Effective working fluid-bath decoupling at the strong coupling regime

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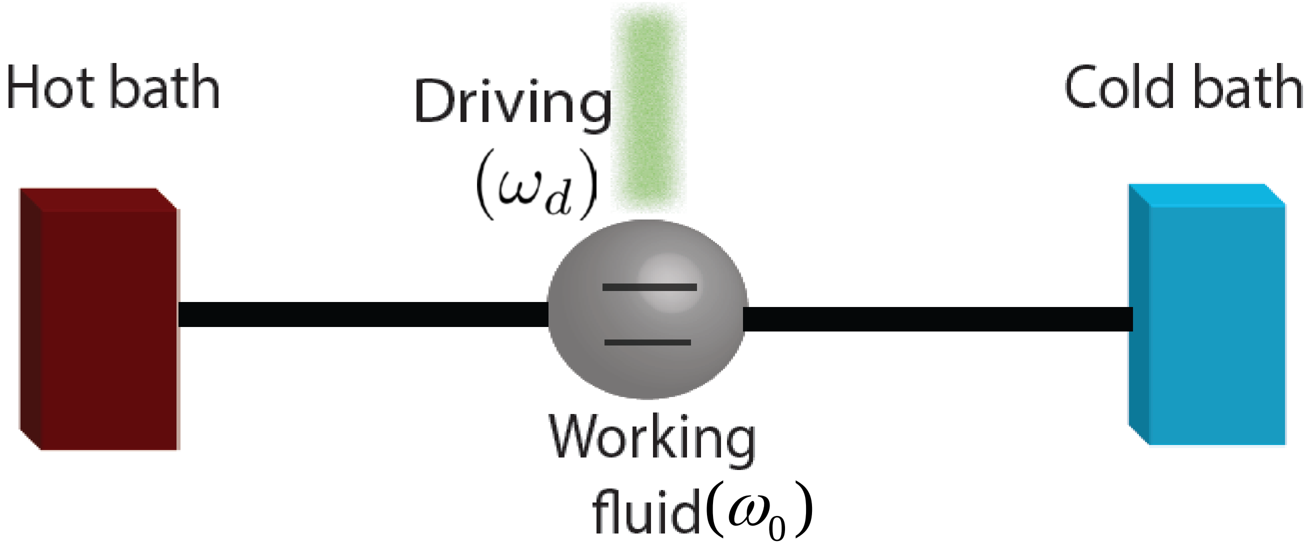
Harvard University

Bad Honnef, April 2017

What is a heat machine?



Components

1. Working fluid: (qubit, TLS).
2. Hot and cold bath
3. A piston (External driving) periodically drives the system and gets or gives work.

$$H_{Tot} = H_S(t) + \sum_i (H_{B_i} + \underline{\xi_i S} \otimes B_i) \quad i \in H, C$$

Review: D. G.-K, W. Niedenzu, G. Kurizki Adv. AMO Physics 64, 329-407 (2015) (arXiv:1503.01195)

Weakly coupled machines

$$H_{Tot} = H_S(t) + \sum_i H_{B_i} + H_{SB_i} \quad i \in H, C$$

(Baths at equilibrium)

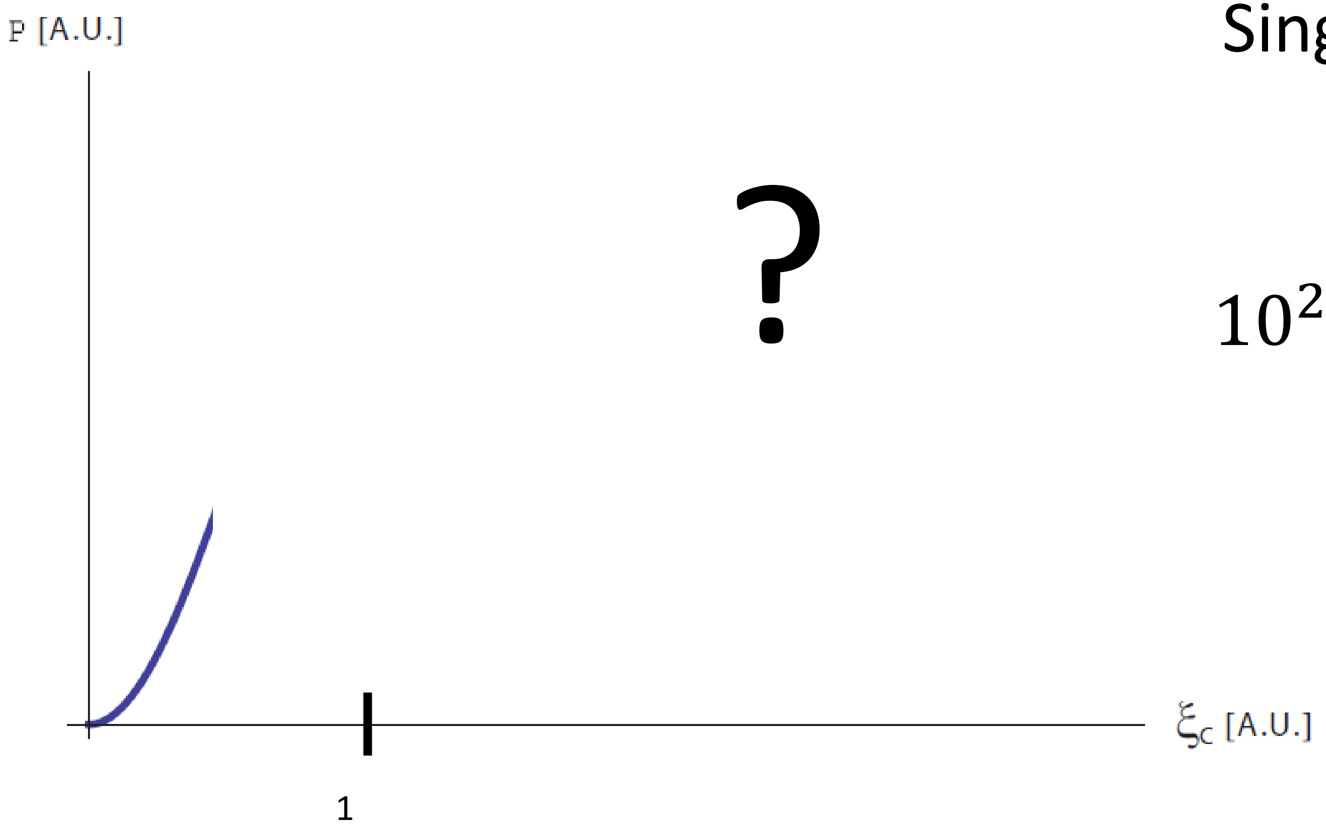
Lindblad master equation
(weak coupling, “small” ξ_i)

$$\rho_S(t)$$

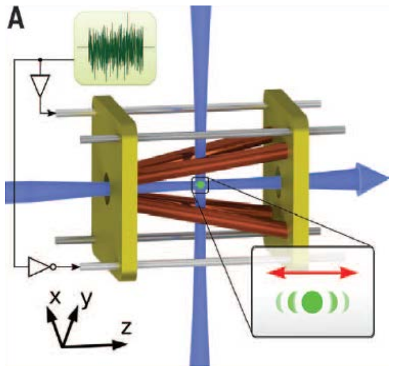
$$J_i(G_i(\omega))$$

Thermodynamic quantities
(analytic expressions)

Weak coupling limitations



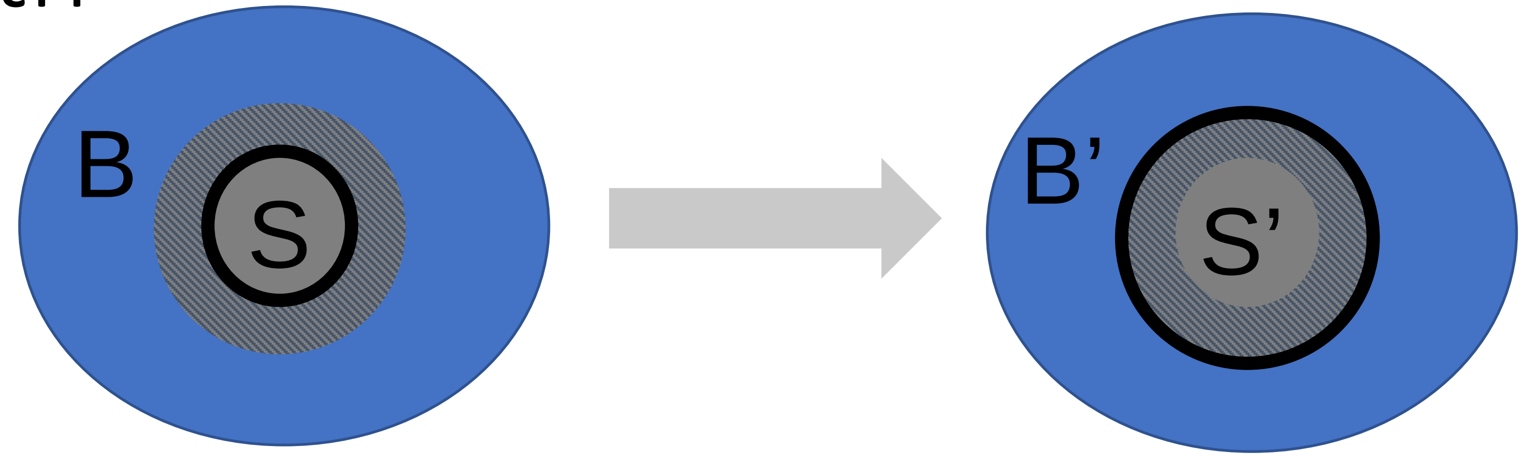
Single atom heat engine power*: $10^{-22} J/s$

$10^{27} X$ 

Power/mass: $1.5 kW/kg$

J Rossnage, S Dawkins, K Tolazzi, O Abah, E Lutz, F Schmidt-kaler, K Singer (2016) *Science* 325-329

Strong coupling: Redefining the system and the bath



S-B strong coupling

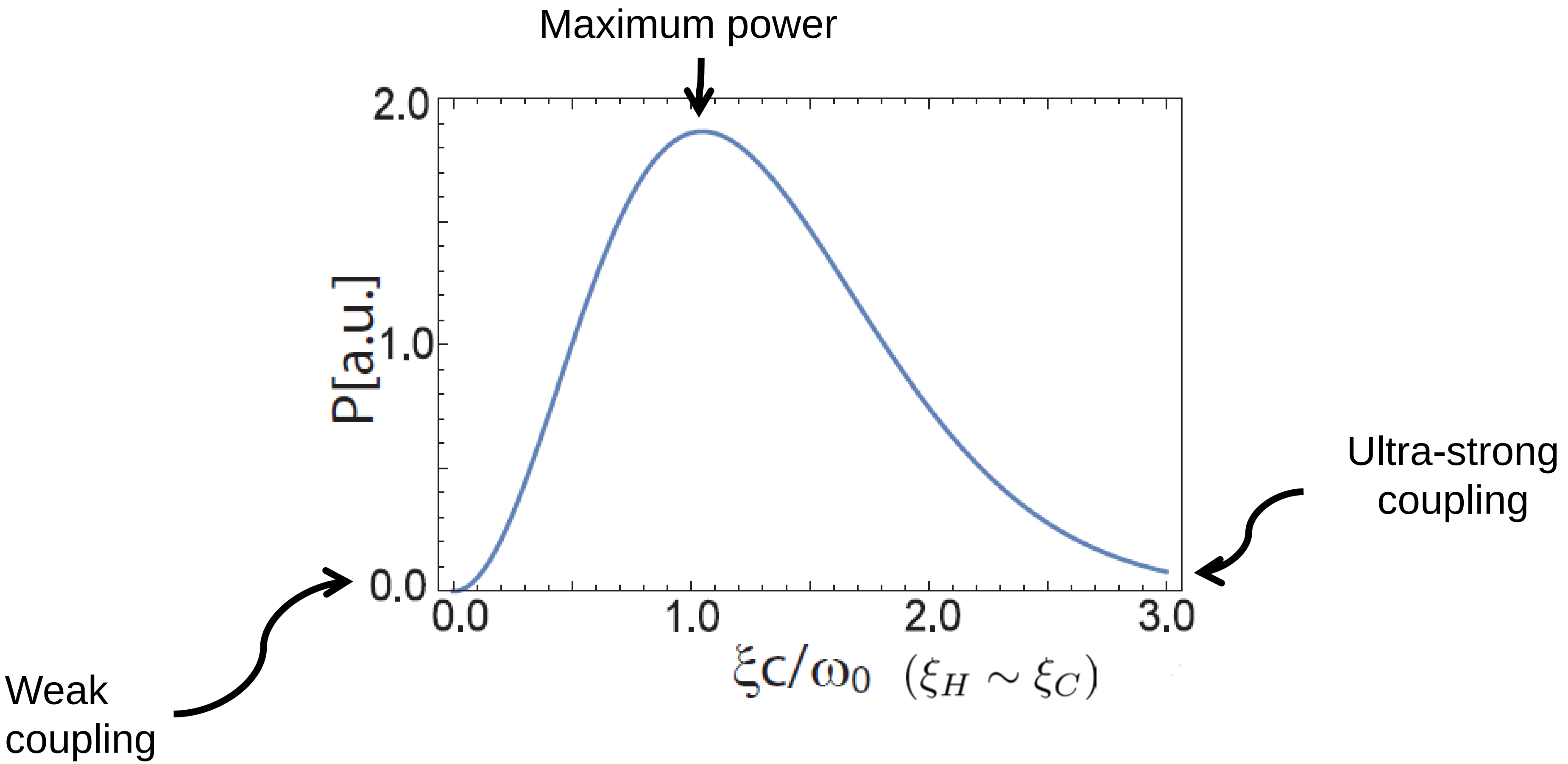
S'-B' effective weak coupling

$$\tilde{\mathcal{H}} \longrightarrow \mathcal{H} = U\tilde{\mathcal{H}}U^{\dagger}$$

$$U \ \text{Polaron transformation}$$

D. P. McCutcheon and A. Nazir, NJP 12, 113042 (2010).
D G-K, A Aspuru-Guzik, JPCL 6 (17), 3477–3482 (2015)

Power “disappears” at the strong coupling



D G-K, A Aspuru-Guzik, JPCL 6 (17), 3477–3482 (2015)

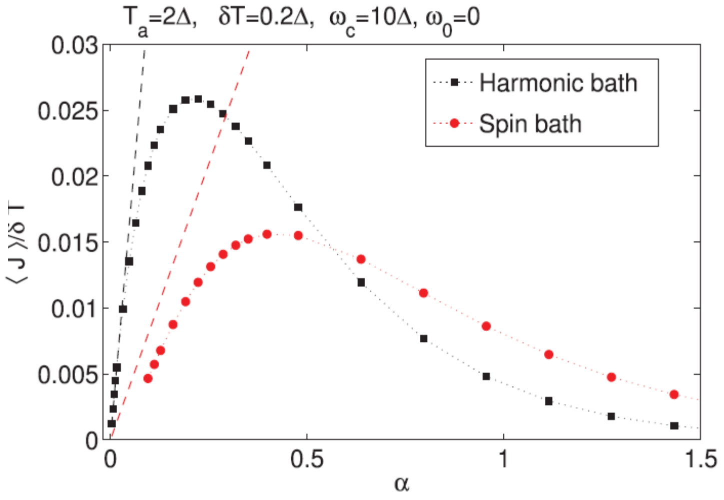
Decay of the current in other systems

THE JOURNAL OF CHEMICAL PHYSICS **140**, 164110 (2014)

Two-level system in spin baths: Non-adiabatic dynamics and heat transport

Dvira Segal
Chemical Physics Theory Group, Department of Chemistry, University of Toronto, 80 Saint George St.,

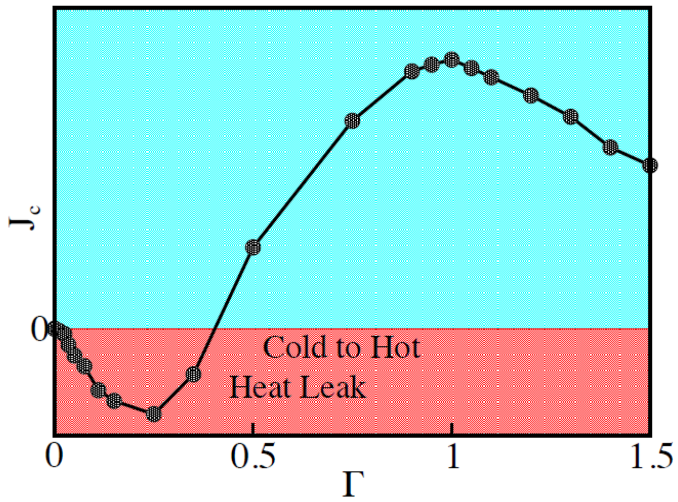
System: Spin
Baths: Spin/Boson
Technique: NIBA



Article

Quantum Thermodynamics in Strong Coupling: Heat Transport and Refrigeration

System: Molecule
Baths: Spin
Technique: Surrogate Hamiltonian

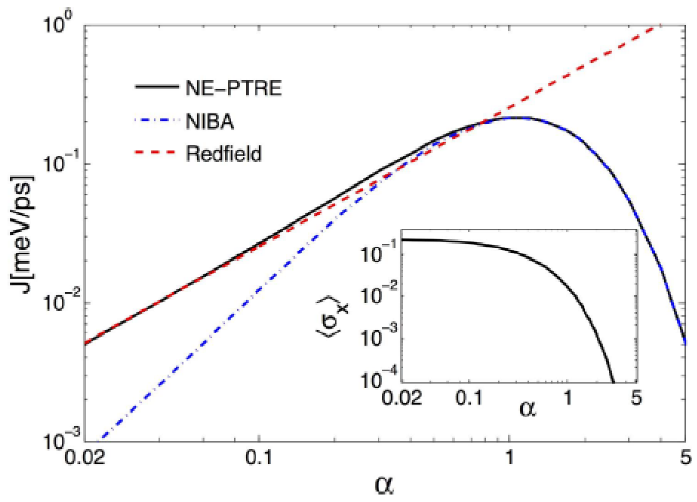


Decay of the current in other systems

Nonequilibrium Energy Transfer at Nanoscale: A Unified Theory from Weak to Strong Coupling

Chen Wang[1,2,3], Jie Ren[1,4] & Jianshu Cao[1,2]

System: Spin
Baths: Bosonic
Technique: NE-PTRE



Quantum phase transition in the multimode Dicke model

Denis Tolkunov* and Dmitry Solenov†
Department of Physics, Clarkson University, Potsdam, New York 13699–5820
(Dated: February 6, 2008)

System: Harmonic oscillator
Baths: Bosonic
Technique: Holstein-Primakoff Transformation

Nonequilibrium thermodynamics in the strong coupling and non-Markovian regime based on a reaction coordinate mapping

Philipp Strasberg[1], Gernot Schaller[1], Neill Lambert[2] and Tobias Brandes[1]

System: Arbitrary
Baths: Bosonic
Technique: Reaction coordinate

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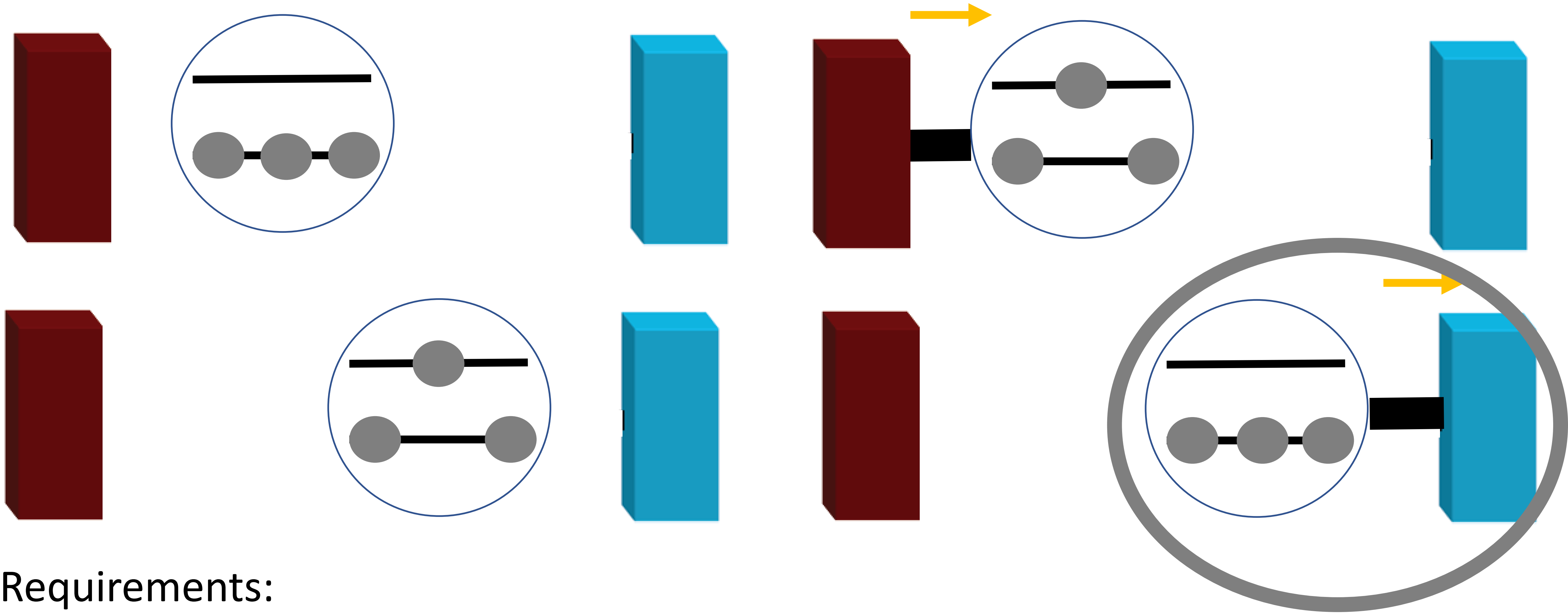
Yes

What is the physical mechanism?

No

Show an example

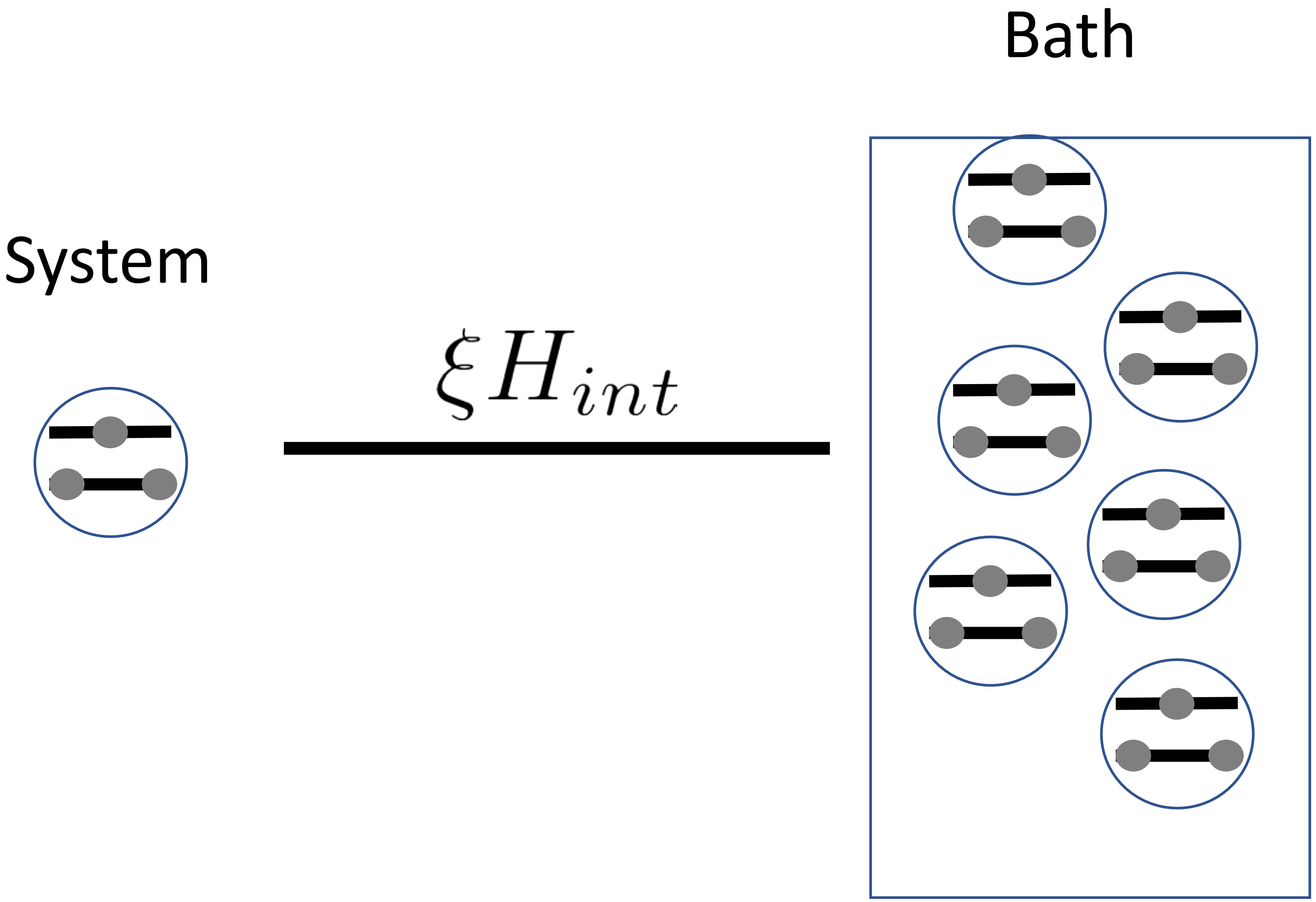
Energy transfer in the strokes engine



Requirements:

- Energy exchange between the system and bath
- Different equilibrium states for different temperatures

Energy exchange between the system and a single thermal bath



$$\rho(0) = \rho_{gg} \otimes \frac{e^{-\beta H_B}}{Z}$$

There are two different mechanisms of effective decoupling…

… or maybe only one?

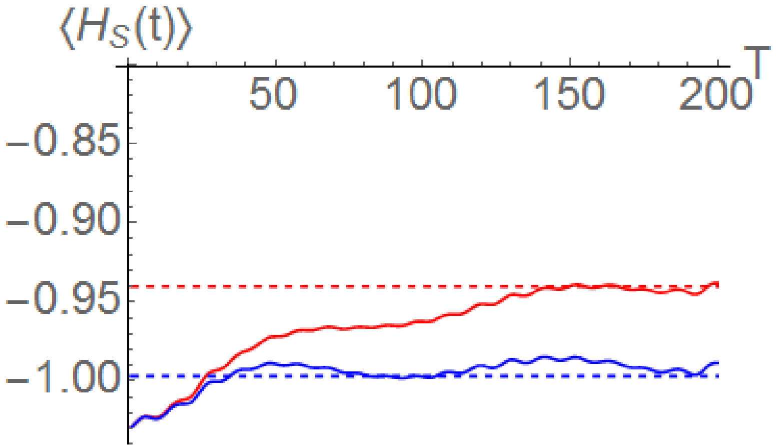
Case 1:"Polaron" Hamiltonian

$H_s = \frac{\omega_0}{2}\sigma_z + A\sigma_x$

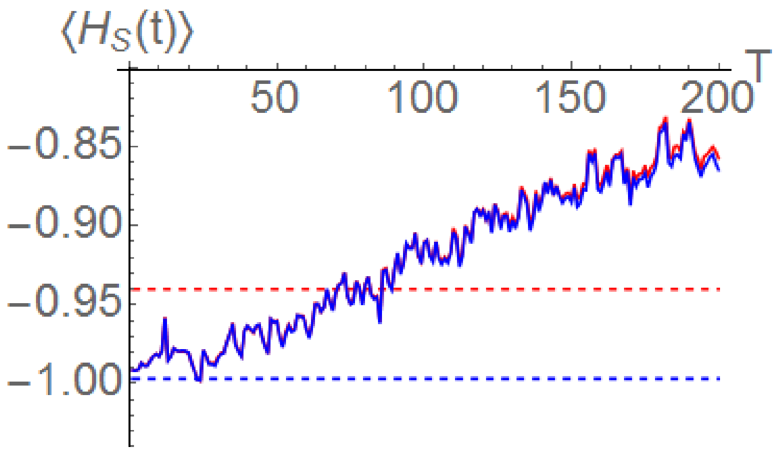
$\xi H_{int} = \xi\sigma_z \otimes B$

Two level system weakly driven by a low frequency laser $A \ll \omega_0$

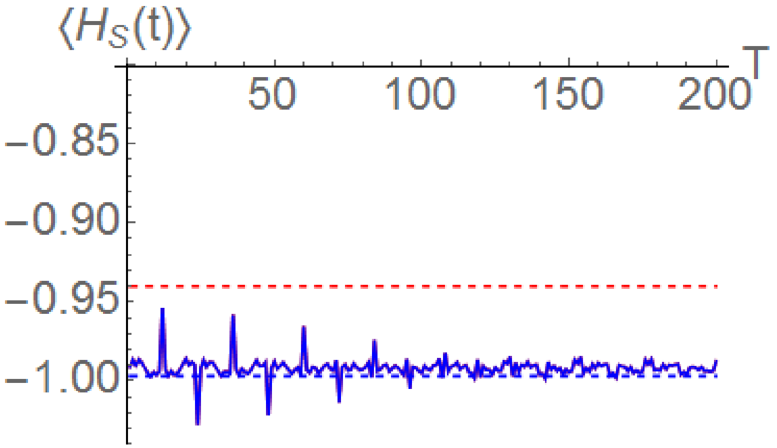
Weak coupling



Intermediate coupling



Strong coupling

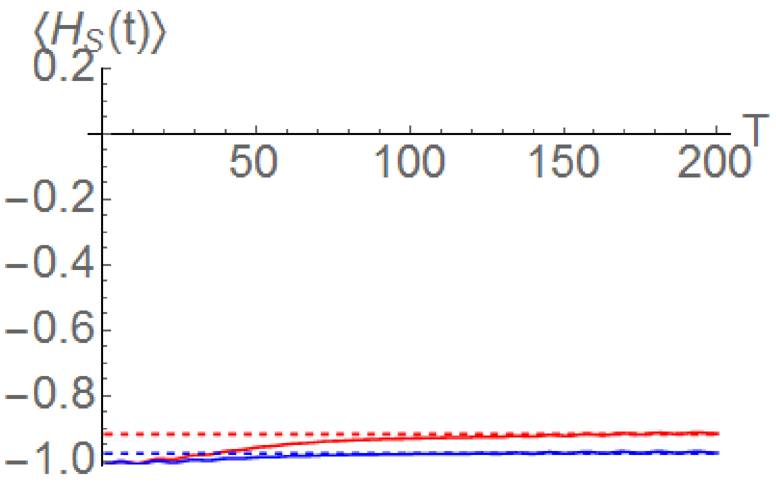


At the strong coupling: the system and the bath do not exchange energy anymore

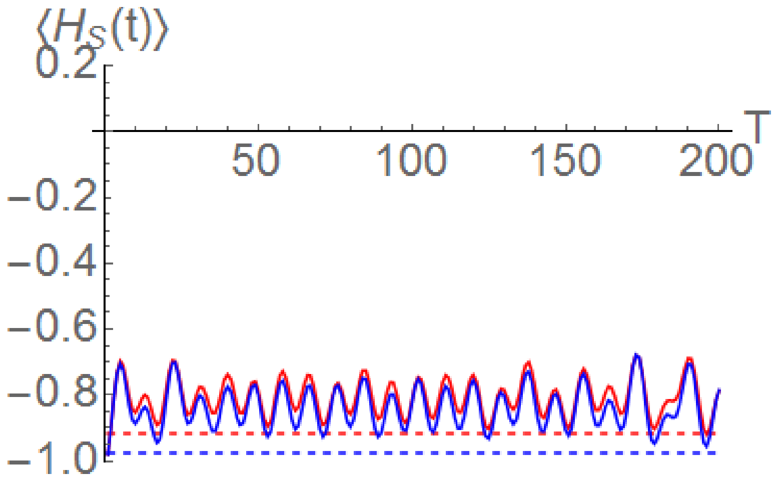
Case 2:“Orthogonal” Hamiltonian

$$H_s = \frac{\omega_0}{2}\sigma_z \qquad \xi H_{int} = \xi \sigma_x \otimes B$$

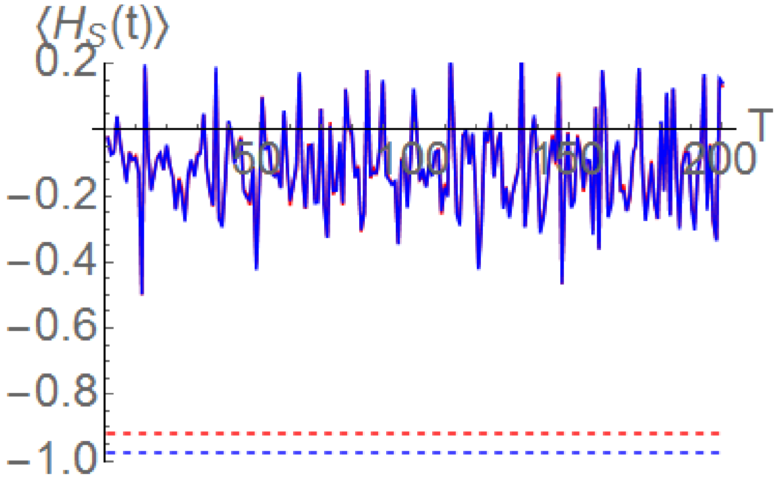
Weak coupling



Intermediate coupling



Strong coupling



At the strong coupling: the system and the bath energy exchange grows

Heisenberg picture: time evolution at any coupling strength

$$H_S(t) = e^{iH_{tot}t} H_s(0) e^{-iH_{tot}t}$$

$$H_{tot}|i\rangle = E_i|i\rangle$$

$$\rho_{tot}(0) = \sum_{ij} \rho_{tot}^{ij}(0)|i\rangle\langle j|$$ (Doesn't evolve in this picture)

$$H_s \otimes I_B(0) = \sum_{ij} H_s^{ij}(0)|i\rangle\langle j|$$

Steady state for any coupling strength

$$\langle H_s(t) \otimes I_B \rangle =$$
$$\sum_i H_s^{ii}(0)\rho_{tot}^{ii}(0) + \sum_{i\neq j} H_s^{ij}(0)\rho_{tot}^{ji}(0)e^{it(E_i - E_j)}$$

Diagonal terms:
Steady state

Off-diagonal terms:
Oscillatory

At the strong coupling: $H_{tot} \approx \xi H_{int}$

Steady state for "polaron" Hamiltonian

$$H_s \otimes I_B = (\tfrac{\omega_0}{2}\sigma_z + A\sigma_x) \otimes I_B \qquad \xi H_{int} = \xi\sigma_z \otimes B$$

$$H_{tot} \approx \xi\sigma_z \otimes B$$

$$\textstyle\sum_i H_s^{ii}(0)\rho_{tot}^{ii}(0) = \langle \frac{\omega_0}{2}\sigma_z(0)\rangle \approx \langle H_s(0)\rangle$$

This result is independent of the bath and its coupling to the system

Steady state for “Orthogonal” Hamiltonian

$$H_s \otimes I_B = \frac{\omega_0}{2}\sigma_z \otimes I_B \qquad \xi H_{int} = \xi \sigma_x \otimes B$$

$$H_{tot} \approx \xi \sigma_x \otimes B$$

$$H_s^{ii}(0) = 0$$

$\sum_i H_s^{ii}(0)\rho_{tot}^{ii}(0) = 0$ Does not depend on the bath temperature

This result is independent of the bath and its coupling to the system

What can we do?

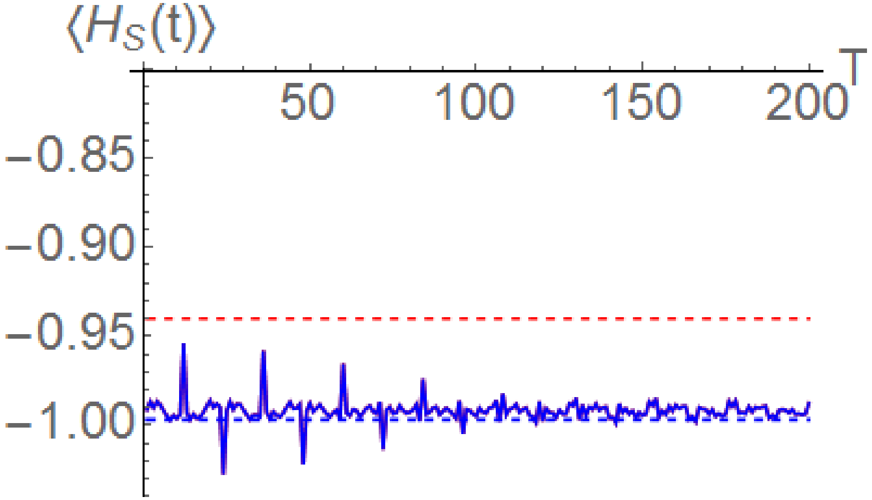
$$\langle H_s(t) \otimes I_B \rangle =$$

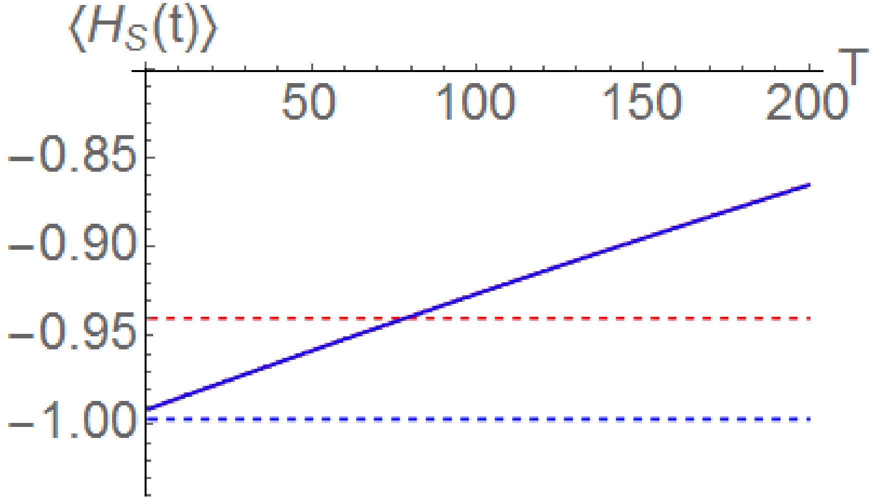
$$\sum_i H_s^{ii}(0)\rho_{tot}^{ii}(0) + \sum_{i\neq j} H_s^{ij}(0)\rho_{tot}^{ji}(0)e^{it(E_i - E_j)}$$

Break the dynamics!

… by periodically disturbing the dynamics!

“polaron” Hamiltonian under disturbances

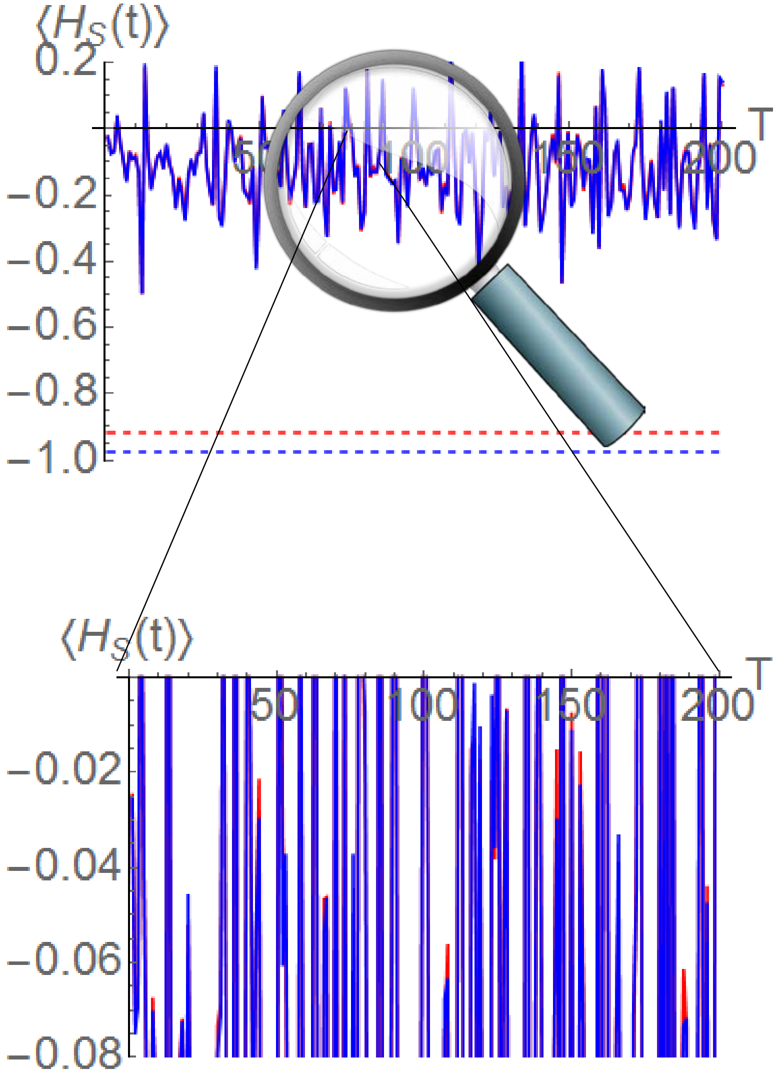


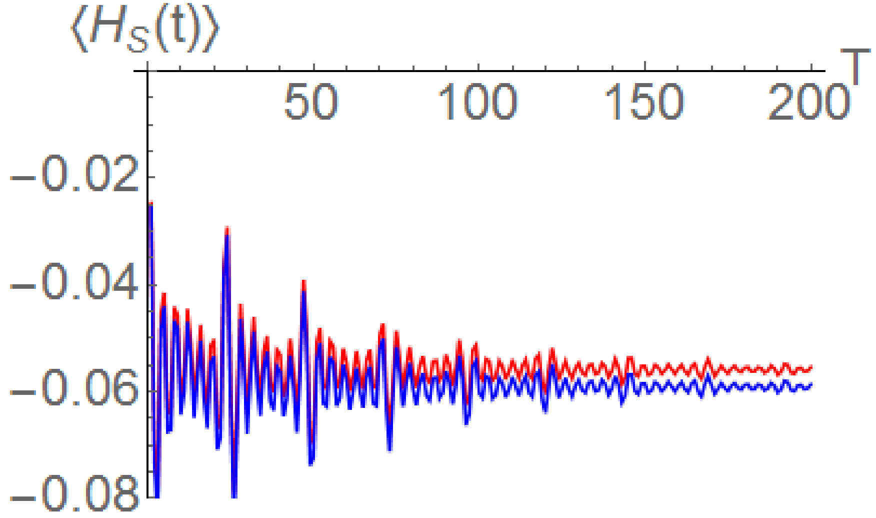


Independent of the bath temperature

No heat currents or power

“Orthogonal” Hamiltonian under disturbances

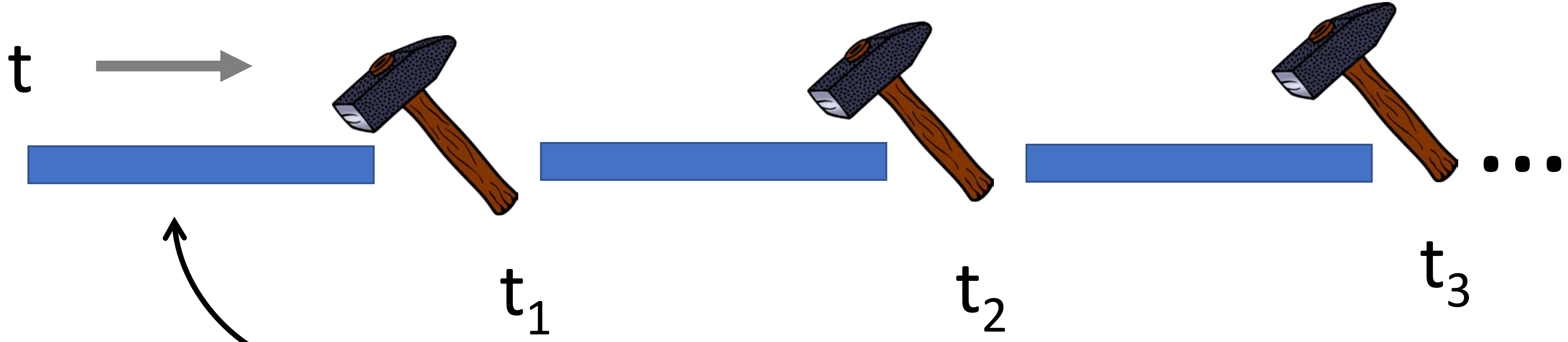




Depends on the bath temperature

Heat currents and power

Frequent perturbations: totally different dynamics



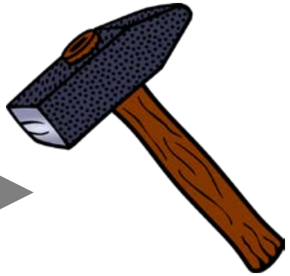
$$e^{iH_{tot}t}H_s(0)e^{-iH_{tot}t} \approx$$
$$H_s(0) + it[H_{tot}, H_s(0)] - \frac{t^2}{2}[H_{tot}, [H_{tot}, H_s(0)]]$$

Recurrent short time dynamics

$$H_s(t) = H_s(0) + it[H_{tot}, H_s(0)] - \frac{t^2}{2}[H_{tot}, [H_{tot}, H_s(0)]] = H_s(0) + f(t)$$

Short time dynamics

$$H_s(t_1) = H_s(t_0) + f(t_1)$$

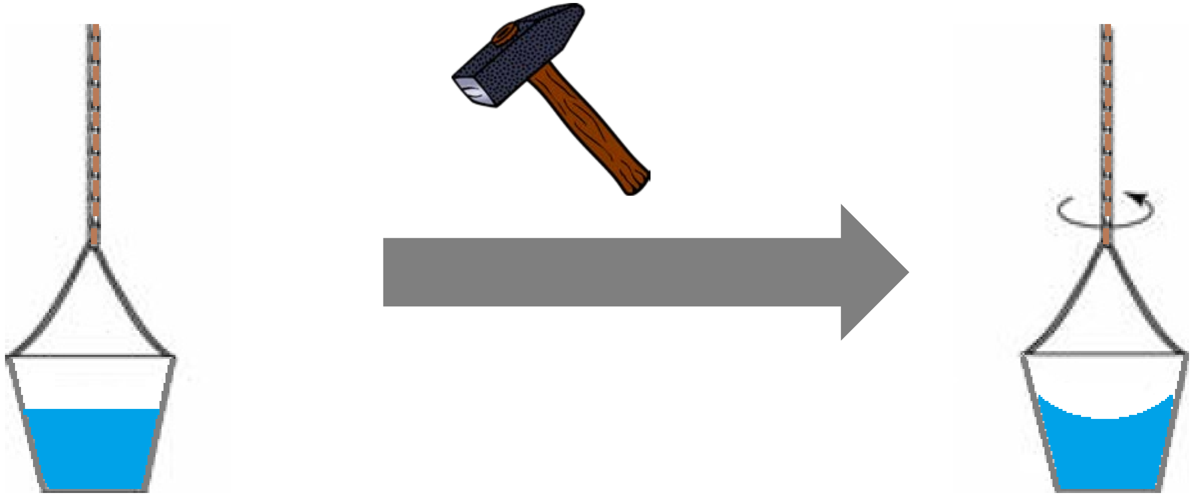


Does not change H_s(t) or H_{tot}

$$H_s(t_2) = H_s(t_1) + f(t_2)$$

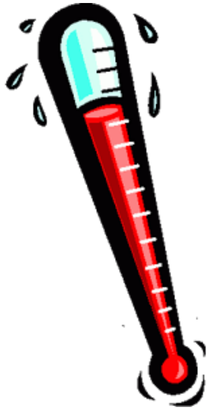
$\vdots$

Effects of frequent perturbations



Change the steady state

$\cancel{\sum_i H_s^{ii} \rho_{tot}^{ii}}$



$f(t)$ may depend on $\langle H_B(0) \rangle$

(Bath temperature)

Conclusions

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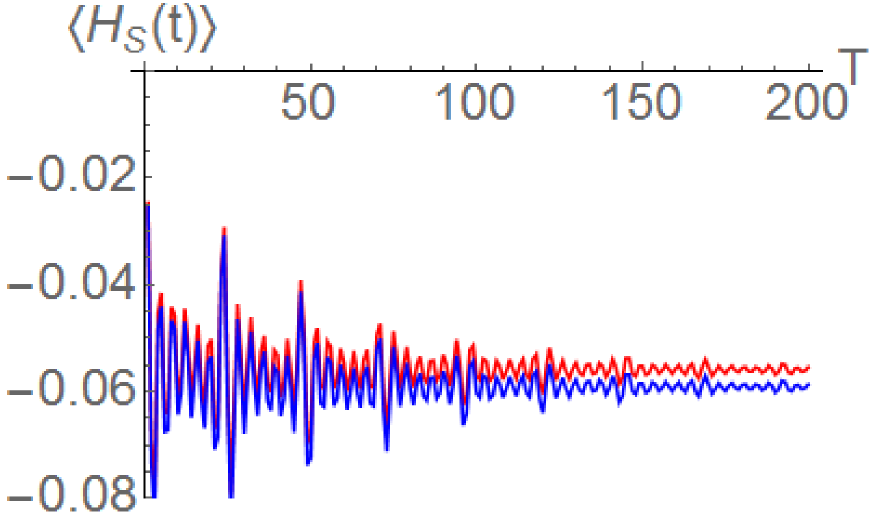
I do not know

$J, P = 0,$ caused by the steady state independence of T



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Nicolas Sawaya

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