

**Einselection
and
Quantum Thermodynamics of Small Systems
Strongly Interacting with Environments**

Ryoichi Kawai

Ketan Goyal
(Student)

*Department of Physics
University of Alabama at Birmingham*

NORDITA, September 14, 2017



RALF EICHHORN,

“Let us remind you that the program is intended to discuss open questions and new ideas in a lively atmosphere. Accordingly, we would prefer talks on such open questions,

but overviews of past work and/or historical perspectives are also welcome.”

Contents

- Motivation
- Review of Quantum Measurement theory, Decoherence and Eigenselection
- A couple of Claims
- Review of Open Quantum Systems
- Model
- Theoretical/Computational Methods
- Thermalization
- Heat Conduction
- Autonomous Quantum Heat Engine
- Conclusions

Thermalization and Decoherence in Energy Eigenbasis

$$\text{Thermalization: } \rho_0 \implies \rho_G = \frac{1}{Z} e^{-\beta H} \quad (\text{Gibbs state})$$

Gibbs state is very special.

- Diagonal in the energy eigenbasis
- Decoherence in the energy eigenbasis
- Decoherence is induced by the environment
- Why and how does the environment select the energy eigenbasis?
- Does it have to be the energy eigenbasis?
- If not, what else is possible?
- In what basis decoherence happens in non-equilibrium steady state?

Quantum Measurement Postulate (Projective Measurement)

system state

$$|\psi_s\rangle = \sum_i c_i |\omega_i\rangle$$

observable

$$\hat{\Omega} |\omega_i\rangle = \omega_i |\omega_i\rangle$$

probability

$$P_i = |c_i|^2$$

Collapse of wavefunction

before measurement

$$\rho_{<} = \sum_{ij} c_i c_j^* |\omega_i\rangle\langle\omega_j|$$

measurement

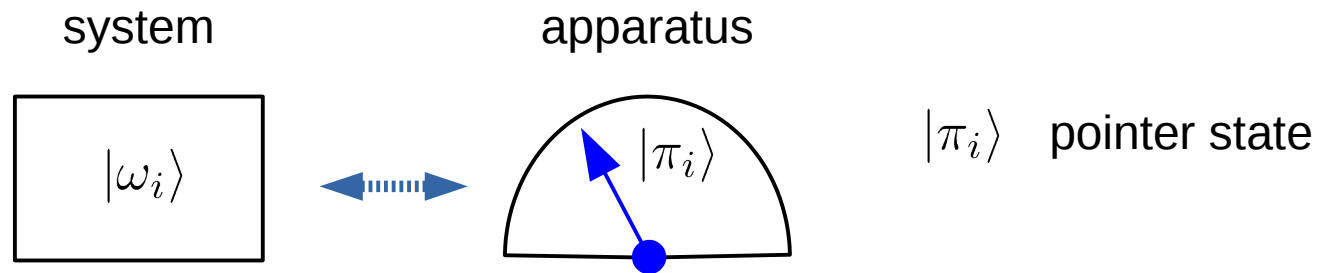
after measurement

$$\rho_{>} = \sum_i |c_i|^2 |\omega_i\rangle\langle\omega_i| = \sum_i |\omega_i\rangle\langle\omega_i| \rho_{<} |\omega_i\rangle\langle\omega_i|$$

Decoherence in Observable Basis

- Decoherence happens for different basis depending on what you measure.
- If the decoherence is induced by the environment, how does the environment know what you measure?

von Neumann - Everett Theory of measurement.



entanglement $|\psi_{SA}\rangle = \sum_i c_i |\omega_i\rangle \otimes |\pi_i\rangle$

This correlation does not solve the problem. $|\psi_{SA}\rangle = \sum_i d_i |\nu_i\rangle \otimes |\xi_i\rangle$

We need collapse of wavefunction

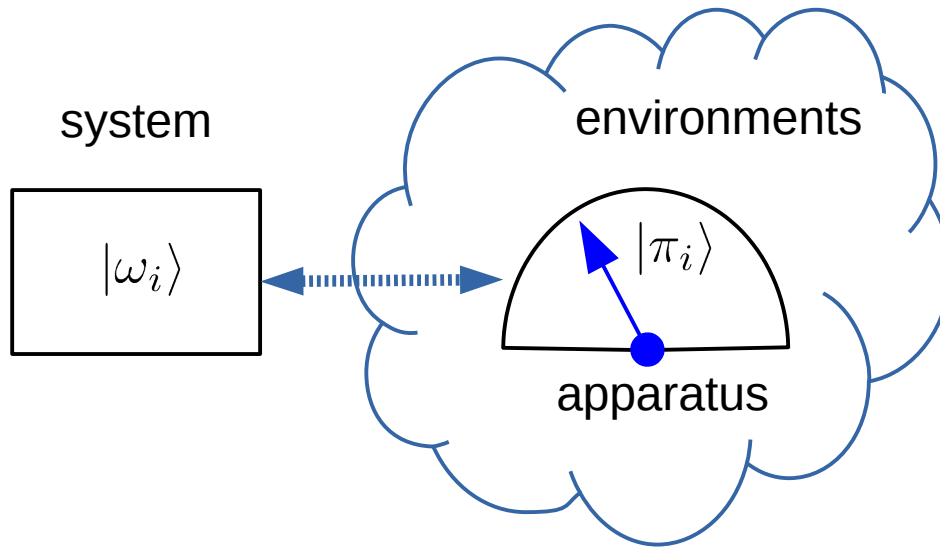
before measurement

$$\rho_{\text{pure}} = \sum_j \sum_j c_j c_j^* |\omega_j\rangle\langle\omega_j| \otimes |\pi_j\rangle\langle\pi_j|$$

after measurement

$$\rho_{\text{mixed}} = \sum_i |c_i|^2 |\omega_i\rangle\langle\omega_i| \otimes |\pi_i\rangle\langle\pi_i|$$

Environment-induced Decoherence



$$\begin{aligned}
 |\Psi\rangle &= \sum_i c_i |\omega_i\rangle \otimes |\pi_i\rangle \otimes |\mathcal{E}_i\rangle \\
 &\neq \sum_i d_i |\nu_i\rangle \otimes |\xi_i\rangle \otimes |\mathcal{F}_i\rangle \\
 \rho_{SA} &= \text{tr}_B |\Psi\rangle\langle\Psi| \\
 &= \sum_i |c_i|^2 |\omega_i\rangle\langle\omega_i| \otimes |\pi_i\rangle\langle\pi_i|
 \end{aligned}$$

Environment picks pointer states and induces decoherence among pointer states.

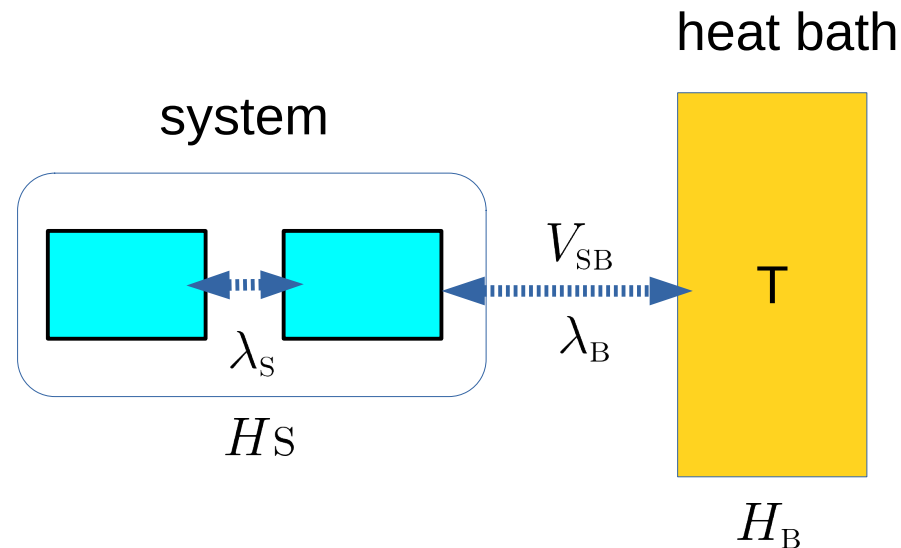
Why is the pointer state? $\rightarrow V_{AE}$ picks the pointer state.

When \hat{V}_{AE} is dominant, the pointer states are determined by:

$$\left[\hat{\Pi} \otimes I^E, \hat{V}_{AE} \right] = 0 \quad \hat{\Pi} |\pi_i\rangle = \pi_i |\pi_i\rangle$$

Environment-induced Eigenselction (Superselection) W. Zurek (1981, 1982)

Thermodynamic Steady State and Eigenselection



$$\lambda_B \ll 1 \quad \rho_s \rightarrow \frac{1}{Z} e^{-\beta H_s}$$

Claims

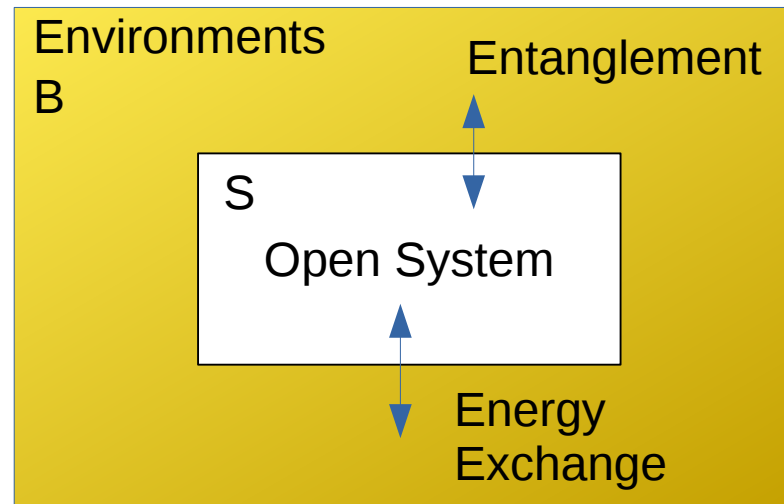
$$\lambda_B \gg |H_S|, \quad \rho_s \rightarrow \frac{1}{Z} \sum_i |\pi_i\rangle\langle\pi_i| e^{-\beta H_s} |\pi_i\rangle\langle\pi_i|$$

$$\lambda_B \sim |H_S|, \quad \langle\pi_i|\rho_s|\pi_i\rangle \approx \frac{1}{Z} \langle\pi_i|e^{-\beta H_s}|\pi_i\rangle$$

Projective measurement by the environment

$$[V_{SB}, \hat{\Pi}], \quad \hat{\Pi} |\pi\rangle = \pi_i |\pi_i\rangle$$

Open Quantum Systems



Assuming that the whole system is completely isolated, how does the system evolve in time?

Hamiltonian:

$$H_{SB} = H_S \otimes I_B + I_S \otimes H_B + V_{SB}$$

Unitary Evolution
Of the Total System

$$i \frac{\partial \rho_{SB}}{\partial t} = [H_{SB}, \rho_{SB}]$$

State of the System

$$\rho_S(t) = \text{tr}_B[\rho_{SB}(t)]$$

Dynamics of System State

Separable Hamiltonian: $H_{\text{SB}} = H_{\text{S}} \otimes I_{\text{B}} + I_{\text{S}} \otimes H_{\text{B}} + \lambda_{\text{B}} X_{\text{S}} \otimes Y_{\text{B}}$

$$i \frac{\partial}{\partial t} \rho_{\text{SB}} = [H_{\text{SB}}, \rho_{\text{SB}}] \quad \xRightarrow{\text{tr}_{\text{B}}} \quad i \frac{\partial}{\partial t} \rho_{\text{S}} = [H_{\text{S}}, \rho_{\text{S}}] + \lambda_{\text{B}} [X_{\text{S}}, \eta_{\text{S}}]$$

$$\eta_{\text{S}} = \text{tr}_{\text{B}} [Y_{\text{B}} \rho_{\text{SB}}]$$

system-dependent mean displacement of environment

If there is no correlation:

$$\rho_{\text{SB}} = \rho_{\text{S}} \otimes \rho_{\text{B}} \implies \eta_{\text{S}} = \rho_{\text{S}} \langle Y_{\text{B}} \rangle$$

If η_{S} is a functional of ρ_{S} , then we have a self-consistent equation of motion for ρ_{S} (ex. Lindblad equation).

Born-Markovian Approximation: Quantum Master Equation

- Weak Coupling between S and B: Born Approximation

$$\rho_{SB}(t) = \rho_S(t) \otimes \rho_G$$

- Short correlation time for B: Markovian Approximation
- Other approximations: Secular, Rotating Wave

$$\frac{\partial \rho_S}{\partial t} = -i [\tilde{H}_S, \rho_S] + D[\rho_S]$$

Dissipator



In energy eigenbasis,

- Off-diagonal element vanishes very quickly (Decoherence)
- The transition between eigenstates is incoherent.
The dynamics is semi-classical.
- Correlation between S and B is considered only perturbatively.
- Steady state exists: Gibbs state.

Not suited for the present issues.

Model: A Pair of Q-bits

Coupled Q-bits

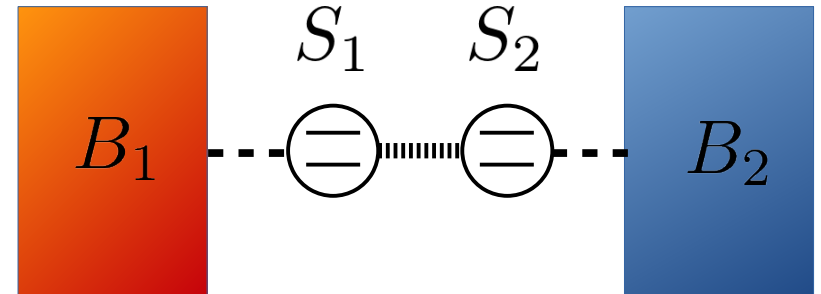
$$\hat{H}_S = \frac{\omega_0}{2} \hat{\sigma}_{S_1}^z + \frac{\omega_0}{2} \hat{\sigma}_{S_2}^z + \lambda_S (\hat{\sigma}_{S_1}^+ \hat{\sigma}_{S_2}^- + \hat{\sigma}_{S_1}^- \hat{\sigma}_{S_2}^+)$$

$$E_1 = -\omega_0, \quad |e_1\rangle = |--\rangle$$

$$E_2 = -\lambda_S, \quad |e_2\rangle = \frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle)$$

$$E_3 = +\lambda_S, \quad |e_3\rangle = \frac{1}{\sqrt{2}} (|+-\rangle + |-+\rangle)$$

$$E_4 = +\omega_0, \quad |e_4\rangle = |++\rangle$$



Boson Baths

$$\hat{H}_{B_i} = \sum_k \omega_{B_i}(k) \hat{a}_{B_i}^\dagger(k) \hat{a}_{B_i}(k), \quad i = 1, 2$$

System-Bath Coupling

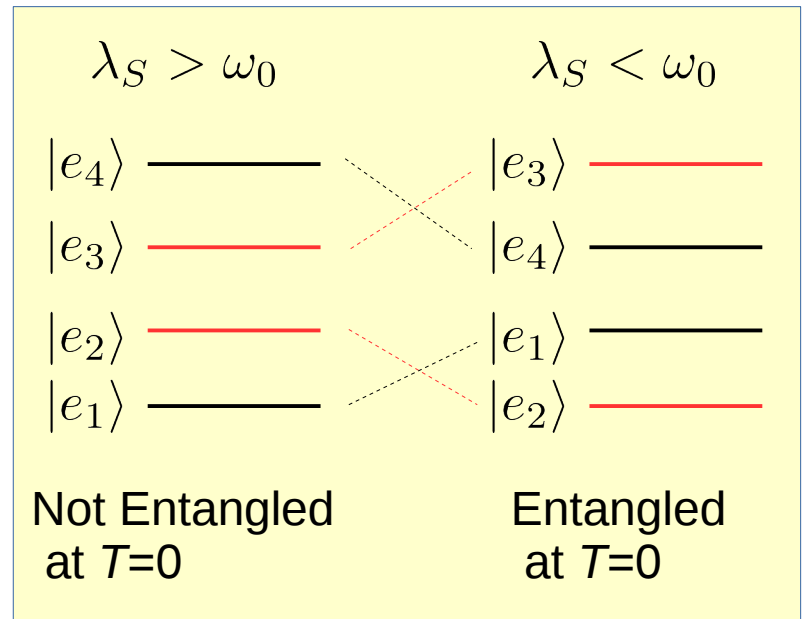
$$\hat{V}_{S_i B_i} = \hat{X}_{S_i} \otimes \hat{Y}_{B_i}$$

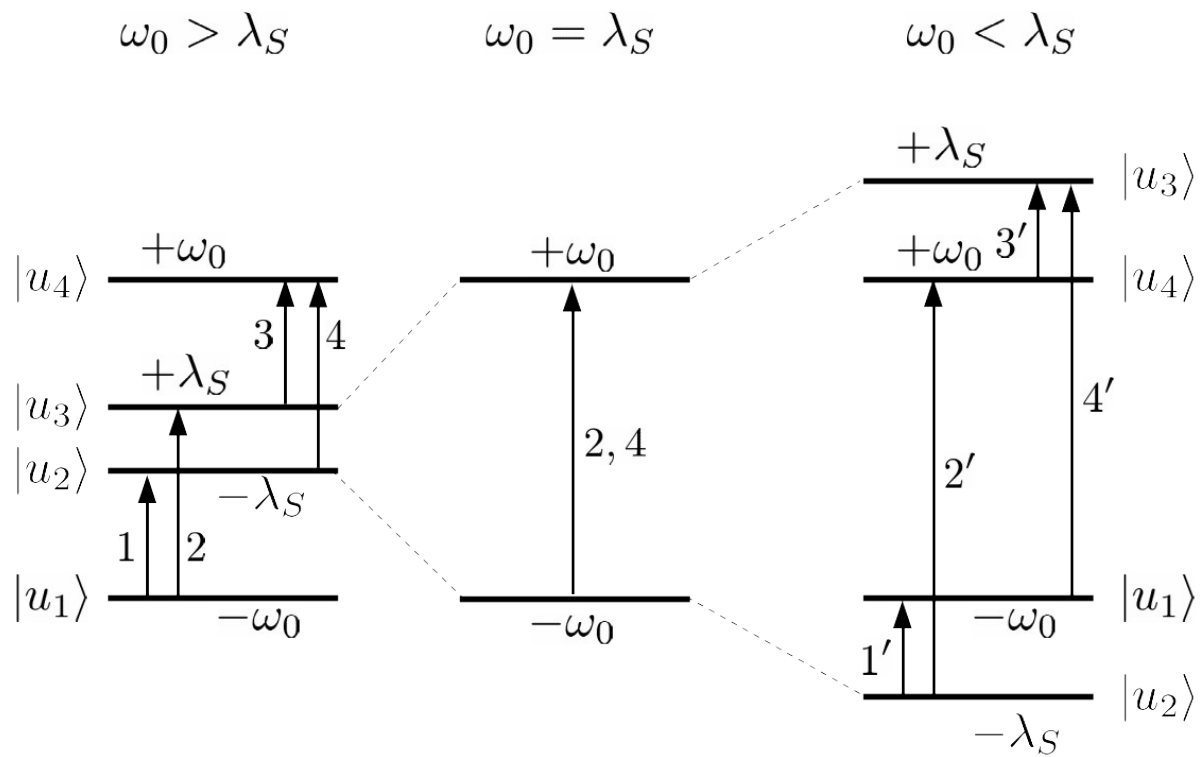
$$\hat{X}_{S_i} = \sigma_{S_i}^+ + \sigma_{S_i}^-$$

$$\hat{Y}_{B_i} = \sum_k \epsilon_{B_i}(k) [\hat{a}_{B_i}^\dagger(k) + \hat{a}_{B_i}(k)]$$

Drude-Lorentzian model

$$\begin{aligned} g_{B_i}(\omega) &= \sum_k |\epsilon_{B_i}(k)| \delta(\omega - \omega_{B_i}(k)) \\ &= \frac{2\lambda_{B_i} \gamma_{B_i} \omega}{\omega^2 + \gamma_{B_i}^2} \end{aligned}$$





Exact Solution: Step 1

$$H_{\text{total}} = \underbrace{H_S + H_{B_1} + H_{B_2}}_{H_0} + \underbrace{X_{S_1} \otimes Y_{B_1}}_{V_1} + \underbrace{X_{S_2} \otimes Y_{B_2}}_{V_2}$$

Interaction Picture

$$i \frac{\partial}{\partial t} \rho_{\text{SB}} = \sum_j [V_j(t), \rho_{\text{SB}}]$$

Unitary Evolution of the total system

$$\rho_{\text{SB}}(t) = \left\{ \overleftarrow{T} \prod_j e^{-i \int_{t_0}^t \hat{V}_j(s) ds} \right\} \rho_{\text{SB}}(t_0) \left\{ \overrightarrow{T} \prod_\ell e^{i \int_{t_0}^t \hat{V}_\ell(s) ds} \right\}$$

Exact Solution: Step 2

$$\rho_S(t) = \text{tr}_B \rho_{SB}(t)$$

This partial trace can be computed if,

1) Initial state: $\rho_{SB}(t_0) = \rho_S(t_0) \otimes \rho_{B_1}(t_0) \otimes \rho_{B_2}(t_0)$

2) $\rho_{B_j}(t_0)$ is a quasi-free state. $\rho_{B_j}(t_0) = \frac{1}{Z_j} e^{-\beta_j \hat{H}_{B_j}}$

$$\rho_S(t) = \overleftarrow{\mathcal{T}} \prod_j e^{-\int_{t_0}^t \int_{t_0}^{t_1} dt_1 dt_2 \mathcal{K}_j(t_1, t_2)} \rho_S(t_0)$$

$$\mathcal{K}_j(t_1, t_2) = \mathcal{S}_j^-(t_1) \text{Im} C_j(t_1 - t_2) \mathcal{S}_j^-(t_2) + i \mathcal{S}_j^-(t_1) \text{Re} C_j(t_1 - t_2) \mathcal{S}_j^+(t_2)$$

$$\mathcal{S}_j^\pm(t) = \left[\hat{X}_{S_j}(t), \cdot \right]_\pm$$

$$C_j(t_1 - t_2) = \left\langle \hat{Y}_{B_j}(t_1) \hat{Y}_{B_j}(t_2) \right\rangle_{t_0}$$

Exact Solution: Step 3

$$i \frac{\partial}{\partial t} \rho_S = \sum_j [X_{S_j}(t), \eta_j]$$

$$\begin{aligned} \eta_j(t) &= -i \overleftarrow{\mathcal{T}} \int_{t_0}^t ds \{ \text{Re } C_j(t-s) \mathcal{S}_j^-(s) + i \text{Im } C_j(t-s) \mathcal{S}_j^+(s) \} \\ &\times \prod_j e^{-\int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \mathcal{K}_j(t_1, t_2)} \rho_S(0). \end{aligned}$$

Numerically tractable if

$$C_j(t) = \lambda_{B_j} [c_j e^{-\gamma_j t} + 2\Delta_j \delta(t)]$$

$$c_j = 2/\beta_j - \gamma_j \Delta_j - i\gamma_j$$

$$\Delta_j = \gamma_j \beta_i / 6$$

$$g_{B_j}(\omega) = \frac{2\lambda_{B_j} \gamma_j \omega^2}{\omega^2 + \gamma_j}$$

Hierarchical Equation of Motion (HEOM) Tanimura-Kubo(1989)

Auxiliary operators

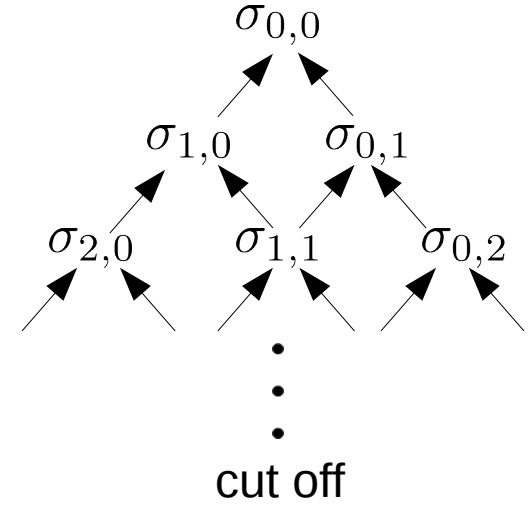
$$\sigma_{n_1, n_2}(t) = \overleftarrow{\mathcal{T}} \prod_{j=1}^2 \left\{ \left[-i \int_{t_0}^t ds e^{-\gamma_j(t-s)} \mathcal{G}_j(s) \right]^{n_j} \right. \\ \times e^{-\lambda_j \int_{t_0}^t \int_{t_0}^{t_1} dt_1 dt_2 \mathcal{S}_j^-(t_1) e^{-\gamma_j(t_1-t_2)} \mathcal{G}_j(t_2)} \\ \left. \times e^{-\lambda_{B_j} \Delta_i \int_{t_0}^t dt_1 \mathcal{S}_j^-(t_1) \mathcal{S}_j^-(t_1)} \right\} \rho_S(t_0)$$

$$\mathcal{G}_i(t) = (2/\beta_i - \gamma_{B_i} \Delta_i) \mathcal{S}^-(t) - i\gamma_{B_i} \mathcal{S}^+(t).$$

$$\rho_S(t) = \sigma_{0,0}$$

$$\eta_1(t) = \lambda_{B_1} [\sigma_{1,0}(t) - i\Delta_1 \mathcal{S}_1^-(t) \sigma_{0,0}(t)]$$

$$\eta_2(t) = \lambda_{B_2} [\sigma_{0,1}(t) - i\Delta_2 \mathcal{S}_2^-(t) \sigma_{0,0}(t)]$$



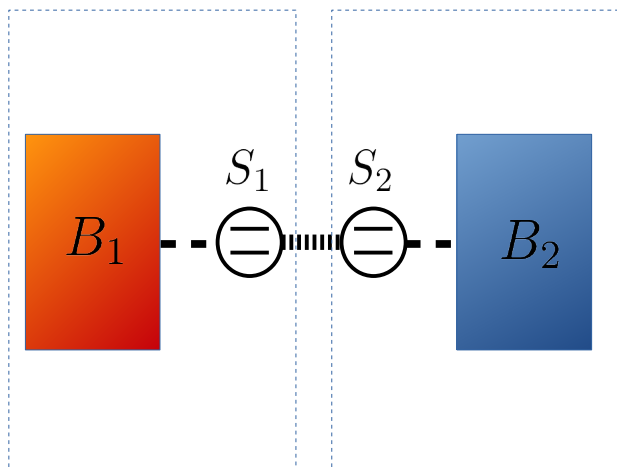
Cut-off at depth=40,
861 auxiliary ops.

8610 coupled ODEs

Equation of Motion

$$\frac{d}{dt} \sigma_{n_1, n_2}(t) = -(\gamma_{B_1} n_1 + \gamma_{B_2} n_2) \sigma_{n_1, n_2}(t) \\ - [\lambda_{B_1} \Delta_1 \mathcal{S}_1^-(t) \mathcal{S}_1^-(t) + \lambda_{B_2} \Delta_2 \mathcal{S}_2^-(t) \mathcal{S}_2^-(t)] \sigma_{n_1, n_2}(t) \\ - i \lambda_{B_1} \mathcal{S}_1^- \sigma_{n_1+1, n_2}(t) - i \lambda_{B_2} \mathcal{S}_2^- \sigma_{n_1, n_2+1}(t) \\ - i n_1 \lambda_{B_1} \mathcal{G}_1(t) \sigma_{n_1-1, n_2}(t) - i n_2 \lambda_{B_2} \mathcal{G}_2(t) \sigma_{n_1, n_2-1}(t)$$

Choice of Basis Sets



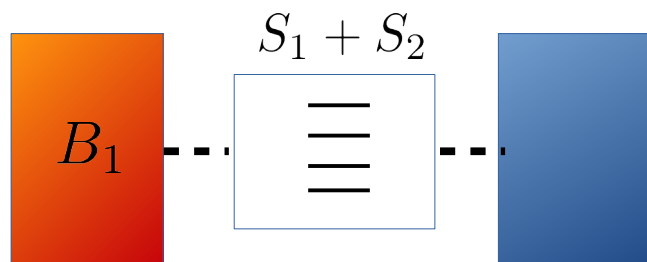
Atom Basis

$$|a_1\rangle = |--\rangle$$

$$|a_2\rangle = |-\rangle|+\rangle$$

$$|a_3\rangle = |+\rangle|-\rangle$$

$$|a_4\rangle = |++\rangle$$



Eigen Basis

$$|e_1\rangle = |--\rangle$$

$$|e_2\rangle = (|-\rangle|+\rangle - |+\rangle|-\rangle) / \sqrt{2}$$

$$|e_3\rangle = (|-\rangle|+\rangle + |+\rangle|-\rangle) / \sqrt{2}$$

$$|e_4\rangle = |++\rangle$$

$$H_s |e_i\rangle = E_i |e_i\rangle$$

$$E = \{-\omega_0, -\lambda_s, +\lambda_s, +\omega_0\}$$

More Basis Sets

Bell Basis

$$|b_1\rangle = |\Phi_+\rangle = (|++\rangle + |--\rangle) / \sqrt{2}$$

$$|b_2\rangle = |\Phi_-\rangle = (|++\rangle - |--\rangle) / \sqrt{2}$$

$$|b_3\rangle = |\Psi_+\rangle = (|+-\rangle + |-+\rangle) / \sqrt{2}$$

$$|b_4\rangle = |\Psi_-\rangle = (|+-\rangle - |-+\rangle) / \sqrt{2}$$

Pointer Basis

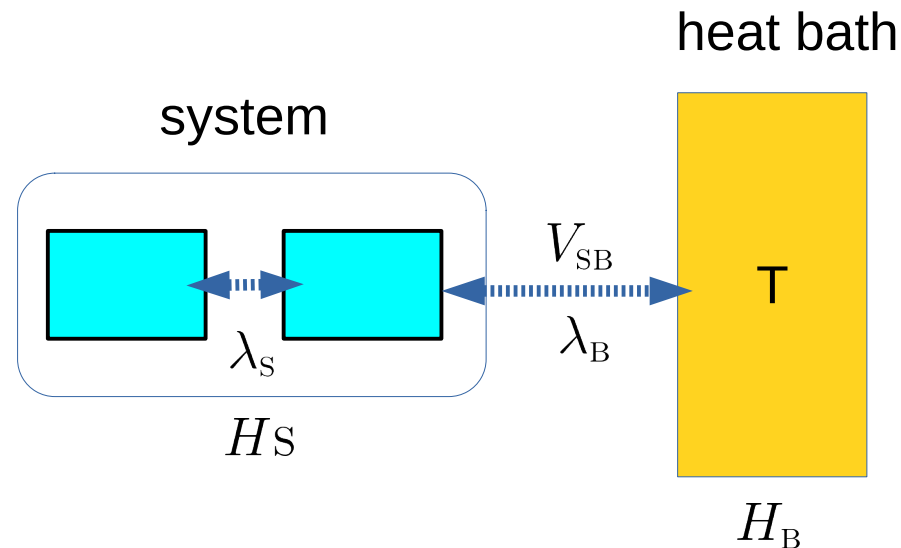
$$\sigma_x^A \otimes I^B |\pi_i\rangle = \lambda_i |\pi_i\rangle \quad |\pi_1\rangle = (|\Phi_+\rangle + |\Psi_+\rangle) / \sqrt{2} = (|++\rangle + |--\rangle + |+-\rangle + |-+\rangle) / 2$$

$$I^A \otimes \sigma_x^B |\pi_i\rangle = \eta_i |\pi_i\rangle \quad |\pi_2\rangle = (|\Phi_+\rangle - |\Psi_+\rangle) / \sqrt{2} = (|++\rangle + |--\rangle - |+-\rangle - |-+\rangle) / 2$$

$$\lambda = \{1, -1, -1, 1\} \quad |\pi_3\rangle = (|\Phi_-\rangle + |\Psi_-\rangle) / \sqrt{2} = (|++\rangle - |--\rangle + |+-\rangle - |-+\rangle) / 2$$

$$\eta = \{1, -1, 1, -1\} \quad |\pi_4\rangle = (|\Phi_-\rangle - |\Psi_-\rangle) / \sqrt{2} = (|++\rangle - |--\rangle - |+-\rangle + |-+\rangle) / 2$$

Thermodynamic Steady State and Eigenselection



$$\lambda_B \ll 1 \quad \rho_s \rightarrow \frac{1}{Z} e^{-\beta H_s}$$

Claims

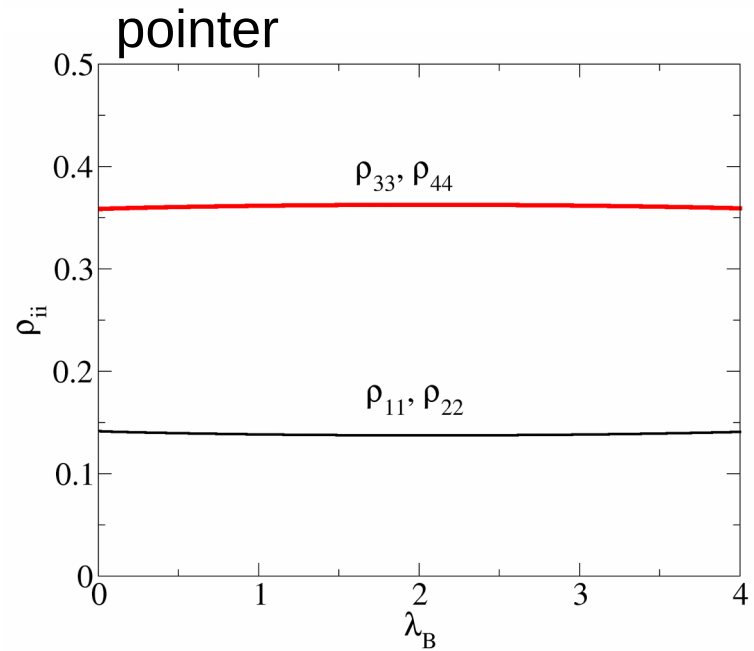
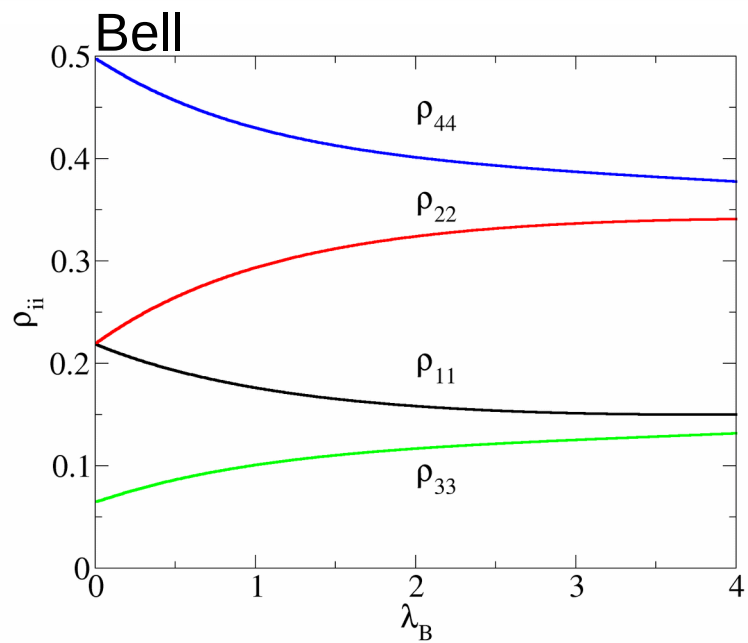
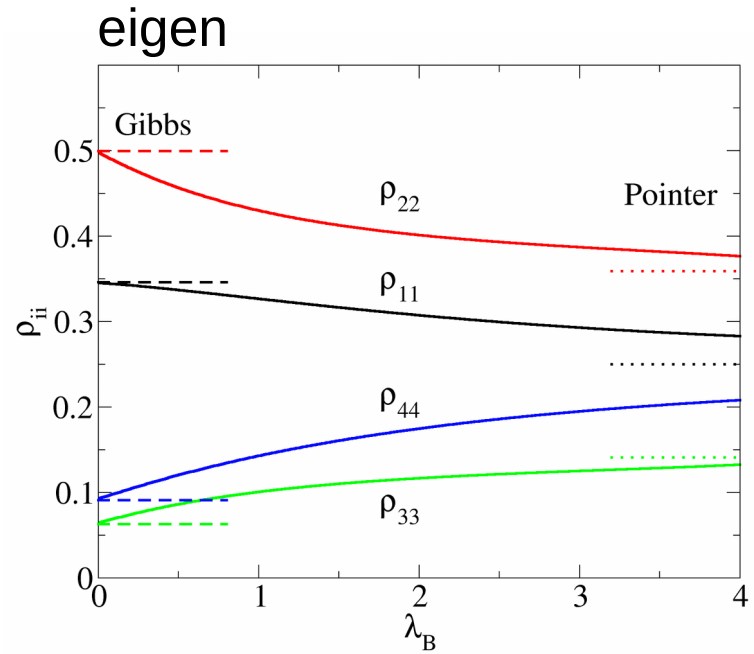
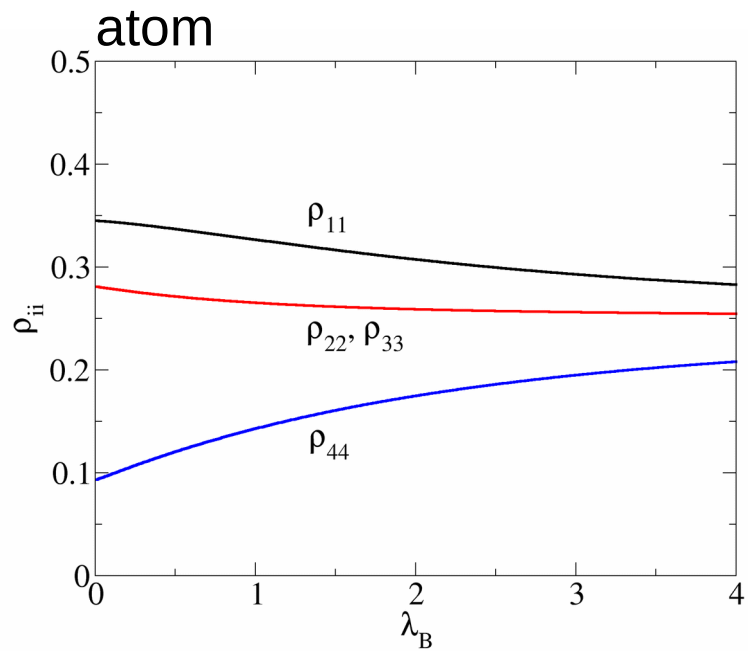
$$\lambda_B \gg |H_S|, \quad \rho_s \rightarrow \frac{1}{Z} \sum_i |\pi_i\rangle\langle\pi_i| e^{-\beta H_s} |\pi_i\rangle\langle\pi_i|$$

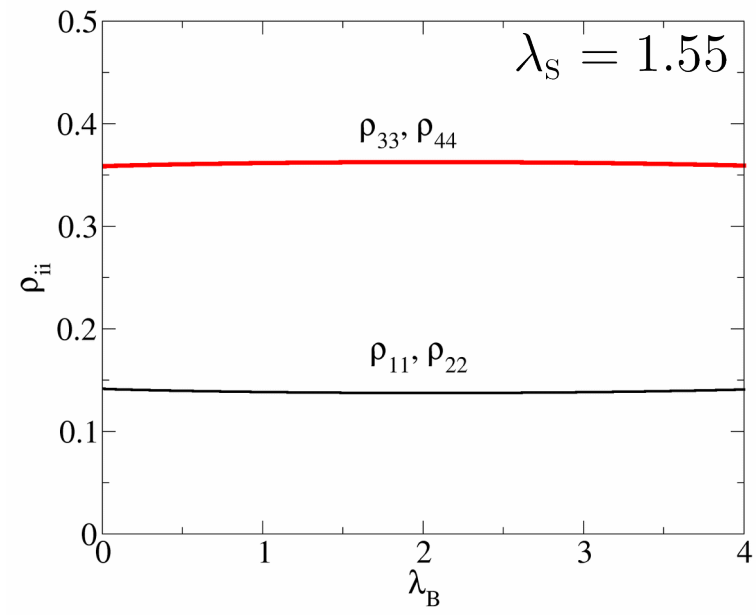
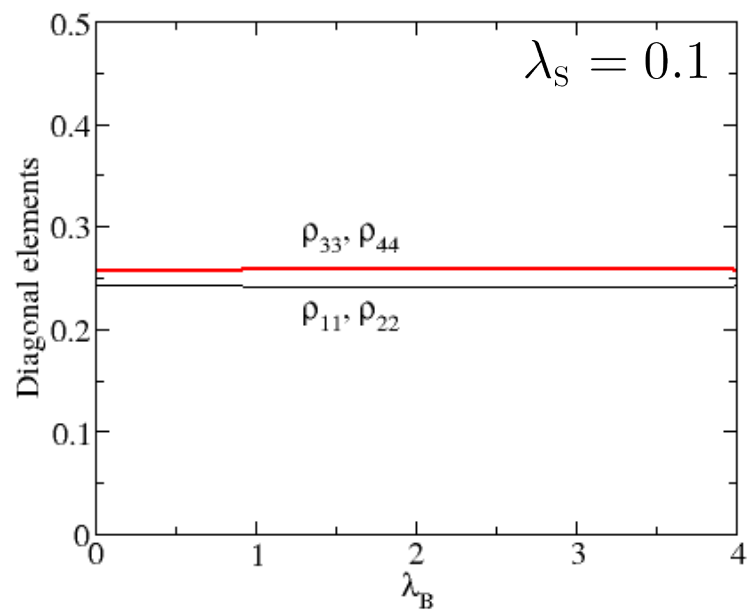
$$\lambda_B \sim |H_S|, \quad \langle\pi_i|\rho_s|\pi_i\rangle \approx \frac{1}{Z} \langle\pi_i|e^{-\beta H_s}|\pi_i\rangle$$

$$[V_{SB}, \hat{\Pi}] = 0, \quad \hat{\Pi} |\pi\rangle = \pi_i |\pi_i\rangle$$

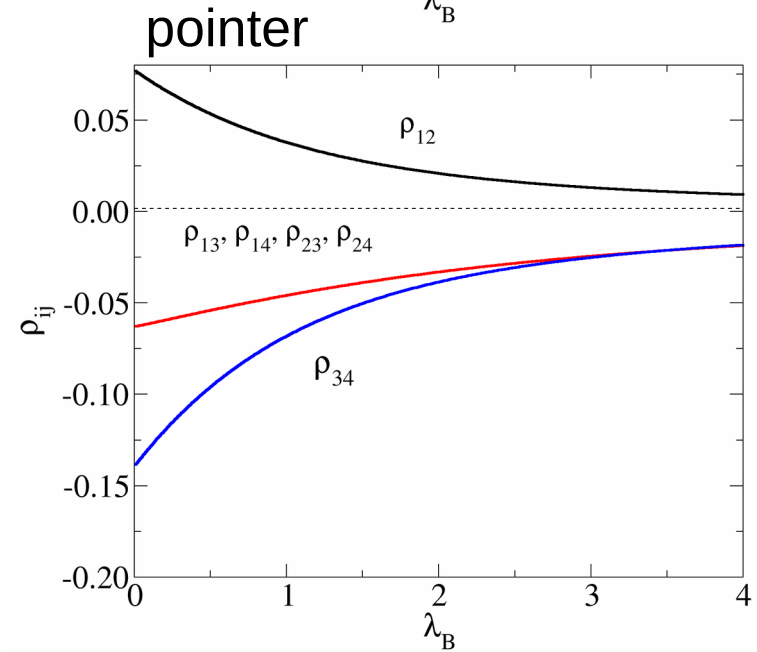
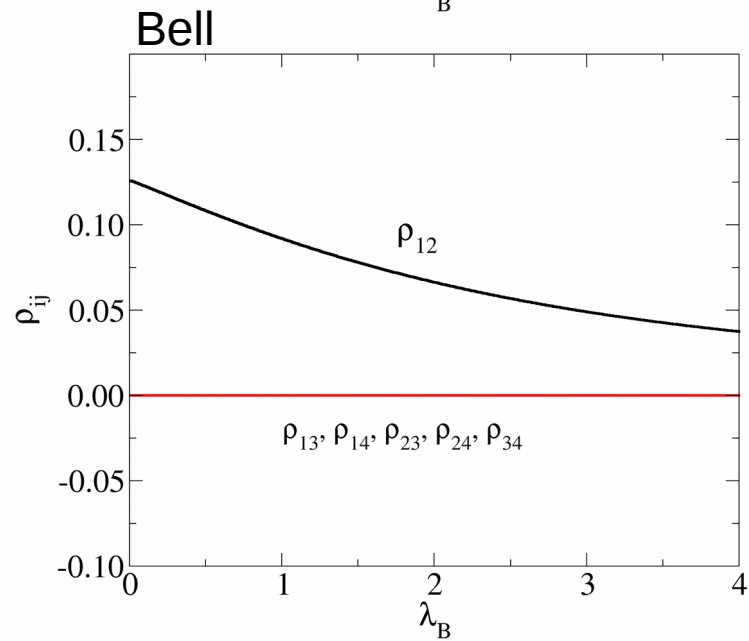
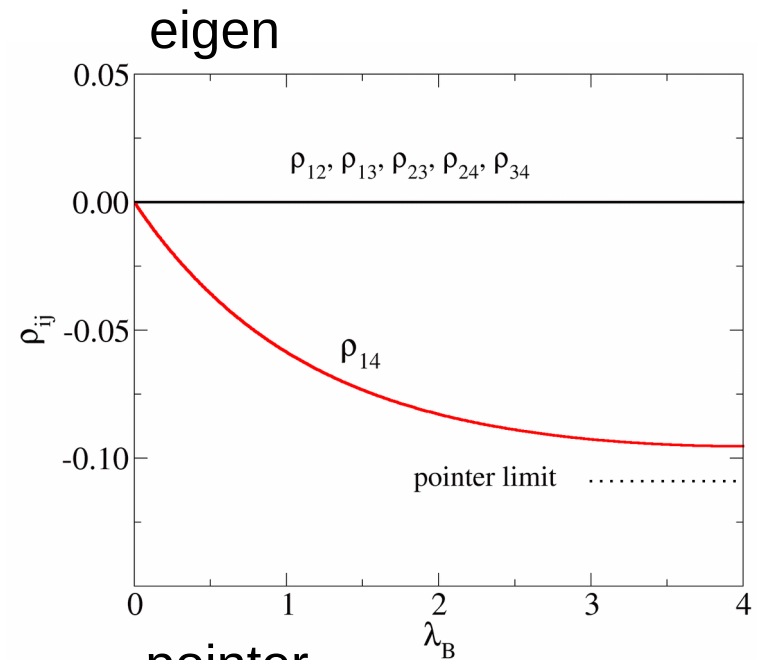
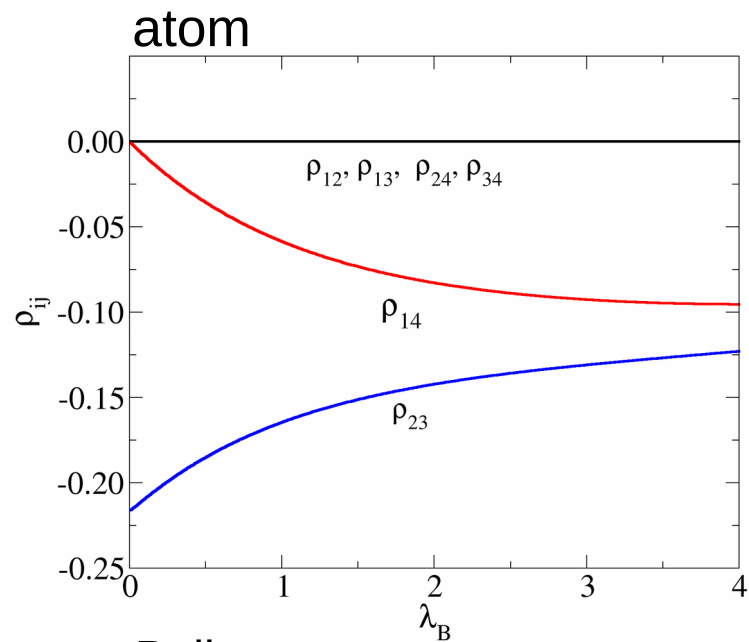
Steady State: Diagonal Elements

$$T_A = T_B = 1.5, \lambda_S = 1.55, \omega_0 = 1$$

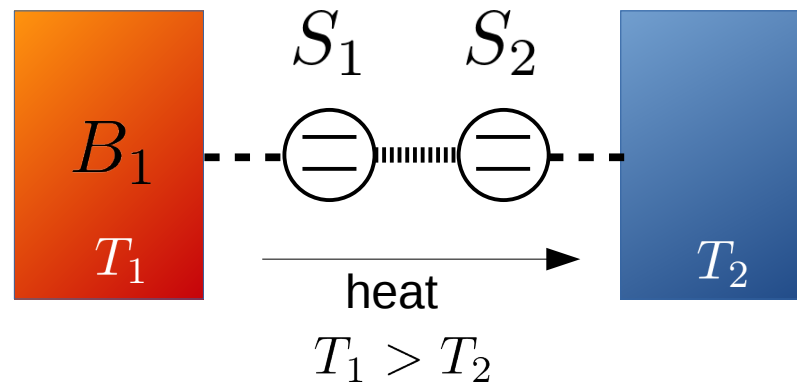




Steady State: Off-Diagonal Elements



Non-Equilibrium Steady State and Heat



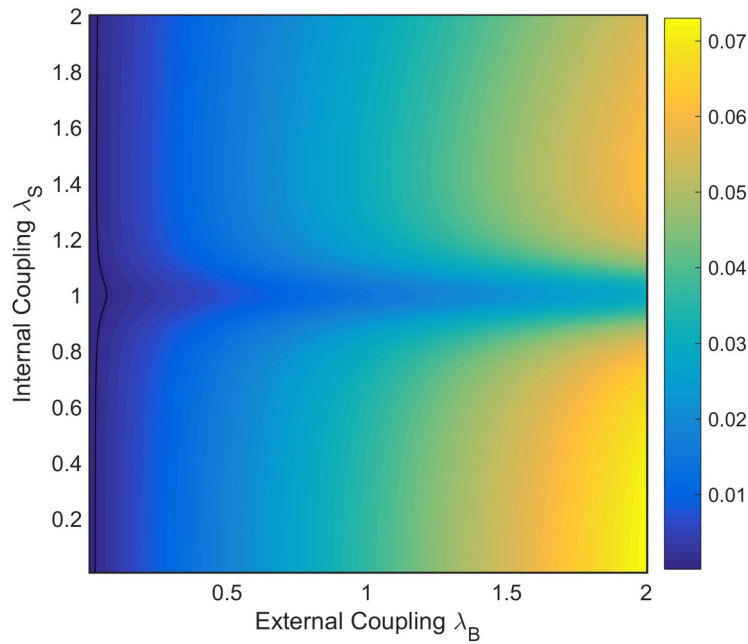
$$J_j = -i \operatorname{tr}_S \left\{ [\hat{X}_{S_j}, \eta_j] \hat{H}_S \right\}$$

Does heat flow under the observation by the environment?

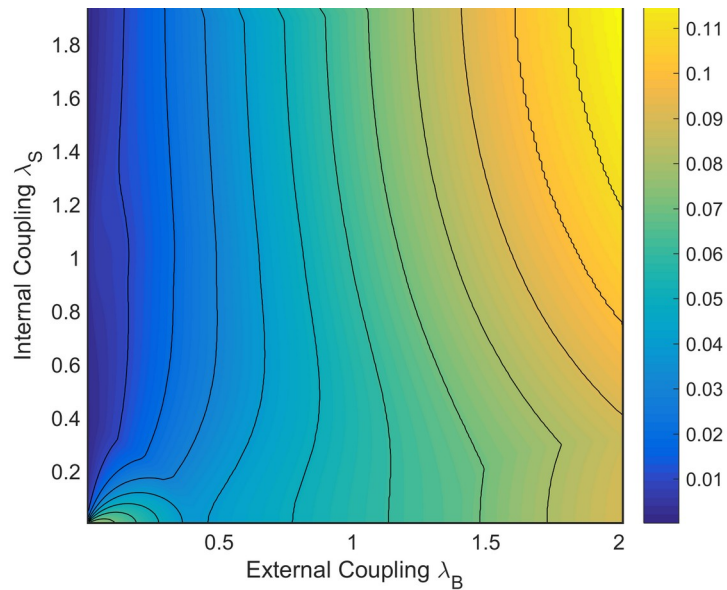
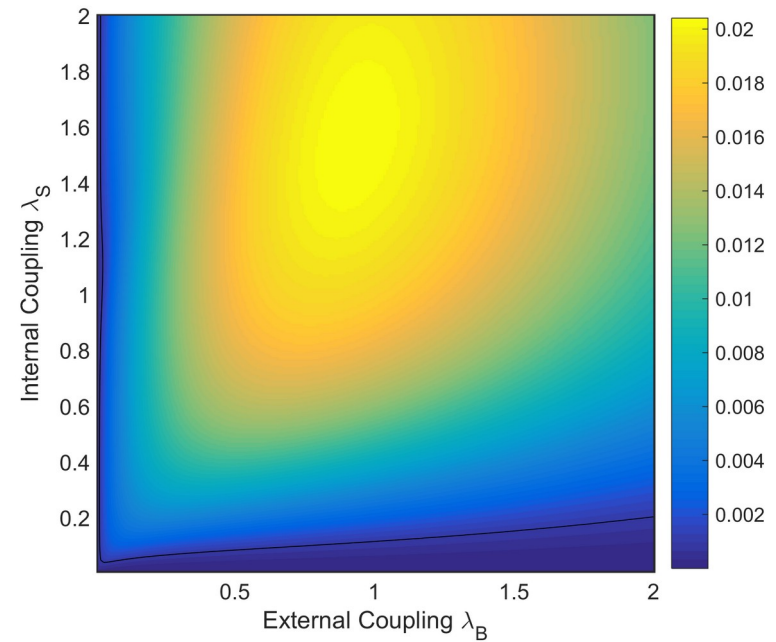
Heat by QME and HEOM

$$T_1 = 2, T_2 = 1$$

Heat Current (QME)



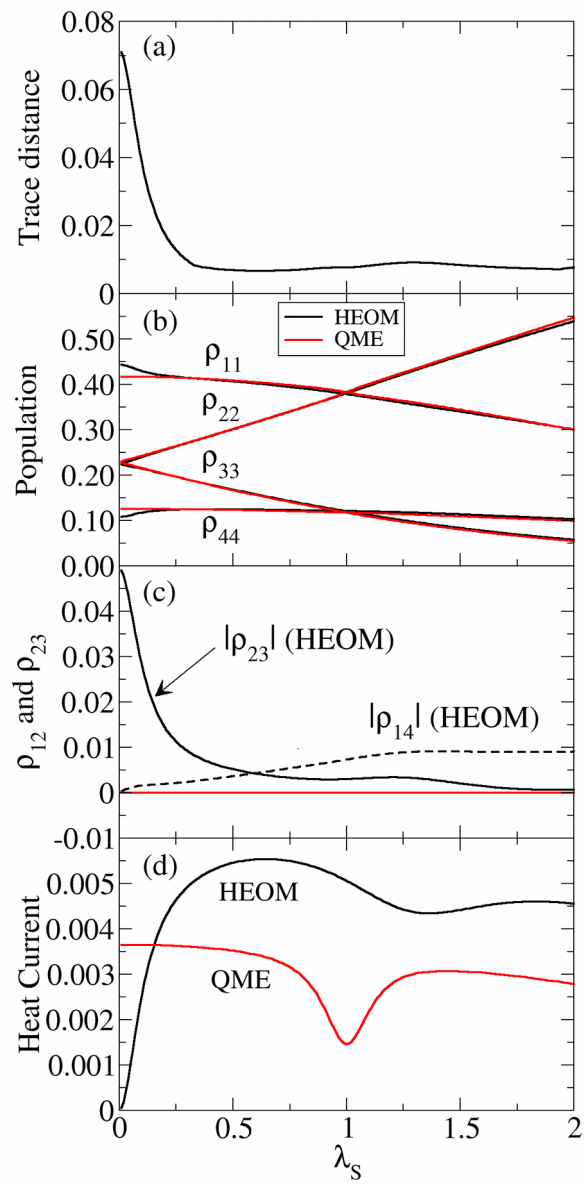
Heat Current (HEOM)



Trace distance: $\|\rho_S^{\text{HEOM}} - \rho_S^{\text{QME}}\|$

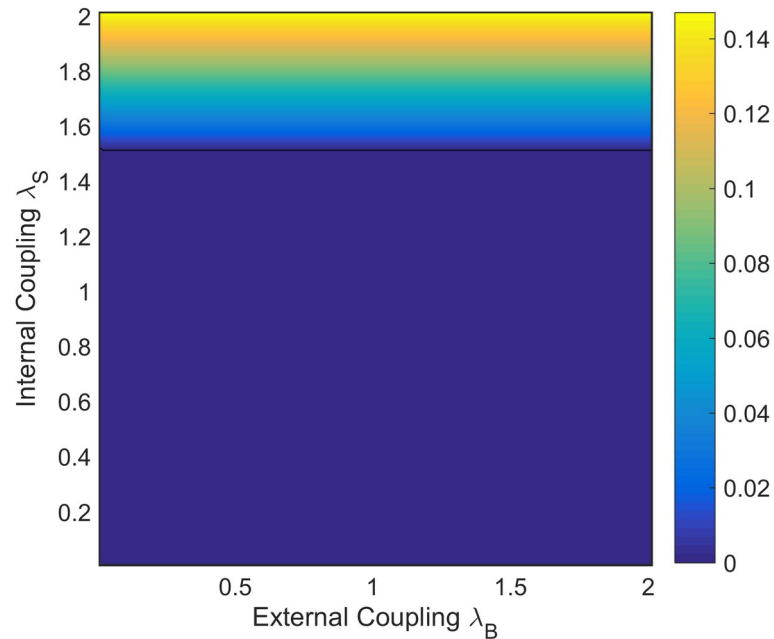
$$\|\rho - \sigma\| = \frac{1}{2} \text{tr} \left[\sqrt{(\rho - \sigma)^\dagger (\rho - \sigma)} \right]$$

QME vs HEOM

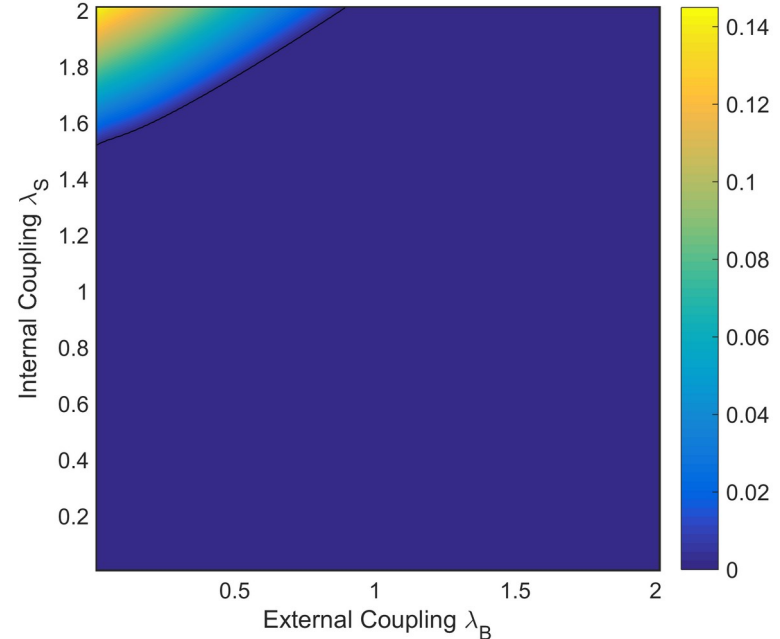


Entanglement between Q-bits

QME (Born+Markov)



HEOM (Non-Markovian)

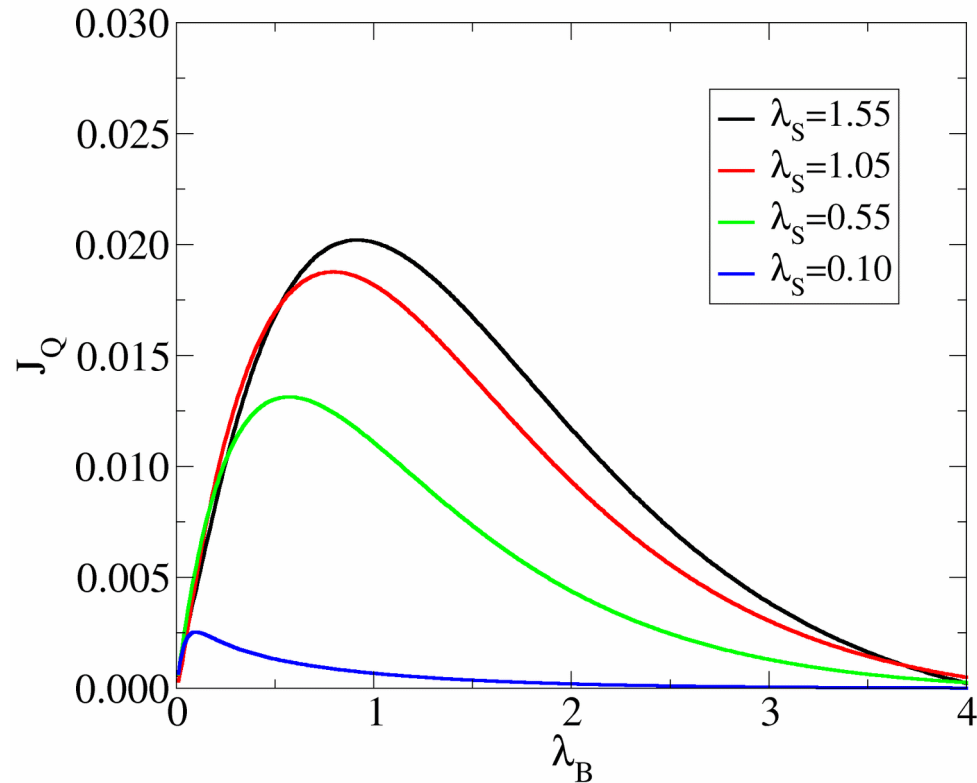


Concurrence $C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$

$\lambda_i =$ eigenvalue of $R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$ in decreasing order

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$$

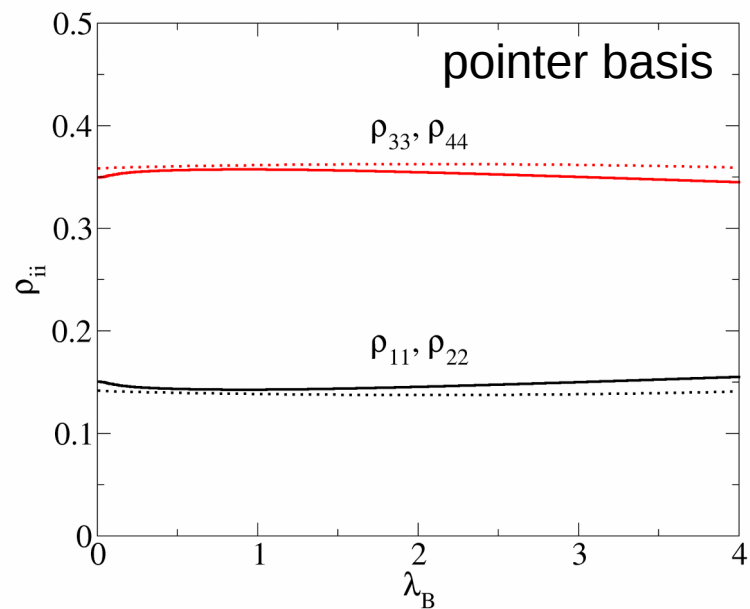
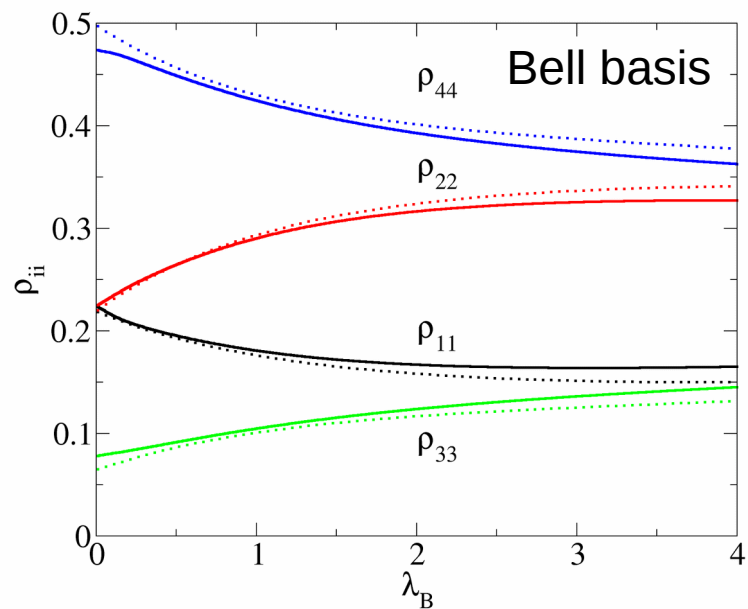
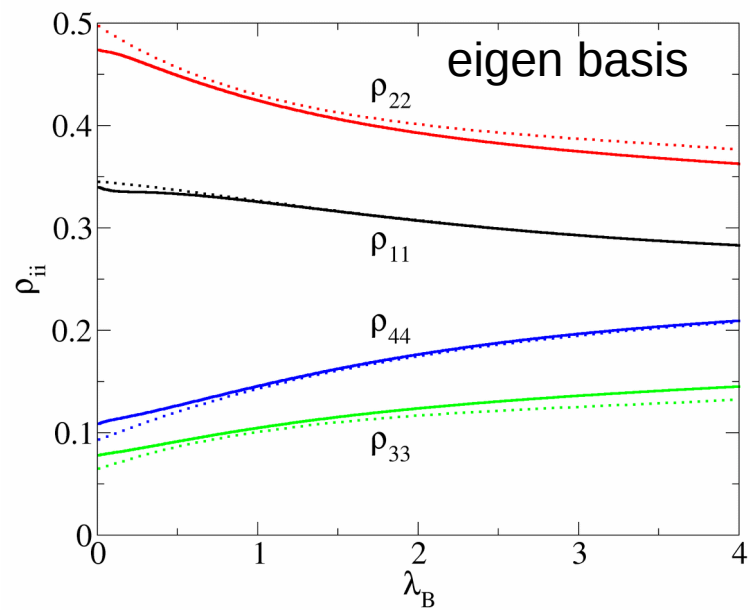
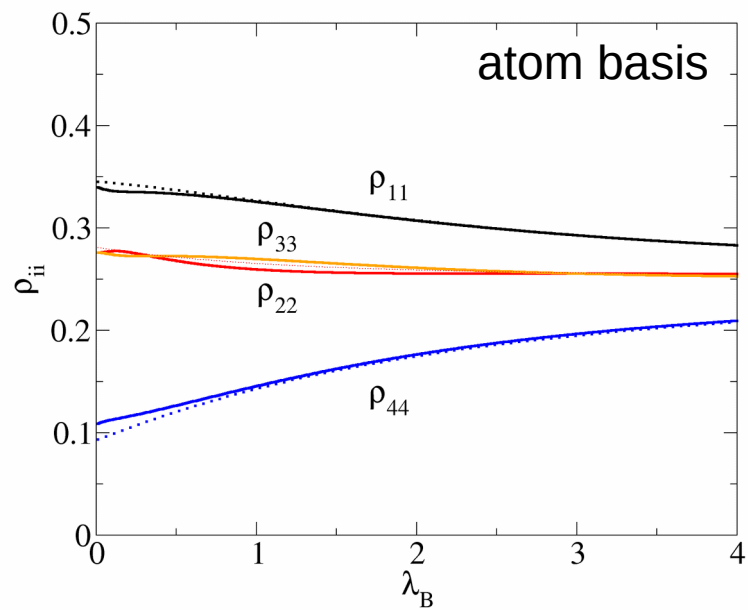
Heat conduction dies off at strong coupling



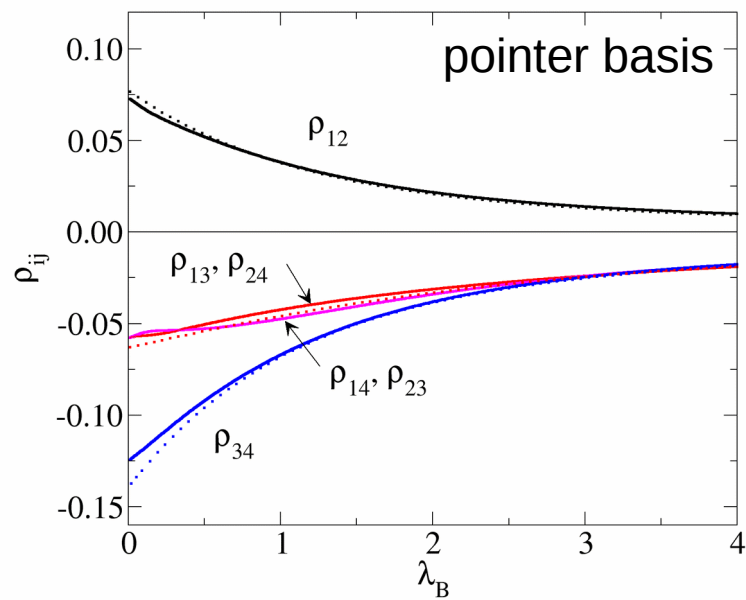
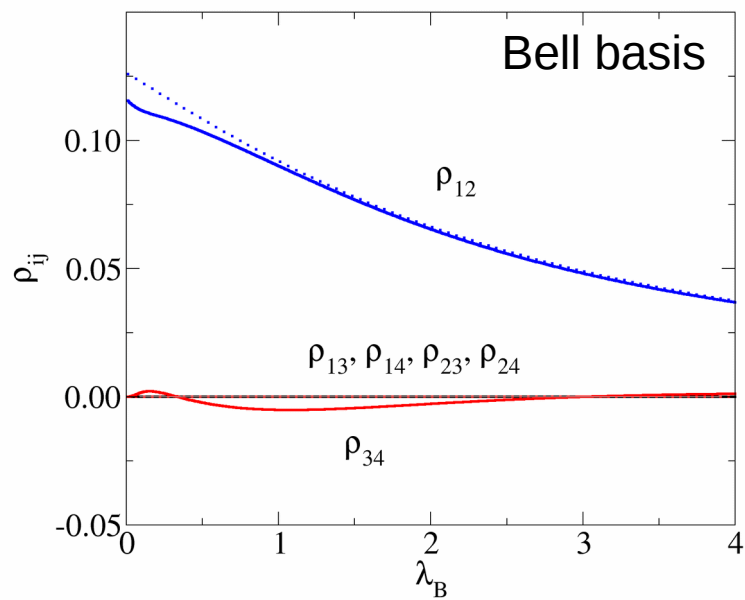
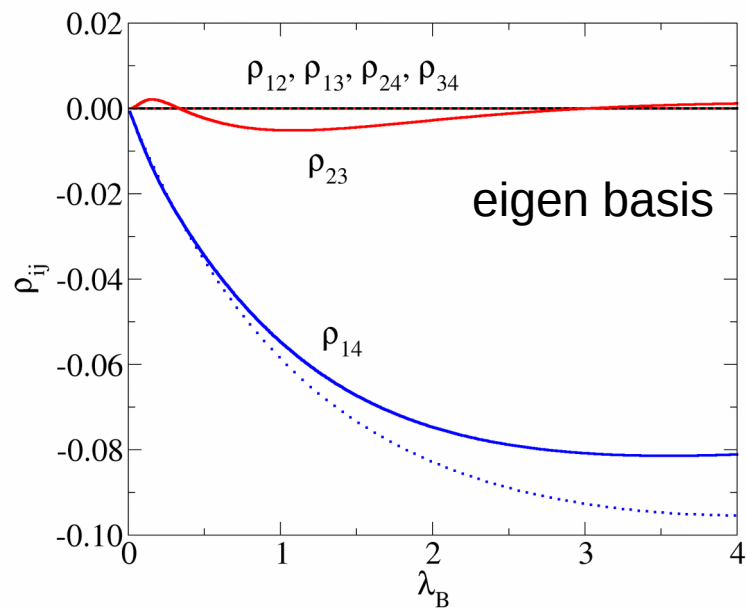
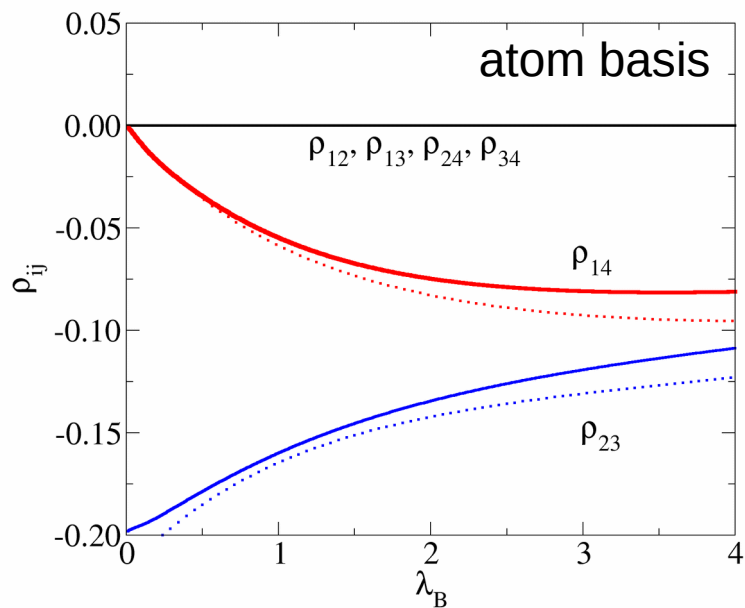
Disappearance of Heat ---> Quantum Zeno effect

Rebentrost *et al.* (2009), Kato-Tanimura (2015)

Non-Equilibrium Steady State: Diagonal Elements



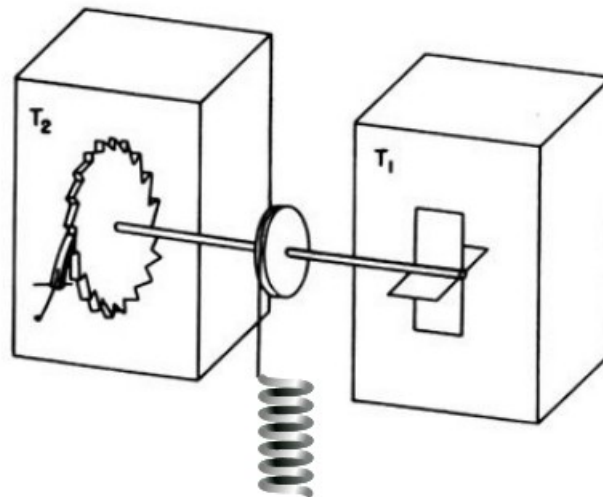
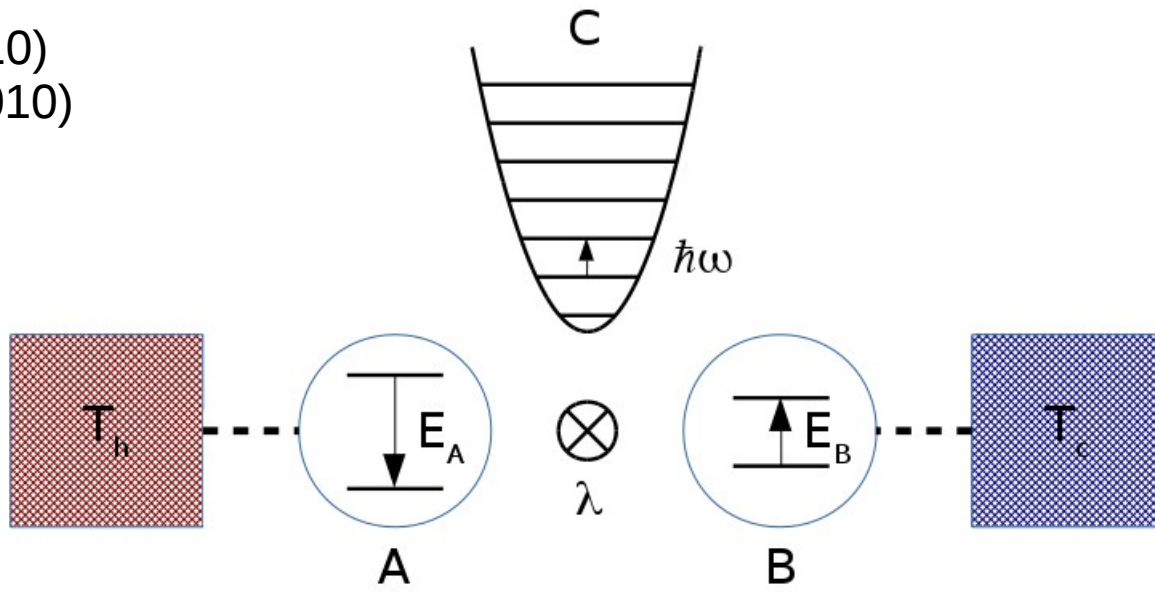
Non-Equilibrium Steady State: Off-Diagonal Elements



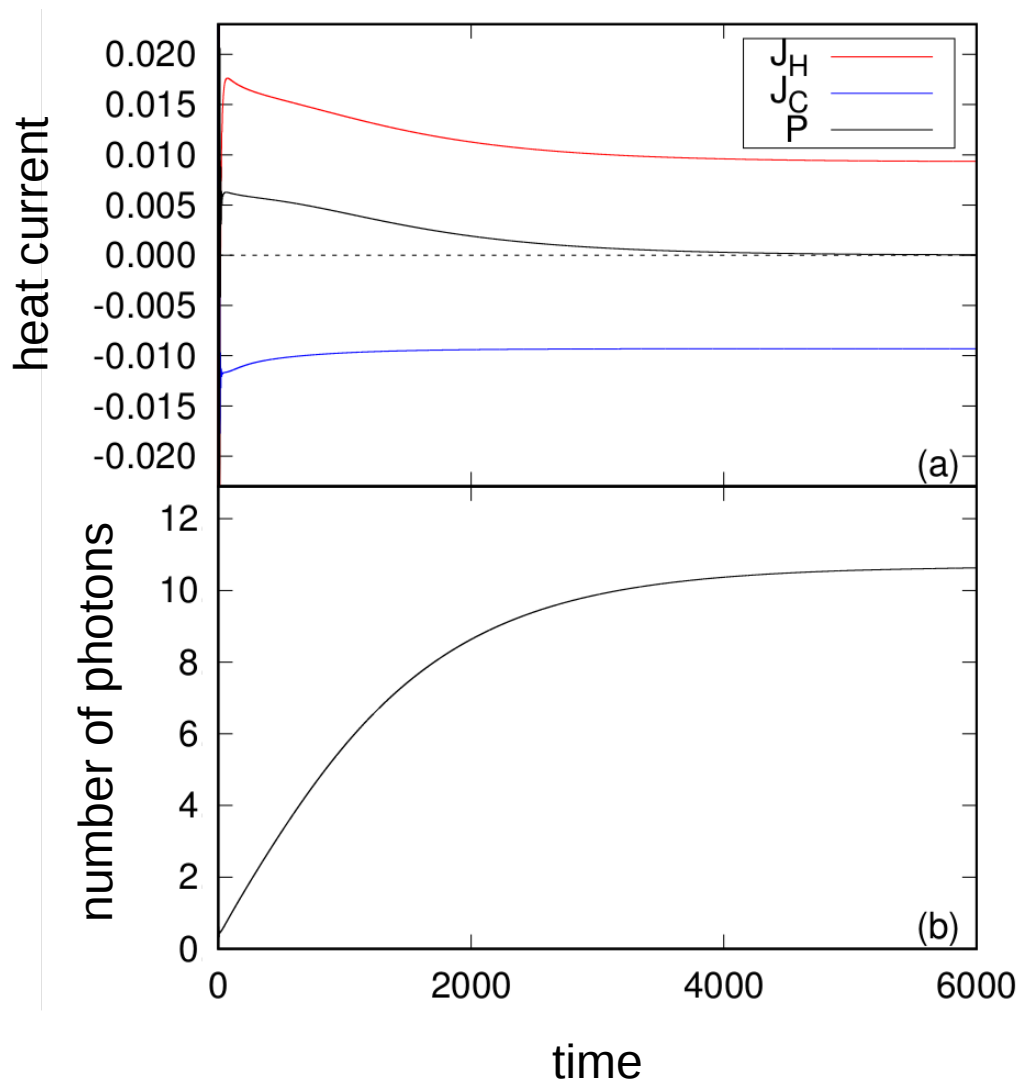
Decoherence strength: Flemming et al. (2012)

Autonomous Quantum Heat Engine

Linden *et al.* (2010)
Youssef *et al.* (2010)



Heat at stalled force



$$T_A = 5, T_B = 1, \lambda_S = 0.5, \lambda_B = 0.05, \hbar\omega = 1$$

Conclusions

Equilibrium

- Continuous measurement by the environment projects Gibbs state to pointer states.
- Probability distribution of pointer states is insensitive to the coupling strength.

Non-Equilibrium

- Continuous measurement by the environments kills heat conduction.

About Born-Markovian quantum master equation

- Decoherence predicted by Born-Markovian quantum master equation predicts the Gibbs state for equilibrium situation but exhibits unrealistic results for non-equilibrium situation.

Numerical Method

- Hierarchical Equation of Motion (HEOM) provides exact numerical solution for open quantum systems.

