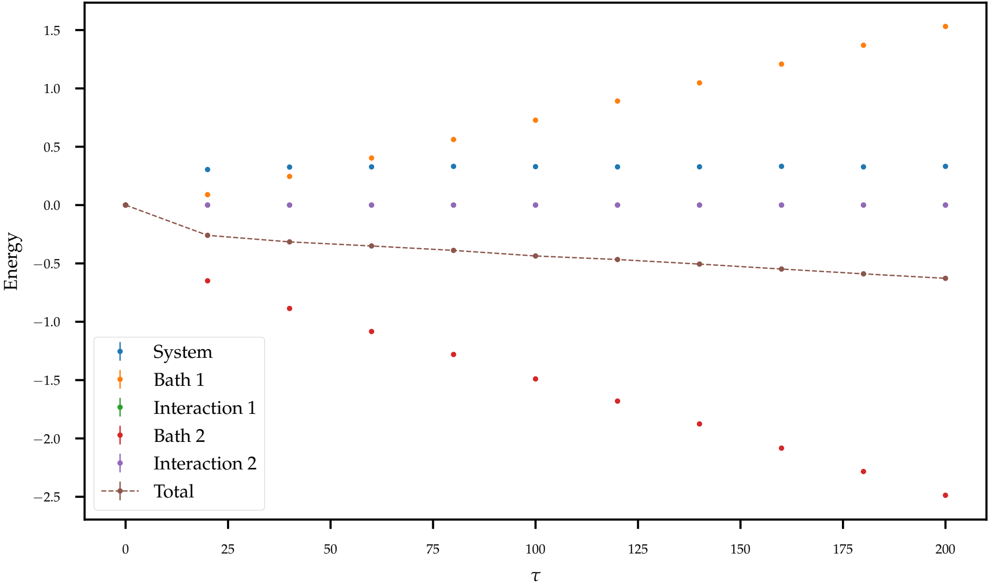
Spin-Boson model with compression of H_S and modulation of L.

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



[4] 4.


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



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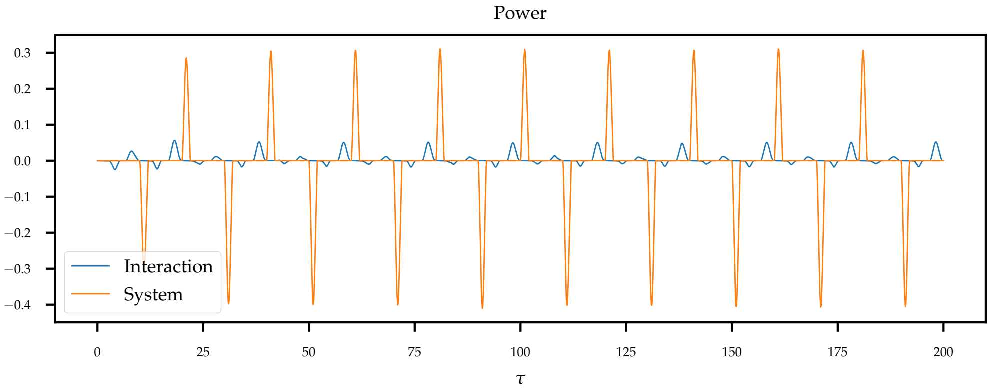


- $\bar{P} = 1.98 \cdot 10^{-3} \pm 2.3 \cdot 10^{-5}$, $\eta \approx 20\%$, $T_c = 1$, $T_h = 20$
- no tuning of parameters, except for resonant coupling
- long bath memory $\omega_c = 1$, but weak-ish coupling

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)

Anti-Zeno Engine

Question

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

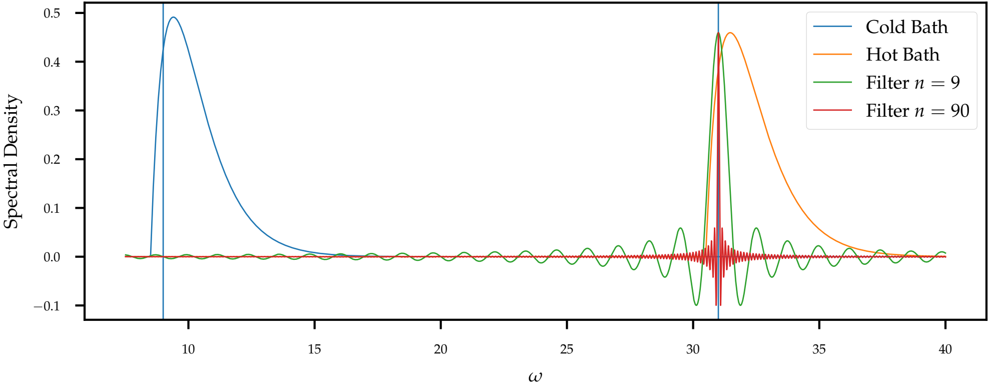
- [5] claims that one can exploit the time-energy uncertainty for quantum advantage[5]

Model

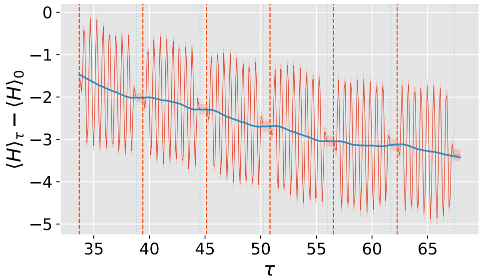
Qubit coupled to two baths of different temperatures (T_c, T_h)

$$H_{\mathrm{S}} = \frac{1}{2}[\omega_0 + \gamma\Delta\sin(\Delta t)]\sigma_z,\ L_{c,h} = \frac{1}{2}\sigma_x \tag{12}$$

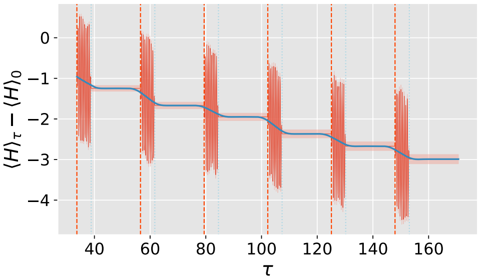
[5] I'd be careful to call this quantum advantage.



- 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?)

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, 57–63, 65).

[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, 57–63, 65).

[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] V. Mukherjee, A. G. Kofman, and G. Kurizki, "Anti-Zeno quantum advantage in fast-driven heat machines", Commun. Phys. **3**, 1–12 (2020) (cit. on p. 38).

[6] 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. 65).

References II

[7] 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. 65).

[8] 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. 65).

[9] 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. 65).

[10] 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. 65).

[11] 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. 65).

References III

[12] P. Talkner and P. Hnggi, “Open system trajectories specify fluctuating work but not heat”, Phys. Rev. E **94**, 022143 (2016) (cit. on p. 65).

[13] 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. 65).

[14] 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. 65).

[15] 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. 65).

[16] J. Klauder and E. Sudarshan, “Fundamentals of quantum optics benjamin”, Inc., New York (1968) (cit. on p. 67).

[17] 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. 67).

References IV

[18] 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. 68–70).

Model

$$H = \frac{\Omega}{4}(p^2 + q^2) + \frac{1}{2} q \sum_{\lambda} \left(g_{\lambda}^{*} b_{\lambda} + g_{\lambda} b_{\lambda}^{\dagger} \right) + \sum_{\lambda} \omega_{\lambda} b_{\lambda}^{\dagger} b_{\lambda}, \tag{13}$$

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...leading to ...

$$\dot{q} = \Omega p \tag{14}$$

$$\dot{p} = -\Omega q - \int_0^t \Im[\alpha_0(t-s)] q(s) \, \mathrm{d}s + W(t) \tag{15}$$

$$\dot{b}_\lambda = -i g_\lambda \frac{q}{2} - i\omega_\lambda b_\lambda \tag{16}$$

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

$$\dot{G}(t) = AG(t) - \int_0^t K(t-s)G(s)\,\mathrm{d}s\,, \quad A = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}, \quad K(t) = \begin{pmatrix} 0 & 0 \\ \Im[\alpha_0(t)] & 0 \end{pmatrix}. \quad (17)$$

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Then

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = G(t)\begin{pmatrix} q(0) \\ p(0) \end{pmatrix} + \int_0^t G(t-s)\begin{pmatrix} 0 \\ W(s) \end{pmatrix}\mathrm{d}s\,. \tag{18}$$

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

Result

Solution

$$G(t) = \sum_{l=1}^{N+1} \left[R_l \begin{pmatrix} \tilde{z}_l & \Omega \\ \frac{\tilde{z}_l^2}{\Omega} & \tilde{z}_l \end{pmatrix} \mathrm{e}^{\tilde{z}_l \cdot t} + \text{c.c.} \right] \tag{19}$$

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

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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

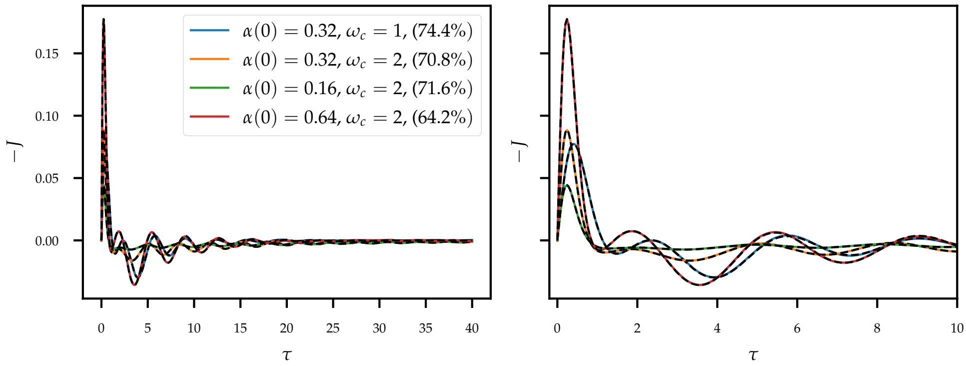
$$
\begin{aligned}
\langle \dot{H}_B \rangle &= \sum_\lambda \omega_\lambda \Big(\Big\langle b_\lambda^\dagger \dot{b}_\lambda \Big\rangle + \text{c.c.} \Big) \\
&= -\frac{1}{2} \Im \Big[\int_0^t \mathrm{d}s \, \langle q(t) q(s) \rangle \, \dot{\alpha}_0(t-s) \Big] \\
&\qquad + \frac{1}{2} G_{12}(t) [\alpha(t) - \alpha_0(t)] - \frac{\Omega}{2} \int_0^t \mathrm{d}s \, G_{11}(s) [\alpha(s) - \alpha_0(s)]
\end{aligned}
\tag{20}
$$

- becomes huge sum of exponentials (thanks Mathematica)

One Bath, Finite Temperature

Parameters

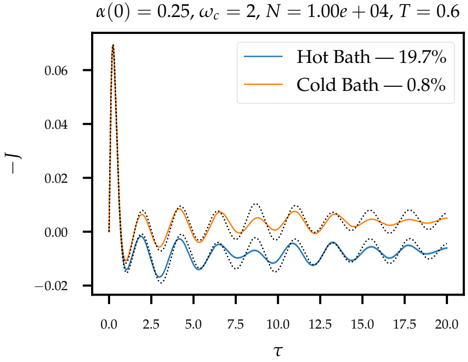
$\Omega = 1$, Ohmic BCF $\frac{\eta}{\pi}(\omega_c/(1 + i\omega_c\tau))^2$ with $(\alpha(0) = 0.64,\ \omega_c = 2)$, $N = 10^5$ samples, 15 Hilbert space dimensions, $|\psi(0)\rangle_S = |1\rangle_S$, $T = 1$

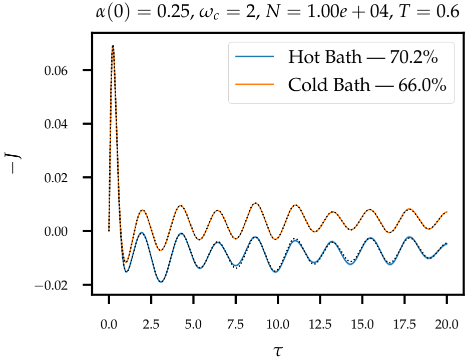


Two Baths, Finite Temperature (Gradient)

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

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

with $[H_S, H_B] = 0$.

[6] even in strong coupling equilibrium...
[7] 1, 2.

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

[6] even in strong coupling equilibrium...
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Generalizations

Finite Temperature

$$J(t) = J_0(t) + \left[\langle L^\dagger \partial_t \xi(t)\rangle + \text{c.c.}\right] \tag{22}$$

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 $J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(w - \omega_\lambda)$.[8]

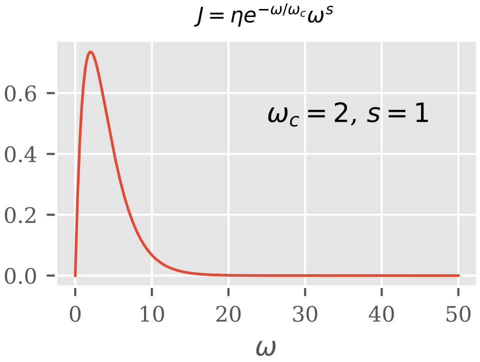
- finite temperatures
- nonlinear NMQSD/HOPS
- multiple baths straight forward
- interaction energy: "removing the dot"...
- general "collective" bath observables $O_\mathrm{S} \otimes (B^a)^\dagger B^b$ with $B = \sum_\lambda g_\lambda a_\lambda$

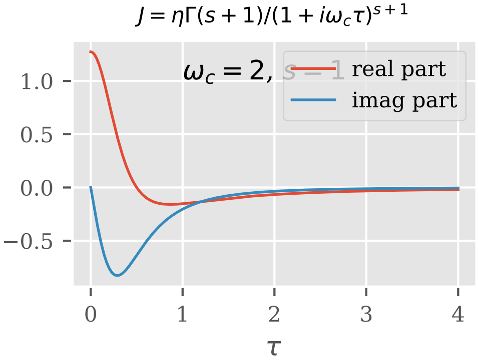
[8] $\partial_t \xi(t)$ exists if correlation function is smooth

More Papers on Thermo

[1, 2, 6–15]

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 [16] $\left\{\left|\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \ldots\right\rangle = |\underline{\mathbf{z}}\rangle\right\}$

$$|\psi(t)\rangle = \int \prod_{n=1}^{N} \left(\frac{\mathrm{d}\mathbf{z}^{(n)}}{\pi^{N_n}} \, \mathrm{e}^{-|\mathbf{z}|^2} \right) |\psi(t, \underline{\mathbf{z}}^*)\rangle \, |\underline{\mathbf{z}}\rangle \,, \tag{23}$$

we obtain

$$\partial_t \psi_t(\boldsymbol{\eta}_t^*) = -iH\psi_t(\boldsymbol{\eta}_t^*) + \mathbf{L} \cdot \boldsymbol{\eta}_t^* \psi_t(\boldsymbol{\eta}_t^*) - \sum_{n=1}^{N} L_n^\dagger \int_0^t \mathrm{d}s \, \alpha_n(t-s) \frac{\delta \psi_t(\boldsymbol{\eta}_t^*)}{\delta \eta_n^*(s)}, \tag{24}$$

with

$$\mathcal{M}(\eta_n^*(t)) = 0, \quad \mathcal{M}(\eta_n(t)\eta_m(s)) = 0, \quad \mathcal{M}(\eta_n(t)\eta_m(s)^*) = \delta_{nm}\alpha_n(t-s), \tag{25}$$

where $\alpha_n(t-s) = \sum_\lambda \left|g_\lambda^{(n)}\right|^2 \mathrm{e}^{-i\omega_\lambda^{(n)}(t-s)} = \langle B(t)B(s)\rangle_{I,\rho(0)}$ [17] (fourier transf. of spectral density $J(\omega) = \pi \sum_\lambda |g_\lambda|^2 \delta(\omega - \omega_\lambda)$).

Fock-Space Embedding

As in Ref. [18] we can define

$$|\Psi\rangle = \sum_{\underline{\mathbf{k}}} \left|\psi^{\underline{\mathbf{k}}}\right\rangle \otimes |\underline{\mathbf{k}}\rangle \tag{26}$$

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

$$\partial_t |\Psi\rangle = \left[-iH_{\mathrm{S}} + \mathbf{L}\cdot\boldsymbol{\eta}^* - \sum_{n=1}^{N}\sum_{\mu=1}^{M_n} b_{n,\mu}^\dagger b_{n,\mu} W_\mu^{(n)} + i\sum_{n=1}^{N}\sum_{\mu=1}^{M_n} \sqrt{G_{n,\mu}}\left(b_{n,\mu}^\dagger L_n + b_{n,\mu} L_n^\dagger\right)\right] |\Psi\rangle\,. \tag{27}$$

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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

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

$$H = \sum_{i\in\{1,2\}} \left[H_O^{(i)} + q_i B^{(i)} + H_B^{(i)}\right] + \frac{\gamma}{4}(q_1 - q_2)^2, \tag{28}$$

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

$$H = \frac{1}{2}\sigma_z + \frac{1}{2}\sum_\lambda \left(g_\lambda \sigma_x^\dagger a_\lambda + g_\lambda^* \sigma_x a_\lambda^\dagger\right) + \sum_\lambda \omega_\lambda a_\lambda^\dagger a_\lambda,\ \left|\psi_0\right\rangle_{\mathrm{S}} = \left|\uparrow\right\rangle \tag{29}$$

- how do we check convergence:

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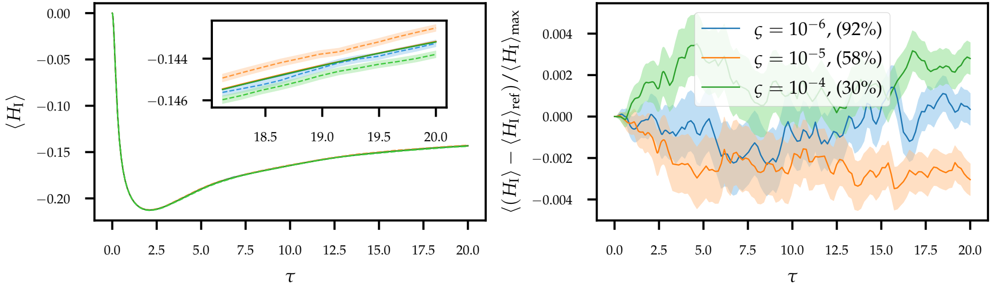
- how do we check convergence:
  - old: difference of results to some “good” configuration
  - new: consistency with energy conservation

Example: Dependence of the Interaction Energy on Stochastic Process Sampling

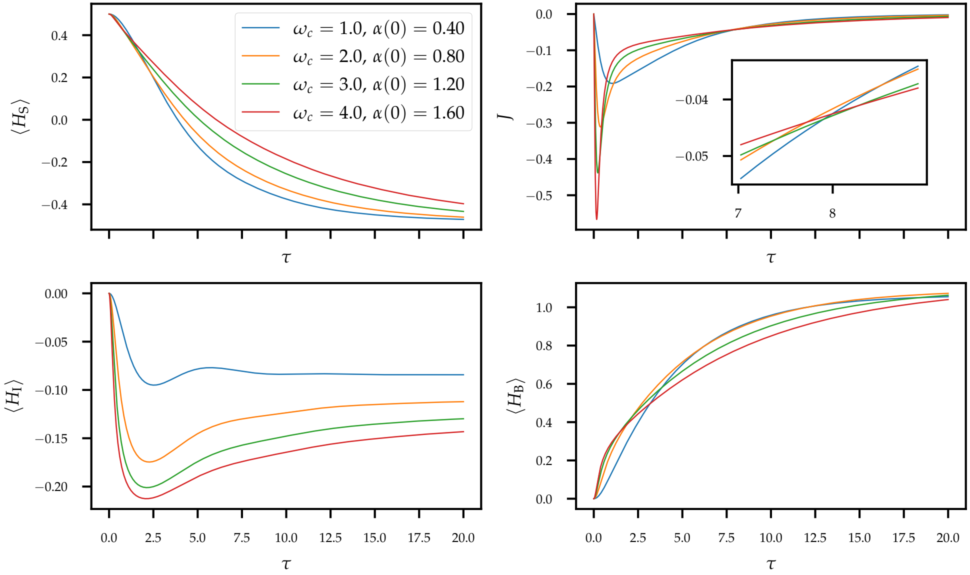


- $\alpha(0) = 1.6$ and $\omega_c = 4 \implies$ stress HOPS through fast decaying BCF
- "perfect" results only with very high accuracy[9] ς
- good qualitative results for less extreme configurations (common theme)

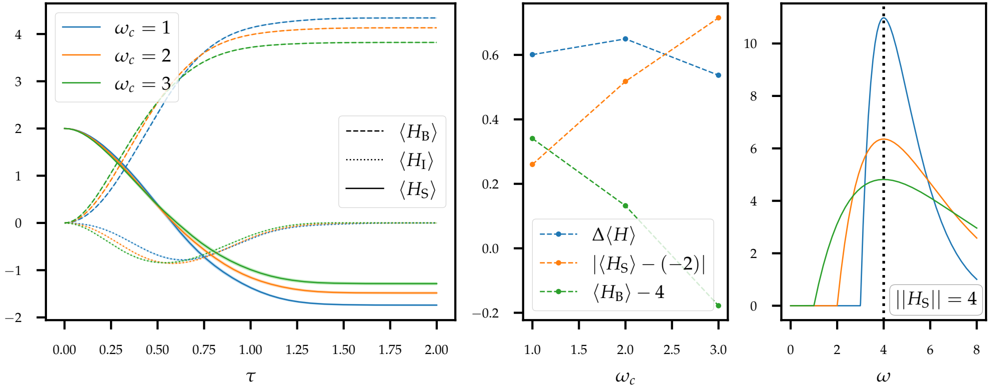
---

[9] smaller ς is better

Various Cutoff Frequencies



Non-Markovian Dynamics



- interaction strengths chosen for approx. same interaction energy

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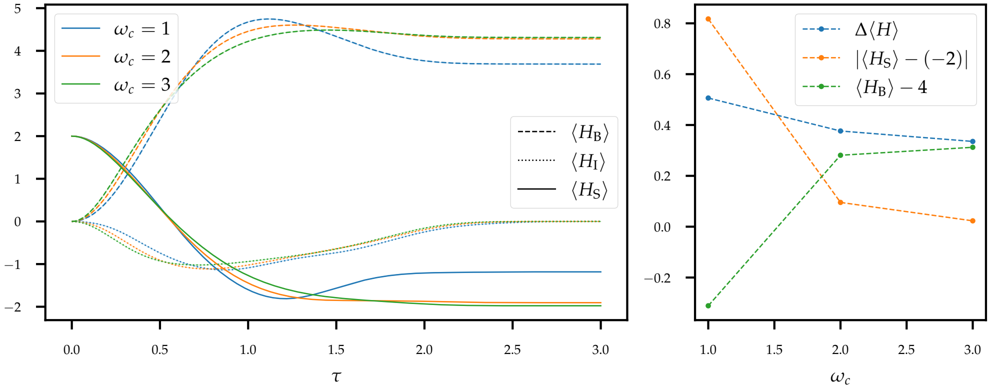


- interaction strengths chosen for approx. same interaction energy
- timing important for energy transfer "performance"

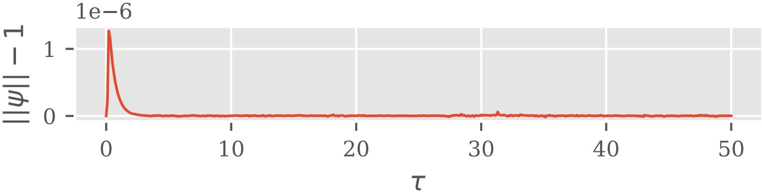
Beware :)

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

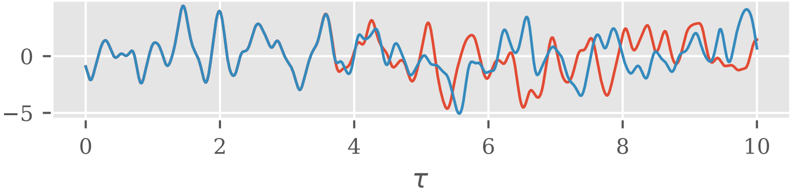
One Bath

Other Projects

- stabilized normalization in nonlinear HOPS



- stochastic process sampling via Cholesky decomposition



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