Introduction to quantum thermodynamics

An open systems perspective

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21 Feb, 2024

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NITheCS
National Institute for
Theoretical and Computational Sciences

QSUN
Quantum Research Group
of Stellenbosch University

Contents

Lecture 1 Feb 7: Background – foundational quantum mechanics, open quantum systems, equilibrium descriptions.

Lecture 2 Feb 14: Markovian master equations – microscopic derivation, 1st and 2nd laws of thermodynamics.

Lecture 3 Feb 21: Quantum thermal machines – discrete heat engines and refrigerators, quantum Otto cycle.

Lecture 4 Feb 28: Strong system-reservoir coupling – mean force Gibbs state, nonequilibrium descriptions.

Last week

Markovian master equation:

- Dynamical semigroup

$$\Phi_{t+s} = \Phi_t \circ \Phi_s \qquad \forall t, s \geq 0$$

Written in form $\Phi_t = e^{\mathcal{L}t}$

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Last week

Markovian master equation:

- Dynamical semigroup

$$\Phi_{t+s} = \Phi_t \circ \Phi_s \qquad \forall t, s \geq 0$$

Written in form $\Phi_t = e^{\mathcal{L}t}$

GKSL theorem

General construction of generator $\mathcal{L}$ of quantum dynamical semigroup:

$$\mathcal{L}(\rho) = -i[H_0, \rho] + \sum_{k=1}^{d^2-1} \gamma_k \left(V_k \rho V_k^\dagger - \frac{1}{2}\{V_k^\dagger V_k, \rho\} \right)$$

where

- H_0 is a self-adjoint operator.
- $V_k \in \mathcal{B}(\mathcal{H}_S)$ are Lindblad operators.
- $\gamma_k \geq 0$ are transition rates.

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

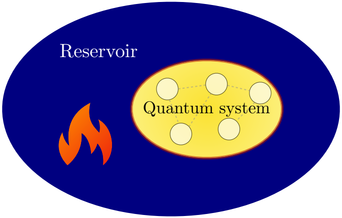
Last week

Markovian master equation:

- Microscopic derivation

$$H = H_S + H_R + \alpha \sum_k A_k \otimes B_k$$

where A_k and B_k are self-adjoint system and reservoir operators.



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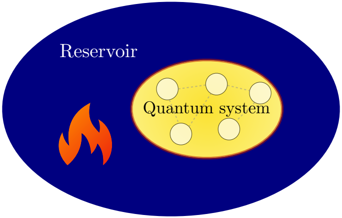

Markovian master equation (GKSL form)

Dynamics of open system in weak contact with thermal reservoir:

$$\frac{d}{dt}\rho_S(t) = \mathcal{L}(\rho_S) = -i[H_S, \rho_S] + \alpha^2 \sum_\omega \sum_{k,l} \gamma_{kl}(\omega) \Big[A_l(\omega)\rho_S A_k^\dagger(\omega) - \frac{1}{2}\{A_k^\dagger(\omega)A_l(\omega), \rho_S\} \Big]$$

where $A_k = \sum_\omega A_k(\omega)$, and $\boldsymbol{\gamma}(\omega) \geq 0$.

- Born approx – $\rho(t) \approx \rho_S(t) \otimes \pi_R(\beta)$
- Markov approx – $\tau_R \ll \tau_I$
- Secular approx – $\tau_S \ll \tau_I$

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Last week

Markovian master equation:

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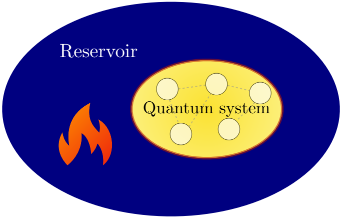

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where $A_k = \sum_\omega A_k(\omega)$, and $\boldsymbol{\gamma}(\omega) \geq 0$.

KMS condition: $\langle \tilde{B}_k(-t) B_l \rangle_\beta = \langle B_l \tilde{B}_k(t - i\beta) \rangle_\beta$

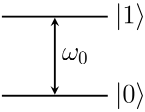
$$\Rightarrow \mathcal{L}(\pi_S^\beta) = 0, \qquad \pi_S^\beta = \frac{e^{-\beta H_S}}{\mathrm{Tr}\, e^{-\beta H_S}}$$

H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002

Two-level system

Hamiltonian:

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sigma_x \otimes B$$



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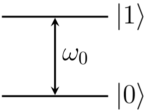

Example (Construction of MME)

- System $\mathcal{H}_S = \mathrm{span}\{|0\rangle, |1\rangle\}$:

$$H_S = \frac{\omega_0}{2}(|1\rangle\langle 1| - |0\rangle\langle 0|) \qquad H_S|0\rangle = -\frac{\omega_0}{2}|0\rangle, \quad H_S|1\rangle = +\frac{\omega_0}{2}|1\rangle$$

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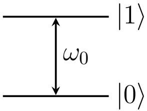

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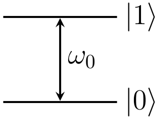
- Reservoir (Bosonic Fock space):

$$H_R = \sum_k \omega_k b_k^\dagger b_k \qquad [H_R, b_k] = -\omega_k b_k, \qquad [H_R, b_k^\dagger] = \omega_k b_k^\dagger$$

- Interaction:

$$A = \sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|, \qquad B = \sum_k (g_k^* b_k + g_k b_k^\dagger)$$

Two-level system



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Example (Construction of MME)

- Lindblad operators $A(\omega) = \sum_{\epsilon' - \epsilon = \omega} \Pi(\epsilon) A \Pi(\epsilon')$, $\quad \epsilon, \epsilon' \in \{\frac{-\omega_0}{2}, \frac{\omega_0}{2}\}$:

$$A(\omega_0) = |0\rangle\langle 0|\sigma_x|1\rangle\langle 1| = \sigma_- \qquad A(-\omega_0) = |1\rangle\langle 1|\sigma_x|0\rangle\langle 0| = \sigma_+$$

where $\sigma_- \equiv \sigma_+^\dagger = |0\rangle\langle 1|$.

Two-level system

Hamiltonian:

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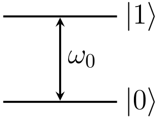

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$$A(\omega_0) = \sigma_- \qquad A(-\omega_0) = \sigma_+$$

- Reservoir correlation functions:

$$C(t) = \langle \tilde{B}(t) B \rangle_\beta = \sum_{k,k'} \left\langle \left[g_k^* \tilde{b}_k(t) + g_k \tilde{b}_k^\dagger(t)\right]\left[g_{k'}^* b_{k'} + g_{k'} b_{k'}^\dagger\right] \right\rangle_\beta$$

Two-level system

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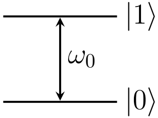

Example (Construction of MME)

- **Lindblad operators** $A(\omega) = \sum_{\epsilon'-\epsilon=\omega} \Pi(\epsilon) A \Pi(\epsilon')$, $\quad \epsilon, \epsilon' \in \{\frac{-\omega_0}{2}, \frac{\omega_0}{2}\}$:

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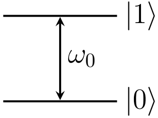
$$\tilde{b}_k(t) = e^{iH_R t} b_k e^{-iH_R t} = b_k e^{-i\omega_k t}, \qquad \tilde{b}_k^\dagger(t) = e^{iH_R t} b_k^\dagger e^{-iH_R t} = b_k^\dagger e^{i\omega_k t}$$

Two-level system

Hamiltonian:

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sigma_x \otimes B$$



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- **Reservoir correlation functions**:

$$C(t) = \langle \tilde{B}(t) B \rangle_\beta = \sum_k |g_k|^2 \left[n_\beta(\omega_k) e^{i\omega_k t} + (1 + n_\beta(\omega_k)) e^{-i\omega_k t} \right]$$

having used $\langle b_k b_{k'}^\dagger \rangle_\beta = (1 + n_\beta(\omega_k))\delta_{kk'}$, $\langle b_k^\dagger b_{k'} \rangle_\beta = n_\beta(\omega_k)\delta_{kk'}$, where

$$n_\beta(\omega) = \frac{1}{e^{\beta\omega} - 1}$$

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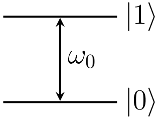

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- Transition rates:

$$\gamma(\omega) = \int_{-\infty}^{\infty} dt\, C(t) e^{i\omega t}$$

Two-level system

Hamiltonian:

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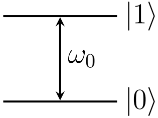

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- Transition rates:

$$\gamma(\omega) = \int_{-\infty}^{\infty} dt\, C(t) e^{i\omega t} = 2\pi \sum_k |g_k|^2 \left[n_\beta(\omega_k) \delta(\omega + \omega_k) + (1 + n_\beta(\omega_k)) \delta(\omega - \omega_k) \right]$$

Two-level system

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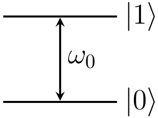

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- Transition rates:

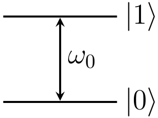
  $$\gamma(\omega) = \int_{-\infty}^{\infty} dt\, C(t) e^{i\omega t} = 2\pi \int_0^\infty d\nu |g(\nu)|^2 \varrho(\nu) \left[n_\beta(\nu)\delta(\omega+\nu) + (1+n_\beta(\nu))\delta(\omega-\nu) \right]$$

  where $\varrho(\omega)$ is the reservoir density of states.

Two-level system

Hamiltonian:

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sigma_x \otimes B$$



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- Transition rates:

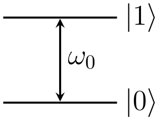
$$\gamma(\omega) = \int_{-\infty}^{\infty} dt\, C(t) e^{i\omega t} = 2\pi \int_0^\infty d\nu |g(\nu)|^2 \varrho(\nu) \Big[n_\beta(\nu)\delta(\omega+\nu) + (1+n_\beta(\nu))\delta(\omega-\nu) \Big]$$

$$\gamma(\omega_0) = 2\pi |g(\omega_0)|^2 \varrho_0 (1 + n_\beta(\omega_0)), \qquad \gamma(-\omega_0) = 2\pi |g(\omega_0)|^2 \varrho_0\, n_\beta(\omega_0)$$

Two-level system

Hamiltonian:

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sigma_x \otimes B$$



Example (Two-level system)

Markovian master equation:

$$\frac{d}{dt}\rho_S(t) = -i[H_S, \rho_S(t)] + \gamma_\beta^\downarrow\left(\sigma_-\rho_S\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_S\}\right) + \gamma_\beta^\uparrow\left(\sigma_+\rho_S\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho_S\}\right)$$

where $\gamma_\beta^\downarrow = 2\pi|g(\omega_0)|^2\varrho_0(1 + n_\beta(\omega_0))$ and $\gamma_\beta^\uparrow = 2\pi|g(\omega_0)|^2\varrho_0\, n_\beta(\omega_0)$.

Two-level system

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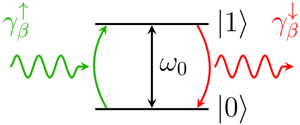


Example (Two-level system)

Markovian master equation:

$$\frac{d}{dt}\rho_S(t) = -i[H_S, \rho_S(t)] + \underbrace{\gamma_\beta^\downarrow \left(\sigma_- \rho_S \sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_S\}\right)}_{\text{Thermal emission}}$$

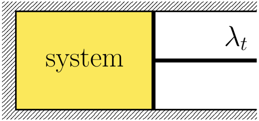
$$+ \underbrace{\gamma_\beta^\uparrow \left(\sigma_+ \rho_S \sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho_S\}\right)}_{\text{Thermal absorption}}$$

where $\gamma_\beta^\downarrow = 2\pi|g(\omega_0)|^2 \varrho_0 (1 + n_\beta(\omega_0))$ and $\gamma_\beta^\uparrow = 2\pi|g(\omega_0)|^2 \varrho_0\, n_\beta(\omega_0)$.

Contents – lecture 3

1st law

Hamiltonian: $H(\lambda_t) = H_S(\lambda_t) + H_R + V$

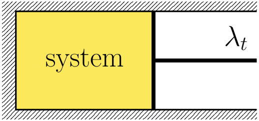


Isolated system $\Delta U = W$:

- Internal energy: $U(t) = \text{Tr}[H(\lambda_t)\rho(t)]$

1st law

Hamiltonian: $H(\lambda_t) = H_S(\lambda_t) + H_R + V$



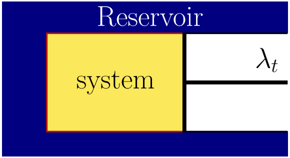
Isolated system $\Delta U = W$:

- Internal energy: $U(t) = \mathrm{Tr}[H(\lambda_t)\rho(t)]$
- Work:

$$\Delta U = \int_0^t ds\, \mathrm{Tr}[\dot{H}(\lambda_s)\rho(s)] = \int_0^t ds\, \mathrm{Tr}_S[\dot{H}_S(\lambda_s)\rho_S(s)] \equiv W$$

1st law

Hamiltonian: $H(\lambda_t) = H_S(\lambda_t) + H_R + V$



Isolated system $\Delta U = W$:

- Internal energy: $U(t) = \text{Tr}[H(\lambda_t)\rho(t)]$
- Work:

$$\Delta U = \int_0^t ds\, \text{Tr}[\dot{H}(\lambda_s)\rho(s)] = \int_0^t ds\, \text{Tr}_S[\dot{H}_S(\lambda_s)\rho_S(s)] \equiv W$$

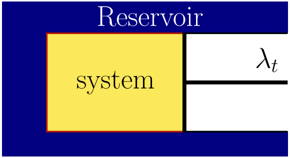
Open system $\Delta U_S = W + Q$ (Vinjanampathy & Anders, CP 2016)

- Internal energy: $\text{Tr}[H(\lambda_t)\rho(t)] \approx \text{Tr}[H_S(\lambda_t)\rho_S(t)] + \text{Tr}[H_R\rho_R(t)]$

$$\Rightarrow \boxed{U_S(t) \approx \text{Tr}[H_S(\lambda_t)\rho_S(t)]}$$

1st law

Hamiltonian: $H(\lambda_t) = H_S(\lambda_t) + H_R + V$



Isolated system $\Delta U = W$:

- Internal energy: $U(t) = \mathrm{Tr}[H(\lambda_t)\rho(t)]$
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$$\Delta U = \int_0^t ds\, \mathrm{Tr}[\dot{H}(\lambda_s)\rho(s)] = \int_0^t ds\, \mathrm{Tr}_S[\dot{H}_S(\lambda_s)\rho_S(s)] \equiv W$$

Open system $\Delta U_S = W + Q$ (Vinjanampathy & Anders, CP 2016)

- Internal energy: $\mathrm{Tr}[H(\lambda_t)\rho(t)] \approx \mathrm{Tr}[H_S(\lambda_t)\rho_S(t)] + \mathrm{Tr}[H_R\rho_R(t)]$

$$\Rightarrow \boxed{U_S(t) \approx \mathrm{Tr}[H_S(\lambda_t)\rho_S(t)]}$$

$$\Delta\dot{U}_S = \mathrm{Tr}[\dot{H}_S(\lambda_t)\rho_S(t)] + \mathrm{Tr}[H_S(\lambda_t)\dot{\rho}_S(t)]$$

- Heat:

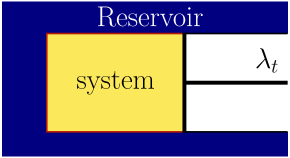
$$\boxed{Q = \int_0^t ds\, \mathrm{Tr}[H_S(\lambda_s)\dot{\rho}_S(s)] = \int_0^t ds\, \mathrm{Tr}[H_S(\lambda_s)\mathcal{L}(\rho_S)]}$$

2nd law

Heat: $Q = \int_0^t ds\, \text{Tr}[H_S(\lambda_s)\mathcal{L}(\rho_S)]$

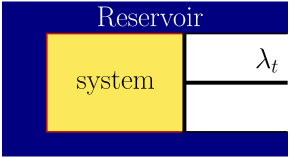
Relative entropy:

$$S(\rho_1||\rho_2) = \text{Tr}[\rho_1(\ln\rho_1 - \ln\rho_2)] \geq 0$$



2nd law

Heat: $Q = \int_0^t ds\, \mathrm{Tr}[H_S(\lambda_s)\mathcal{L}(\rho_S)]$



Relative entropy:

$$S(\rho_1||\rho_2) = \mathrm{Tr}[\rho_1(\ln\rho_1 - \ln\rho_2)] \geq 0$$

Open system $\dot{\sigma}_S \geq 0$ (Vinjanampathy & Anders, CP 2016)

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H. Spohn, *Entropy production for quantum dynamical semigroups*, 1978

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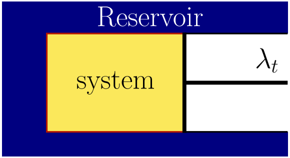

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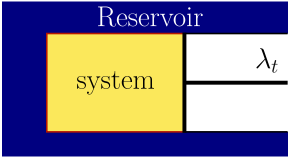

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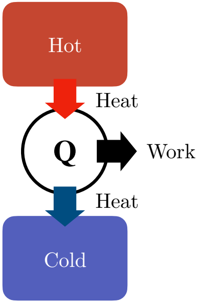
Continuous and reciprocating machines

Continuous thermal machines:

$$\frac{d}{dt}\rho_S(t) = -i[H_S(\lambda_t), \rho_S(t)] + \sum_{\alpha=h,c} \mathcal{D}_{\beta_\alpha}(\rho_S)$$

where $\lambda_t = \lambda_{t+T}$.



S. Bhattacharjeea, A. Dutta *Quantum thermal machines and batteries*, 2021

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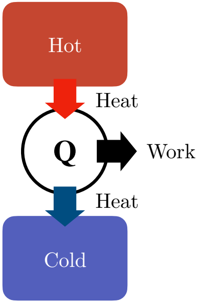

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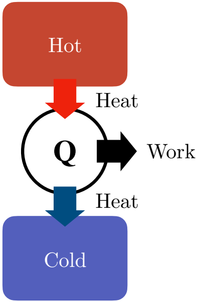
- Work and heat exchange occur continuously.
- Power:

$$\mathcal{P} = \dot{W}_{\text{out}} = -\text{Tr}\left[\frac{\partial H_S(\lambda_t)}{\partial t}\rho_S(t)\right]$$

- Heat currents:

$$J_\alpha = \dot{Q}_\alpha = \text{Tr}[H_S(\lambda_t)\mathcal{D}_{\beta_\alpha}(\rho_S)]$$

Heat engine $\mathcal{P} > 0$.



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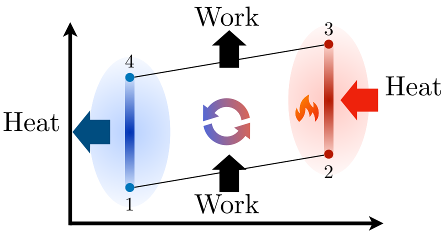
Continuous and reciprocating machines

Reciprocating thermal machines:

- Work and heat exchange occur over sequence of strokes.



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Continuous and reciprocating machines

Reciprocating thermal machines:

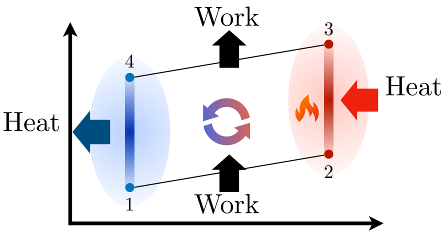
- Work and heat exchange occur over sequence of strokes.
- Power:

$$\mathcal{P} = \frac{W_{\text{out}}}{t_1 + t_2 + t_h + t_c}$$

- Efficiency:

$$\eta = \frac{W_{\text{out}}}{Q_h}$$

Heat engine $\mathcal{P} > 0$.



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Reciprocating heat engine

Quantum Otto cycle (4-stroke):

$$\Phi^{\text{Otto}} = \Phi_{t_c} \circ \Phi_{t_2} \circ \Phi_{t_h} \circ \Phi_{t_1}$$

Working medium $H_S(\lambda_t) = \frac{\lambda_t}{2}(\sigma_z + \mathbb{1})$

1. $1 \to 2$: Adiabatic compression ($\lambda_2 > \lambda_1$)

$$W_1 = \text{Tr}\{[H_S(\lambda_2) - H_S(\lambda_1)]\pi_S^{\beta_c}\}$$

2. $2 \to 3$: Hot isochore

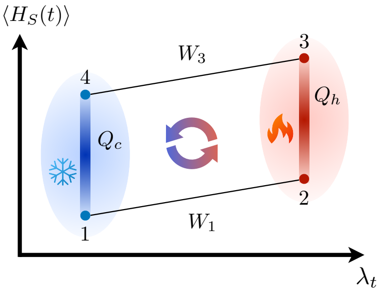
$$Q_h = \text{Tr}\{H_S(\lambda_2)[\pi_S^{\beta_h} - \pi_S^{\beta_c}]\}$$

3. $3 \to 4$: Adiabatic expansion ($\lambda_1 < \lambda_2$)

$$W_2 = \text{Tr}\{[H_S(\lambda_1) - H_S(\lambda_2)]\pi_S^{\beta_h}\}$$

4. $4 \to 1$: Cold isochore

$$Q_c = \text{Tr}\{H_S(\lambda_1)[\pi_S^{\beta_c} - \pi_S^{\beta_h}]\}$$



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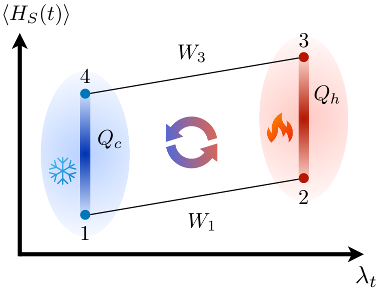

'coherence free'

$$[H_S(t), H_S(t')] = 0, \forall t, t'$$

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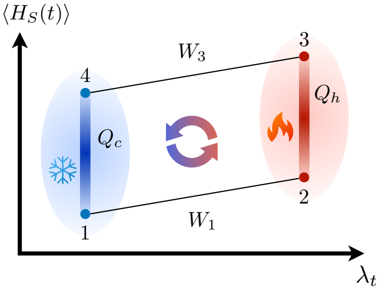

Efficiency

$$\eta = \frac{-W_1 - W_2}{Q_h} = 1 - \frac{\lambda_1}{\lambda_2}$$

Overview

In this lecture we have:

- Derived the Markovian master equation for a two-level system.
- Developed the 1st and 2nd laws of thermodynamics with the MME framework.
- Analyzed a quantum Otto cycle.

Next lecture:

- Extensions to strong system-reservoir coupling.

Thank you

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