Introduction to quantum thermodynamics

An open systems perspective

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NITheCS Mini-School
28 Feb, 2024

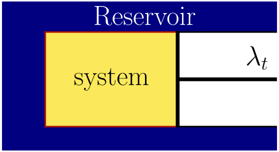
Contents

Last week – 1st law

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

- Internal energy: $U(t) \equiv \text{Tr}[H(\lambda_t)\rho(t)] \approx \langle H_S(\lambda_t)\rangle + \langle H_R\rangle_\beta$

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



R. Alicki and R. Kosloff, *Introduction to Quantum Thermodynamics: History and Prospects*, 2018

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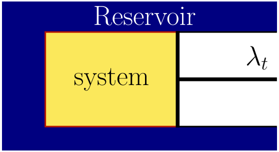

1st law $\dot{U}_S = \dot{W} + \dot{Q}$:

$$\boxed{\dot{U}_S(t) = \text{Tr}[\dot{H}_S(\lambda_t)\rho_S(t)] + \sum_j \text{Tr}[H_S(\lambda_t)\mathcal{D}_j(\rho_S)]}$$

where $\rho_S(t)$ obeys the Markovian master equation*:

$$\dot{\rho}_S = \mathcal{L}(\rho_S) = -i[H_S(\lambda_t), \rho_S(t)] + \sum_j \mathcal{D}_j(\rho_S)$$

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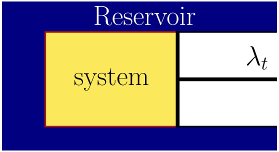

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Power and heat currents:

$$\mathcal{P} = \dot{W} = \left\langle \frac{\partial H_S(\lambda_t)}{\partial t} \right\rangle, \qquad \mathcal{I}_j = \dot{Q}_j = \text{Tr}[H_S(\lambda_t)\mathcal{D}_j(\rho_S)]$$

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Last week – 2nd law

Heat currents: $\mathcal{I}_j = \text{Tr}[H_S(\lambda_t)\mathcal{D}_j(\rho_S)]$

- Von Neumann entropy $S(\rho_S) = -\text{Tr}[\rho_S \ln \rho_S]$

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

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2nd law $\dot{\sigma}_S \geq 0$:

$$\dot{S}(\rho_S) - \sum_j \beta_j \mathcal{I}_j = \dot{S}(\rho_S) + \sum_j \text{Tr}[\mathcal{D}_j(\rho_S)\ln e^{-\beta_j H_S(\lambda_t)}]$$

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$$\begin{aligned}\dot{S}(\rho_S) - \sum_j \beta_j \mathcal{I}_j &= \dot{S}(\rho_S) + \sum_j \mathrm{Tr}[\mathcal{D}_j(\rho_S)\ln e^{-\beta_j H_S(\lambda_t)}] \\ &= \dot{S}(\rho_S) + \sum_j \mathrm{Tr}[\mathcal{D}_j(\rho_S)\ln \pi_S^{\beta_j}], \qquad \pi_S^{\beta_j} = e^{-\beta_j H_S(\lambda_t)}/Z_{S_j}(t).\end{aligned}$$

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Spohn's inequality: $-\text{Tr}[\mathcal{D}_j(\rho_S)(\ln \rho_S(t) - \ln \pi_S^{\beta_j})] \geq 0$ if $\mathcal{D}_j(\pi_S^{\beta_j}) = 0$

$$\Rightarrow \boxed{\dot{\sigma}_S = \dot{S}(\rho_S) - \sum_j \beta_j \mathcal{I}_j \geq 0}$$

where $\dot{\sigma}_S$ is the entropy production rate.

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Contents – lecture 4

1. Recap
   - 1st and 2nd laws
2. Thermal machines – heat engines and refrigerators
   - Continuous machines
   - Reciprocating machines
3. Quantum Otto cycle
4. Strong system-reservoir coupling
5. Summary

Continuous thermal machines

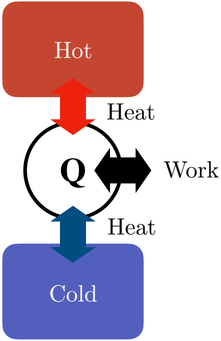
Continuous coupling of working medium to heat source and sink.

(H.E.D. Scovil, E.O. , Schulz-DuBois, *Three-level masers as heat engines*, PRL 1959)

- Markovian master equation:

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

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



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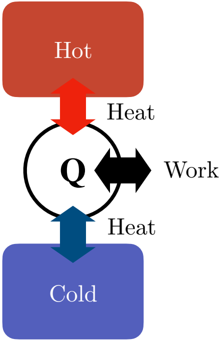
- Driven machines – external control to drive heat currents (right).
- Autonomous machines – external drive replaced by work reservoir.

  (A. Levy, R. Kosloff, *The Quantum Absorption Refrigerator*, PRL 2011)



Continuous (driven) thermal machines

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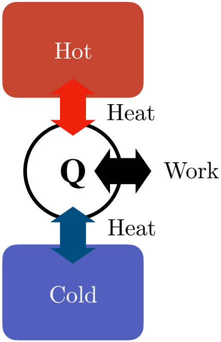

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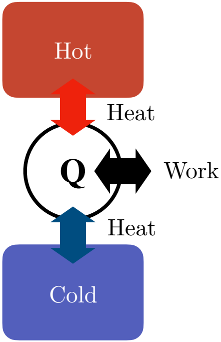
- Floquet formalism: MME for any periodic Hamiltonian $H_S(\lambda_{t+T}) = H_S(\lambda_t)$.
  (H.-P Breuer, F. Petruccione, *The theory of open quantum systems*, 2002)

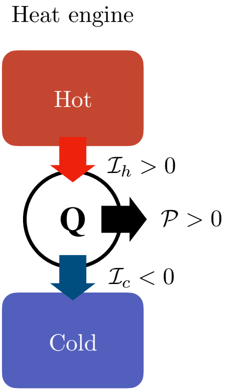
- Operated out of equilibrium in periodic steady state

$$\boxed{\rho_S^{ss}(t+T) = \rho_S^{ss}(t)}$$



Continuous (driven) thermal machines

Heat engine: $\mathcal{P}_{\text{out}} = -\langle \dot{H}_S(t) \rangle > 0$



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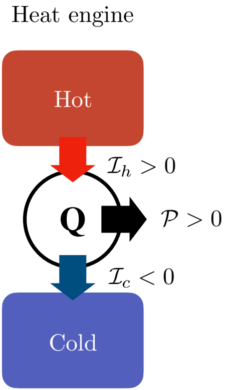
$$\dot{\tilde{\rho}}_S^{ss} = 0 \quad \Rightarrow \quad \dot{U}_S^{ss}(t) = 0$$



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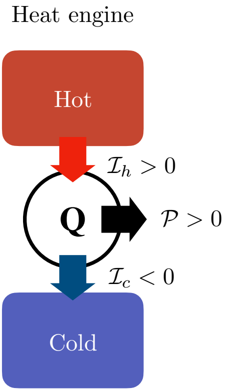

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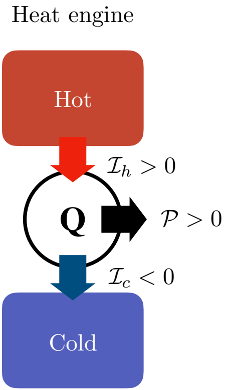
- 2nd law: $\dot{S}(\rho_S) - \sum_j \beta_j \mathcal{I}_j \geq 0$

$$S(\rho_S^{ss}) = S(\tilde{\rho}_S^{ss}) \Rightarrow \boxed{\beta_c \mathcal{I}_c \geq \beta_h \mathcal{I}_h}$$



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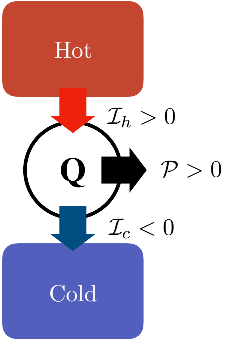
- Efficiency:

$$\eta = \frac{\mathcal{P}_{\text{out}}}{\mathcal{I}_h} = 1 + \frac{\mathcal{I}_c}{\mathcal{I}_h} \leq \boxed{1 - \frac{T_c}{T_h} = \eta_C}$$

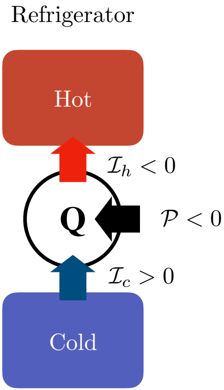
where η_C is the Carnot efficiency.

Heat engine



Continuous (driven) thermal machines

Refrigerator: $\mathcal{P}_{\text{out}} = -\langle \dot{H}_S(t) \rangle < 0$

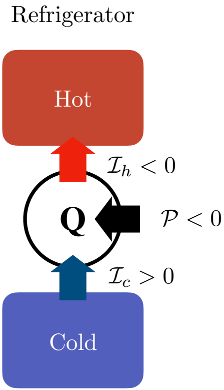


Continuous (driven) thermal machines

Refrigerator: $\mathcal{P}_{\text{out}} = -\langle \dot{H}_S(t) \rangle < 0$

- 1st law: $\dot{U}_S = \sum_j \mathcal{I}_j + \mathcal{P}_{\text{in}}$

$$\boxed{\mathcal{P}_{\text{in}} = -(\mathcal{I}_h + \mathcal{I}_c) > 0}$$



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- 2nd law: $\dot{S}(\rho_S) - \sum_j \beta_j \mathcal{I}_j \geq 0$

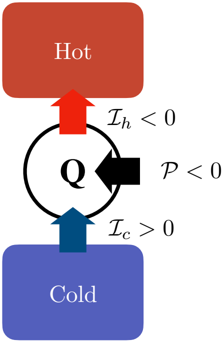
$$S(\rho_S^{ss}) = S(\tilde{\rho}_S^{ss}) \Rightarrow \boxed{\beta_c \mathcal{I}_c \geq \beta_h \mathcal{I}_h}$$

- Coefficient of performance (COP):

$$\epsilon = \frac{\mathcal{I}_c}{\mathcal{P}_{\text{in}}} = -\frac{1}{1 + \frac{\mathcal{I}_h}{\mathcal{I}_c}} \leq \boxed{\frac{T_c}{T_h - T_c} = \epsilon_C}$$

where ϵ_C is the Carnot COP.

Refrigerator



Reciprocating thermal machines

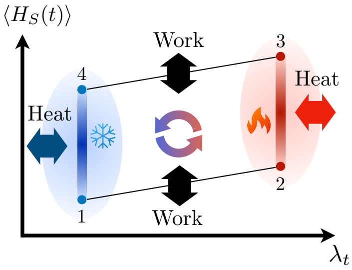
Work and heat exchange occur over sequence of strokes.

- Quantum Otto cycle (right)

  (J. Roßnagel et al, *A single-atom heat engine*, Science 2016)

  (J. Klatzow, et al, *Experimental Demonstration of Quantum Effects in the Operation of Microscopic Heat Engines*, PRL 2019)

- Carnot cycle (reversible)



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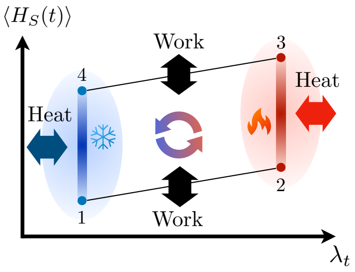
- Adiabaticity:

$$[H_S(\lambda_t), H_S(\lambda_{t'})] = 0 \quad \forall t, t'$$

Shortcuts to adiabaticity –

(A. Del Campo, J. Goold, M. Paternostro, *More bang for your buck: Super-adiabatic quantum engines*, Sci. Rep. 2014)



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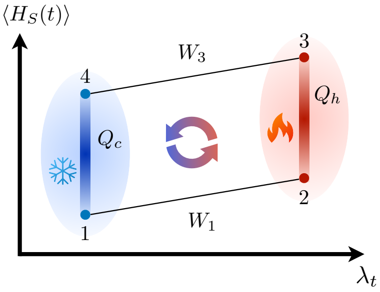
$$\Phi^{\text{Otto}} = \Phi_{t_c} \circ \Phi_{t_2} \circ \Phi_{t_h} \circ \Phi_{t_1}$$



1. $1 \to 2$: Isoentropic 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. $3 \to 4$: Isoentropic expansion

   $$W_3 = \text{Tr}\{[H_S(\lambda_1) - H_S(\lambda_2)]\pi_S^{\beta_h}\}$$

4. $4 \to 1$: Cold isochore

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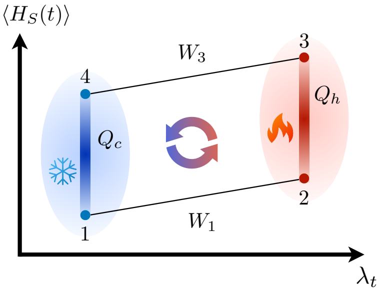

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$$\Rightarrow \boxed{W_1 + Q_h + W_3 + Q_c = 0}$$

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

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$$W_1 = (\lambda_2 - \lambda_1)\frac{e^{-\beta_c \lambda_1}}{1 + e^{-\beta_c \lambda_1}}$$

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$$Q_h = \lambda_2 \left[\frac{e^{-\beta_h \lambda_2}}{1 + e^{-\beta_h \lambda_2}} - \frac{e^{-\beta_c \lambda_1}}{1 + e^{-\beta_c \lambda_1}}\right]$$

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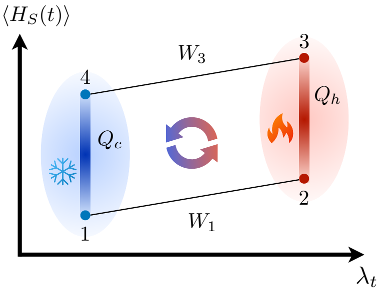

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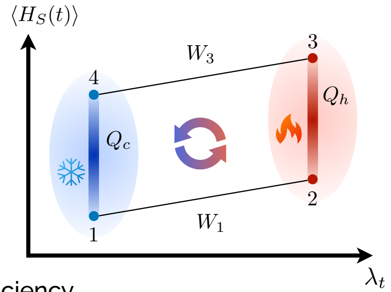

Efficiency

$$\boxed{\eta = \frac{-W_1 - W_3}{Q_h} = 1 - \frac{\lambda_1}{\lambda_2} \leq \eta_C}$$

Quantum thermodynamics — strong reservoir coupling

Isolated system: $H(\lambda_t) = H_S(\lambda_t) + H_R + V(t)$

- Internal energy $U(t) = \mathrm{Tr}[H(\lambda_t)\rho(t)]$
- Von Neumann equation $\dot{\rho}(t) = -i[H(\lambda_t), \rho(t)]$

Quantum thermodynamics — strong reservoir coupling

Isolated system: $H(\lambda_t) = H_S(\lambda_t) + H_R + V(t)$

- Internal energy $U(t) = \mathrm{Tr}[H(\lambda_t)\rho(t)]$
- Von Neumann equation $\dot{\rho}(t) = -i[H(\lambda_t), \rho(t)]$

1st law: $\Delta U = W + Q$ (Esposito *et al.* NJP 2010; Kato & Tanimura, JCP 2016)

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

- Strong coupling: $\frac{d}{dt}\mathrm{Tr}[(H_S(t) + V(t))\rho(t)] = \dot{W} - \mathrm{Tr}[H_R\dot{\rho}_R(t)]$,

$$\boxed{U_S^*(t) = \mathrm{Tr}[(H_S(\lambda_t) + V(t))\rho(t)]}$$

- Heat: $Q = -\mathrm{Tr}\{H_R[\rho_R(t) - \rho_R(0)]\}$

Quantum thermodynamics — strong reservoir coupling

Isolated system: $H(\lambda_t) = H_S(\lambda_t) + H_R + V(t)$

- Internal energy $U(t) = \text{Tr}[H(\lambda_t)\rho(t)]$
- Von Neumann equation $\dot{\rho}(t) = -i[H(\lambda_t), \rho(t)]$

2nd law: $\Delta S - \beta Q \geq 0$ (Esposito *et al.* NJP 2010)

$$Q = -\int_0^t ds\, \text{Tr}[H_R \dot{\rho}_R(s)]$$

- Monotonicity of relative entropy: $S(\rho_{SR}||\rho_S\pi_R^\beta) \equiv \text{Tr}[\rho_{SR}\ln\rho_{SR}] - \text{Tr}[\rho_{SR}\ln\rho_S\pi_R^\beta] \geq 0$,

$$\boxed{S(\rho_{SR}||\rho_S \otimes \pi_R^\beta) = \Delta S - \frac{Q}{T} \geq 0}$$

where $\Delta S = -\text{Tr}[\rho_S(t)\ln\rho_S(t)] + \text{Tr}[\rho_S(0)\ln\rho_S(0)]$.

Quantum thermodynamics — strong reservoir coupling

Other possible formulations — mean force Gibbs state:

(Kirkwood, J. Therm. Phys. **3**, 300, 1935; Seifert, PRL, **116**, 020601 2016)

- Equilibrium state of isolated system (canonical ensemble):

$$\pi^{\beta}_{SR} = \frac{e^{-\beta H(\lambda)}}{Z(\lambda)}$$

- Equilibrium reduced system state:

$$\pi^{*}_{S}(\beta) = \mathrm{Tr}_R \frac{e^{-\beta H(\lambda)}}{Z(\lambda)} \boxed{\equiv \frac{e^{-\beta H^{*}_{S}(\lambda,\beta)}}{Z^{*}_{S}(\lambda,\beta)} \neq \pi^{\beta}_{S}}$$

Quantum thermodynamics — strong reservoir coupling

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Strong coupling corrections to work & power:

(Perarnau-Llobet et al, PRL, **120**, 120602, 2018)

- Maximal work extraction, $W \leq W^{\text{weak}}$
- Decrease in thermalization time $\Rightarrow$ power enhancement?

Overview

In this lecture we have:

- Introduced continuous and reciprocating thermal machines.
- Calculated efficiency and coefficient of performance for driven continuous heat engines and refrigerators.
- Analyzed a quantum Otto cycle.
- Introduced possible approaches to treating quantum thermodynamics at strong coupling.

Thank you

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