# Optimal quantum driving of a thermal machine

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## Outline



## **1. Slow driving of quantum thermal machines** (close to thermodynamic equilibrium)

- General theory of slowly driven master equations
- Efficiency at maximum power for heat engines



## **2. Optimal driving of quantum thermal machines** (strongly out of equilibrium)

- Optimality of finite-time Carnot cycles
- Full solution for a two-level system heat engine

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## Master equations

#### Classical Markov process

$$\mathbf{p} = (p_1, p_2, \dots, p_n)^\top$$

$$\dot{\mathbf{p}}(t) = L(t)\mathbf{p}(t)$$

Liouvillian matrix

$$L_{i \neq j}(t) \ge 0 \qquad \sum_{i} L_{ij}(t) = 0$$

#### Quantum Markov process

$$\rho = \sum_{i,j=1}^{n} \rho_{ij} |i\rangle \langle j|$$

$$\dot{\rho}(t) = \mathcal{L}(t)\rho(t)$$

Liouvillian superoperator

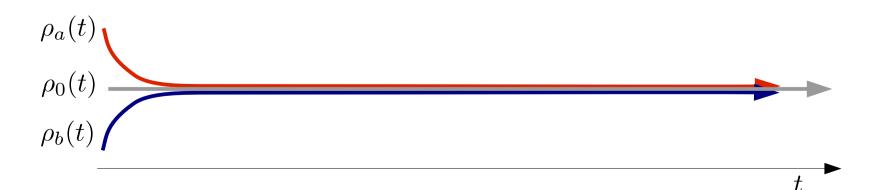
$$\mathcal{L}\rho = -i[H,\rho] + \sum_{j=1}^{n^2 - 1} 2L_j \rho L_j^{\dagger} - L_j^{\dagger} L_j \rho - \rho L_j^{\dagger} L_j$$

## Equilibrium states

 $\dot{\rho}_0 = \mathcal{L}\rho_0 = 0$   $\longrightarrow$   $\rho_0$  is a **fixed point** of the map = **equilibrium state**   $\rho_0$  corresponds to an eigenvector of  $\mathcal{L}$  with eigenvalue zero  $\mathcal{L}^{\dagger}(\mathbb{I}) = 0$ (trace preserving condition)  $\longrightarrow$  There is at least one equilibrium state  $\rho_0$ 

If  $\rho_0$  is **unique** the master equation is usually called "**mixing**" or "**relaxing**" (assuming convergence from every initial state)

#### **Mixing process**



## Slowly driven master equations

Time dependent master equation:  $\dot{\rho}(t) = \mathcal{L}(t)\rho(t)$ 

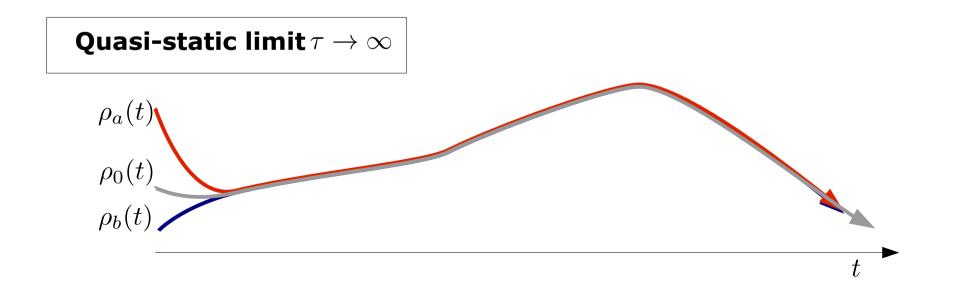
If  $\mathcal{L}(t)$  is relaxing for every t:  $\mathcal{L}(t)$ 

$$\mathcal{L}(t)\rho_0(t) = 0$$

unique instantaneous equilibrium state

#### Slow driving regime

[external driving time-scale]  $\tau \gg \tau_S$  [characteristic time-scale of the system]



## Slowly driven master equations

Time dependent master equation:  $\dot{\rho}(t) = \mathcal{L}(t)\rho(t)$ 

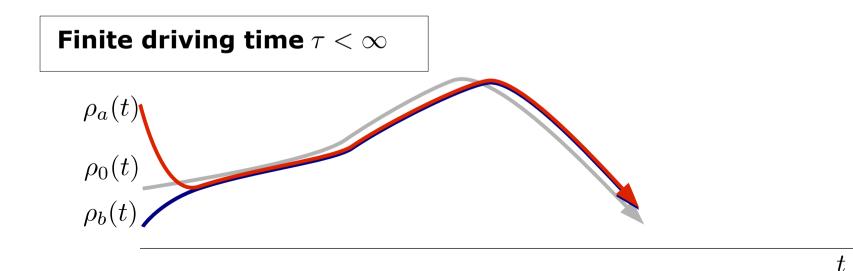
If  $\mathcal{L}(t)$  is relaxing for every t:  $\mathcal{L}$ 

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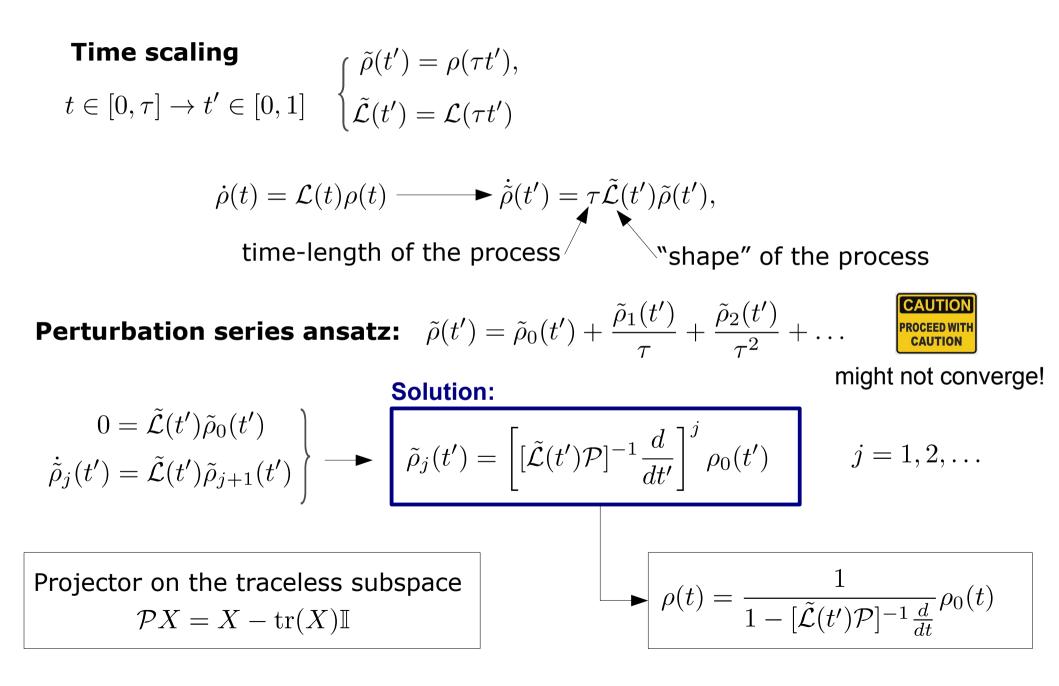
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#### Slow driving regime

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## Perturbation theory of slowly driven quantum systems



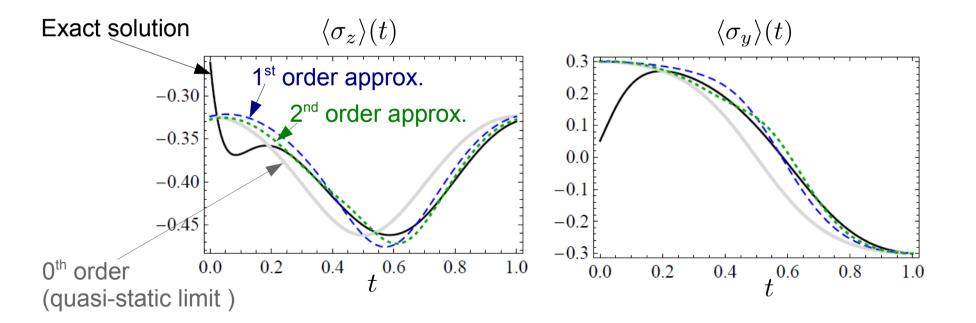
## Example: slowly driven two-level system

modulation (sinusoidal in this case)  

$$N(t) = [\exp(\beta\hbar\omega(t)) - 1]^{-1}$$

$$\dot{\phi}(t) = -\frac{i}{2\hbar} [\rho(t), \Delta(t)\sigma_x] + \gamma (N(t) + 1) \left(\sigma_-\rho(t)\sigma_+ - \frac{1}{2} \{\sigma_+\sigma_-, \rho(t)\}\right)$$

$$+ \gamma N(t) \left(\sigma_+\rho(t)\sigma_- - \frac{1}{2} \{\sigma_-\sigma_+, \rho(t)\}\right)$$



## Finite-time thermodynamics

Thermal master equations:  $\langle$ 

$$\begin{cases} \mathcal{L}(t)\rho_0(t) = 0\\ \rho_0(t) = \frac{\exp[-\beta H(t)]}{Z(t)}, \quad Z(t) = \operatorname{tr}\{\exp[-\beta H(t)]\} \end{cases}$$

 $\tilde{\rho}(t') = \tilde{\rho}_0(t') + \frac{\tilde{\rho}_1(t')}{\tau} + \frac{\tilde{\rho}_2(t')}{\tau^2} + \dots$ Quasi-static evolution

$$\tilde{\rho}_j(t') = \left[ [\tilde{\mathcal{L}}(t')\mathcal{P}]^{-1} \frac{d}{dt'} \right]^j \frac{\exp[-\beta \tilde{H}(t')]}{\tilde{Z}(t')}$$

#### Finite-time corrections

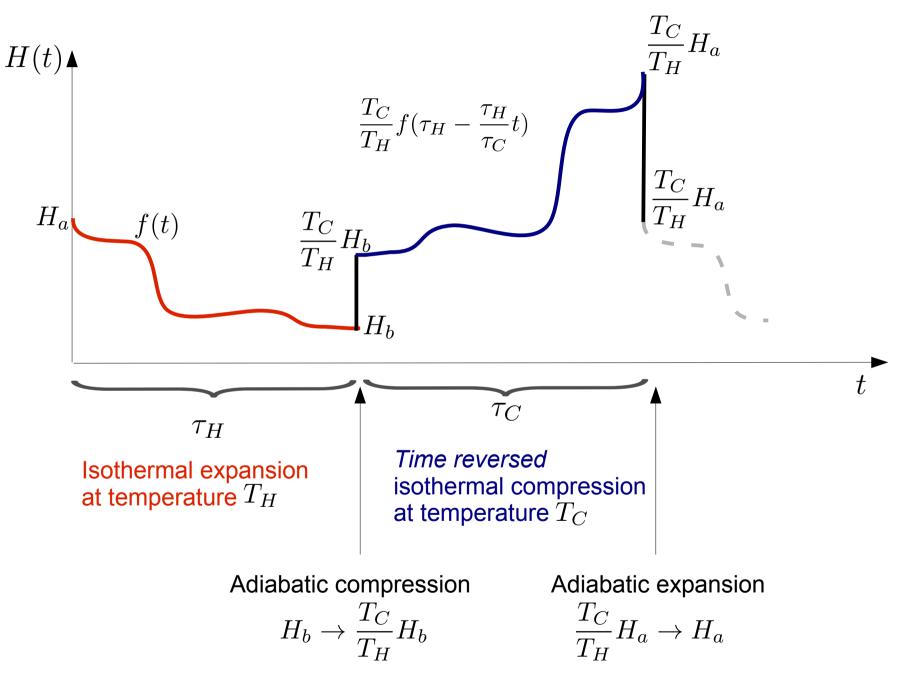
$$\begin{split} S(t) &= -\mathrm{tr}[\rho(t)\mathrm{log}(\rho(t))] &= S_0(t) + S_1(t)/\tau + S_2(t)/\tau^2 + \dots \\ U(t) &= \mathrm{tr}[H(t)\rho(t)] &= U_0(t) + U_1(t)/\tau + U_2(t)/\tau^2 + \dots \\ Q &= \int_0^\tau \mathrm{Tr}[\dot{\rho}(t)H(t)]dt = \int_0^1 \mathrm{Tr}[\dot{\tilde{\rho}}(t')\tilde{H}(t')]dt' &= Q_0(t) + Q_1/\tau + Q_2/\tau^2 + \dots \\ W &= \int_0^\tau \mathrm{Tr}[\rho(t)\dot{H}(t)]dt = \int_0^1 \mathrm{Tr}[\tilde{\rho}(t')\dot{\tilde{H}}(t')]dt' &= W_0(t) + W_1/\tau + W_2/\tau^2 + \dots \\ \mathbf{Reversible} \checkmark & \mathbf{Irreversible corrections} \\ \mathbf{thermodynamics} & \mathbf{Irreversible corrections} \end{split}$$

## First order irreversible corrections

$$\begin{split} U_1(t) &= \operatorname{tr} \left[ \tilde{H}(t')\rho_1(t') \right]_{t'=t/\tau}, \\ &= \operatorname{tr} \left[ \tilde{H}(t')[\tilde{\mathcal{L}}(t')\mathcal{P}]^{-1} \frac{d}{dt'} \tilde{\rho}_0(t') \right]_{t'=t/\tau}, \\ S_1(t) &= -\operatorname{Tr}[\tilde{\rho}_1(t')\log(\tilde{\rho}_0(t'))]_{t'=t/\tau} = \beta U_1(t), \\ Q_1 &= \int_0^1 \operatorname{tr} \left[ \tilde{H}(t')\dot{\tilde{\rho}}_1(t') \right] dt' \\ &= \int_0^1 \operatorname{tr} \left[ \tilde{H}(t')\tilde{\mathcal{L}}(t')\tilde{\rho}_2(t') \right] dt' \\ &= \int_0^1 \operatorname{tr} \left[ \tilde{H}(t')\frac{d}{dt'} [\tilde{\mathcal{L}}(t')\mathcal{P}]^{-1}\frac{d}{dt'}\tilde{\rho}_0(t') \right] dt', \\ \mathbf{1}^{\mathrm{st}} \operatorname{Iaw} \ W_1 &= \Delta U_1 - Q_1. \end{split}$$

**Important property**:  $Q_1$  is invariant for a time reversed protocol

## Finite-time Carnot cycle



Limit of many cycles -

#### **1**<sup>st</sup> order perturbation theory

Initial conditions are lost and also the quantum state becomes periodic,  $\Delta U = 0$ 

$$W = \Delta U - Q^H - Q^C$$

$$\begin{array}{l} \textbf{Power} \\ P = \frac{-W}{\tau_H + \tau_C} \simeq \frac{Q_0^H + Q_1^H / \tau_H + Q_0^C + Q_1^C / \tau_C}{\tau_H + \tau_C} \end{array}$$

#### Efficiency

**Carnot efficiency** 

Max Power 
$$P^* = \max_{\tau_H, \tau_C} P$$
  
Efficiency at max Power  $\eta^* = \left[\frac{2}{\eta_C} - \frac{1}{1 + \sqrt{Q_1^C/Q_1^H}}\right]^{-1}$   
We know how to compute finite-time heat corrections  
Schmiedl, Seifert. EPL 81.2 20003 (2007)  
Esposito *et al.*, PRL 105, 150603 (2010)

$$\eta^* = \left[\frac{2}{\eta_C} - \frac{1}{1 + \sqrt{Q_1^C / Q_1^H}}\right]^{-1}$$

If  $\beta(t)H(t)$  is continuous and differentiable

$$P_1^{(H,C)} = \int_0^1 \operatorname{tr} \left[ \tilde{H}^{(H,C)}(t') \frac{d}{dt'} [\tilde{\mathcal{L}}^{(H,C)}(t')\mathcal{P}]^{-1} \frac{d}{dt'} \tilde{\rho}_0^{(H,C)}(t') \right] dt'$$

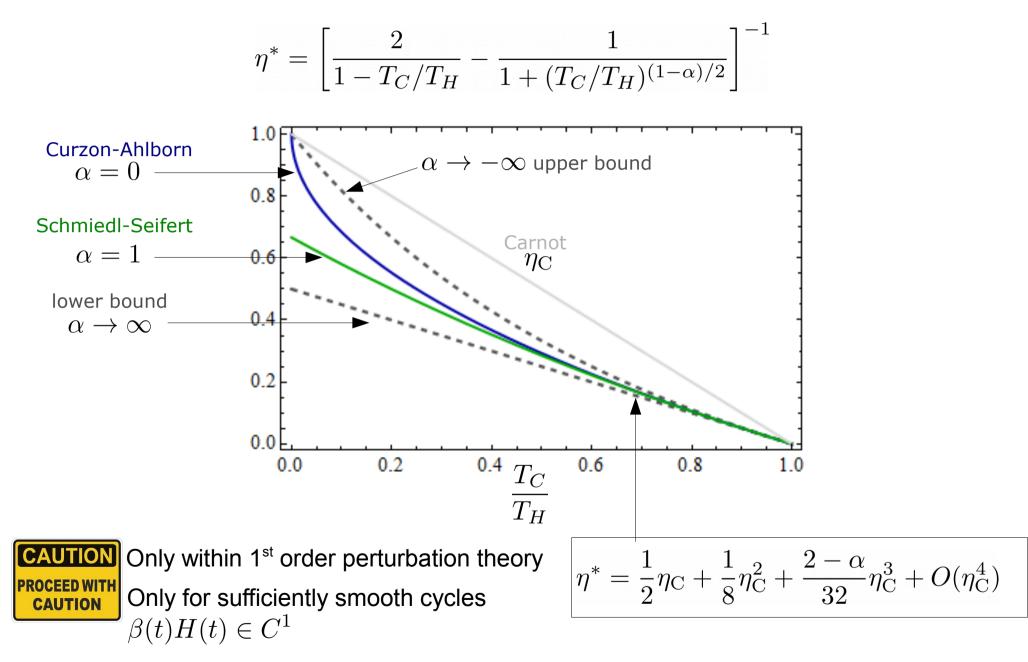
(depends on the particular protocol)

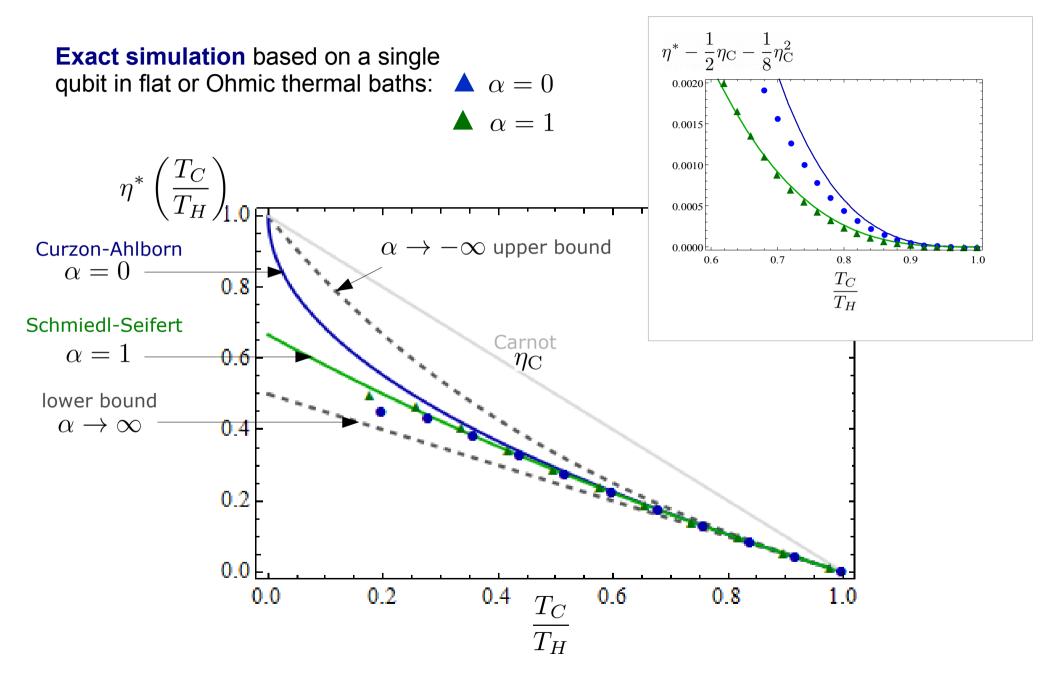
## Pseudo-time reversal symmetry of the cycle $\tilde{H}^{(C)}(t') = \frac{T_C}{T_H} \tilde{H}^{(H)}(1-t')$ $\left(\frac{T_C}{T_{\mu}}\right)^{1-\alpha}$ $\frac{Q_1^C}{O^H} = \left( \right.$ **Scaling properties of thermal Liouvillians** (derives from macroscopic derivation) **Universal scaling** $\mathcal{L}(\lambda H, \{L_i\}, \lambda^{-1}\beta) = \mathcal{L}(H, \{\lambda^{\alpha}L_i\}, \beta)$ for all protocols Spectral density exponent $J(\omega) = \eta \omega^{\alpha}$

#### Thermal bath spectral density

$$J(\omega) = \eta \omega^{\alpha} \qquad \qquad \eta^* = \left[\frac{2}{1 - T_C/T_H} - \frac{1}{1 + (T_C/T_H)^{(1-\alpha)/2}}\right]^{-1}$$

Flat bath
$$J(\omega) = \eta$$
 $\eta^*|_{\alpha=0} = 1 - \sqrt{\frac{T_C}{T_H}}$ Curzon, Ahlborn, AJP 43, 22 (1975)  
Chambadal, L.c..n., 4 1-58 (1957)Ohmic bath $J(\omega) = \eta \omega$  $\eta^*|_{\alpha=1} = 2\eta_C/(4 - \eta_C)$   
Schmiedl, Seifert. EPL 81.2 20003 (2007)Infinitely  
super-Ohmic bath $J(\omega) = \eta \omega^{\alpha \to \infty}$  $\eta^*|_{\alpha \to \infty} = \frac{\eta_C}{2}$ Esposito et al., PRL 105, 150603 (2010)  
Schmiedl, Seifert. EPL 81.2 20003 (2007)Infinitely  
sub-Ohmic bath $J(\omega) = \eta \omega^{\alpha \to -\infty}$  $\eta^*|_{\alpha \to -\infty} = \frac{2\eta_C}{2 - \eta_C}$ Esposito et al., PRL 105, 150603 (2010)  
Schmiedl, Seifert. EPL 81.2 20003 (2007)





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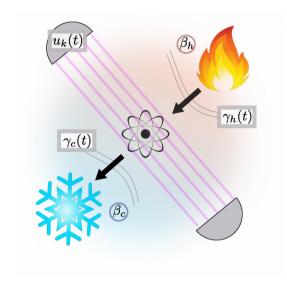
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- Optimality of finite-time Carnot cycles
- Full solution for a two-level system heat engine

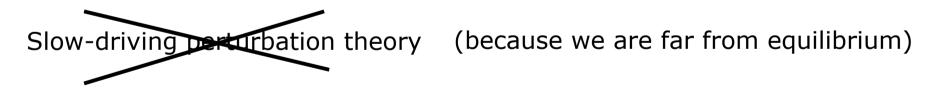
## **General questions**

*What is the optimal driving of a thermal machine ?* 

Given a d-level quantum system and two heat baths, what is the maximum power that we can extract?

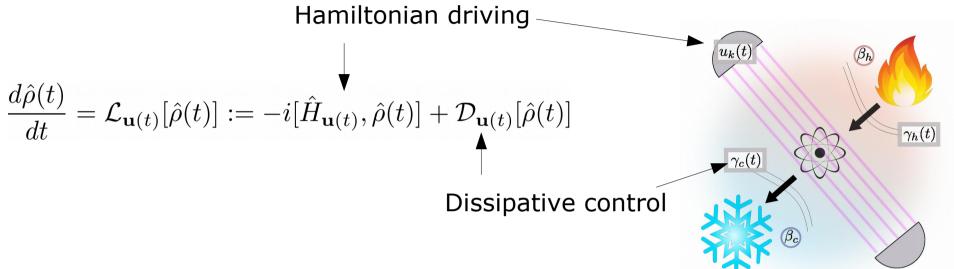


## Methods



Optimal control theory approach (Pontryagin's minimum principle)

## Optimal control of a thermal machine



Heat released by the system:

$$Q := -\int_0^\tau \left\langle \hat{H}_{\mathbf{u}(t)} \mathcal{L}_{\mathbf{u}(t)} [\hat{\rho}(t)] \right\rangle dt$$

Work done by the system:

$$W := -\int_0^\tau \left\langle \hat{\rho}(t) \; \frac{d\hat{H}_{\mathbf{u}(t)}}{dt} \right\rangle dt$$

### **Optimal control problem**

minimize Q

with respect to all control strategies  $\mathbf{u}(t)$ 

for fixed:  $\tau, \rho(0), \rho(\tau)$ 

## Pontryagin's approach

(similar to Hamiltonian formalism applied to control theory)

Extended functional

Lagrange multipliers

$$\mathcal{J} := Q + \int_0^\tau \left\{ \lambda(t) (\langle \hat{\rho}(t) \rangle - 1) + \left\langle \hat{\pi}(t) \left( \mathcal{L}_{\mathbf{u}(t)}[\hat{\rho}(t)] - \frac{d\hat{\rho}(t)}{dt} \right) \right\rangle \right\} dt$$

normalization

master equation

Pseudo Hamiltonian

$$\mathcal{H}(t) := \left\langle (\hat{\pi}(t) - \hat{H}_{\mathbf{u}(t)}) \mathcal{L}_{\mathbf{u}(t)}[\hat{\rho}(t)] \right\rangle + \lambda(t) (\langle \hat{\rho}(t) \rangle - 1)$$
$$\mathcal{J} = \int_{0}^{\tau} \left\{ \mathcal{H}(t) - \left\langle \hat{\pi}(t) \frac{d\hat{\rho}(t)}{dt} \right\rangle \right\} dt$$

Analogue of Hamilton equations:

$$\frac{d\hat{\rho}(t)}{dt} = \frac{\partial\mathcal{H}(t)}{\partial\hat{\pi}(t)} , \qquad \frac{d\hat{\pi}(t)}{dt} = -\frac{\partial\mathcal{H}(t)}{\partial\hat{\rho}(t)} ,$$

Analogue of energy conservation:  $\mathcal{H}(t) = \mathcal{K}$  (constant conserved quantity)

## Pontryagin's minimum principle

Necessary conditions for optimal control strategies minimizing the extended functional

$$\mathcal{J} := Q + \int_0^\tau \left\{ \lambda(t) (\langle \hat{\rho}(t) \rangle - 1) + \left\langle \hat{\pi}(t) \left( \mathcal{L}_{\mathbf{u}(t)}[\hat{\rho}(t)] - \frac{d\hat{\rho}(t)}{dt} \right) \right\rangle \right\} dt$$

are such that:

**1.** there exists a non-zero costate  $\hat{\pi}(t)$  evolving according to:

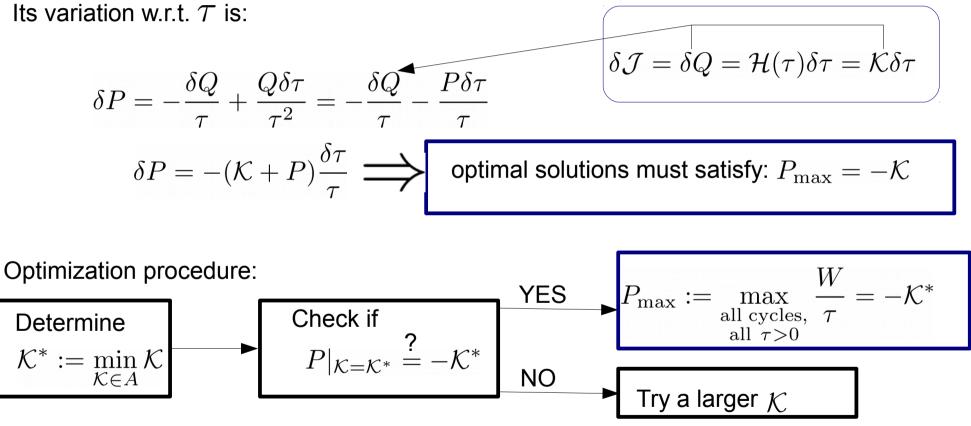
$$\frac{d\hat{\pi}(t)}{dt} = -\frac{\partial\mathcal{H}(t)}{\partial\hat{\rho}(t)} = -\left\{\mathcal{L}^{\dagger}_{\mathbf{u}(t)}[\hat{\pi}(t) - \hat{H}_{\mathbf{u}(t)}] + \lambda(t)\right\}$$

- **2.** the pseudo Hamiltonian  $\mathcal{H}(t) := \left\langle (\hat{\pi}(t) \hat{H}_{\mathbf{u}(t)}) \mathcal{L}_{\mathbf{u}(t)}[\hat{\rho}(t)] \right\rangle + \lambda(t)(\langle \hat{\rho}(t) \rangle 1)$  is minimized by the control function  $\mathbf{u}(t)$  for all  $t \in [0, \tau]$
- **3.** the pseudo Hamiltonian is constant  $\mathcal{H}(t) = \mathcal{K}$

## Thermodynamic link between $\mathcal K$ and maximum power

Does  $\mathcal{K}$  have a physical meaning?

Assume that we want to maximize the power of a cyclic engine  $P = W/\tau = -Q/\tau$ 



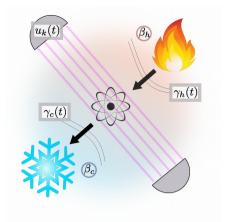
The optimal driving of a generic quantum heat engine reduces to the optimization of a **single degree of freedom**  $\mathcal{K}$  within its accessible region A.

Optimal cycle for a d-level quantum heat engine

$$\frac{d\hat{\rho}(t)}{dt} = -i[\hat{H}_{\mathbf{u}(t)}, \hat{\rho}(t)] + \gamma_c(t)\mathcal{D}_{\mathbf{u}(t)}^{(c)}[\hat{\rho}(t)] + \gamma_h(t)\mathcal{D}_{\mathbf{u}(t)}^{(h)}[\hat{\rho}(t)]$$

Upper bound on the total dissipation rate:

$$\gamma_c(t) + \gamma_h(t) \le \Gamma$$



The optimal control for  $\gamma_c(t)$  and  $\gamma_h(t)$  turns out to be of "bang-bang" type:

## 2 alternatives: $\gamma_c(t) = \Gamma, \ \gamma_h(t) = 0$ (strong coupling **only** with the cold bath) $\gamma_h(t) = \Gamma, \ \gamma_c(t) = 0$ (strong coupling **only** with the hot bath)

Optimal control for the Hamiltonian  $\hat{H}_{\mathbf{u}(t)}$  turns out to be given by differentiable solutions (**isothermal processes**) separated by discontinuous jumps (**adiabatic quenches**).

Maximum power quantum heat engines are achieved by a finite-time Carnot cycle

Power maximization: take the minimum  $\mathcal{K}$  such that  $P = -\mathcal{K}$ 

## Example: full solution for a 2-level system

$$\begin{array}{l} \mbox{control on the energy level} & \mbox{Gibbs thermalizing dissipators} \\ \hat{H}(t) = u(t)|1\rangle\langle 1| & \\ \mathcal{D}_{u(t)}^{(c,h)}[\hat{\rho}(t)] = \frac{e^{-\beta_{(c,h)}u(t)}|1\rangle\langle 1| + |0\rangle\langle 0|}{e^{-\beta_{(c,h)}} + 1} - \hat{\rho}(t) \end{array}$$

Quantum state (diagonal):  $\hat{\rho}(t):=p(t)|1\rangle\langle 1|+[1-p(t)]|0\rangle\langle 0|$ 

Pontryagin's costate:

$$\hat{\pi}(t) = q(t)(|0\rangle\langle 0| - |1\rangle\langle 1|)$$

Pseudo Hamiltonian:

$$\mathcal{H} = \Gamma(-p + \frac{1}{1 + e^{\beta_{c,h}}})(2q + u) = \mathcal{K}$$

(constant of motion)

Pseudo Hamilton equations:

$$\frac{dp(t)}{dt} = \Gamma \Big[ \frac{1}{1 + e^{\beta_{c,h} u(t)}} - p(t) \Big]$$

(master equation)

 $\frac{dq(t)}{dt} = \frac{\Gamma}{2} [2q(t) + u(t)]$  (costate equation)

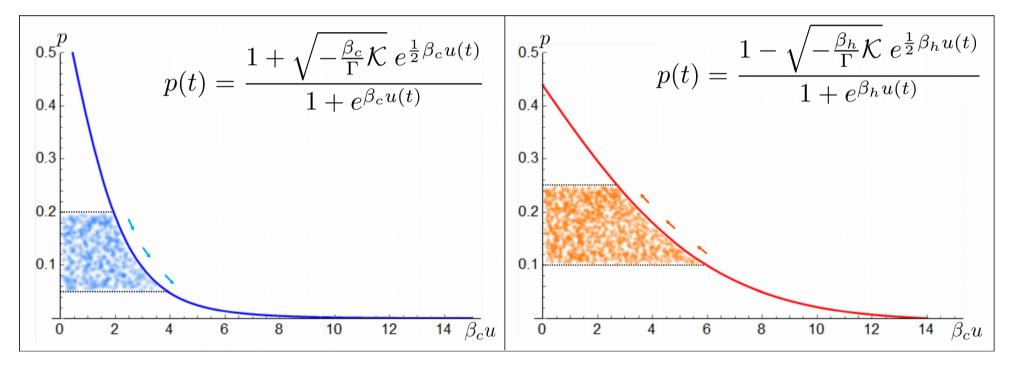
## Optimal solutions for a 2-level system

$$\hat{H}(t) = u(t)|1\rangle\langle 1]$$
  
$$\hat{\rho}(t) = p(t)|1\rangle\langle 1| + [1 - p(t)]|0\rangle\langle 0|$$

Optimal trajectories in the (u, p) plane

Cold isotherm

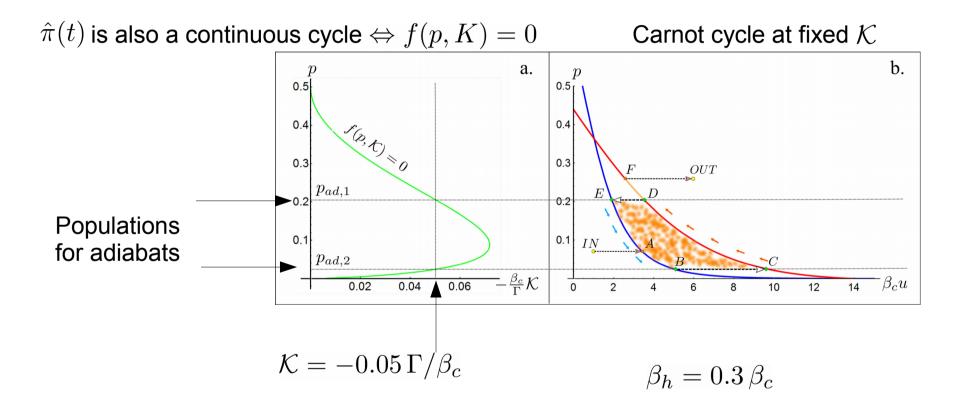
Hot isotherm



 $\mathcal{K} = -0.05 \, \Gamma / \beta_c \qquad \beta_h = 0.3 \, \beta_c$ 

## Optimal solutions for a 2-level system

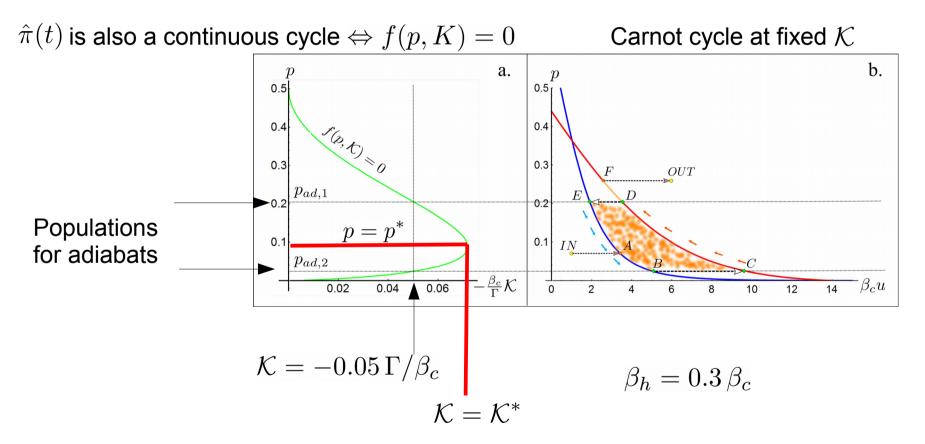
$$\hat{H}(t) = u(t)|1\rangle\langle 1]$$
  
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 $\mathcal{K}$  completely determines the Carnot cycle.

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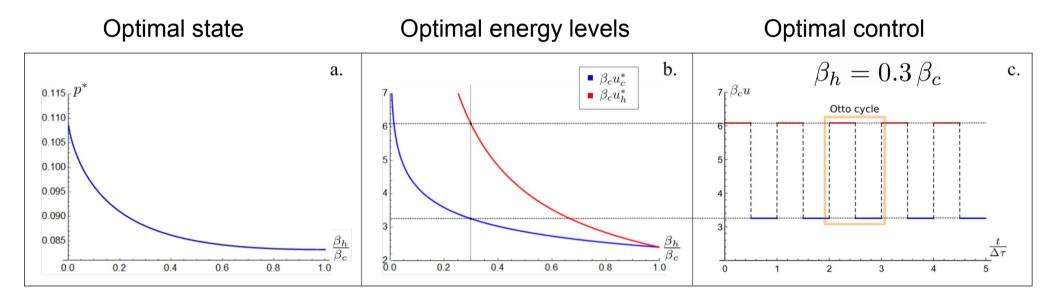


 ${\cal K}$  completely determines the Carnot cycle.

The maximum power is achieved for  $\mathcal{K} = \mathcal{K}^*$  corresponding to an infinitesimal cycle performed around the optimal non-equilibrium state  $p = p^*$ 

## Maximum power cycle for a 2-level system

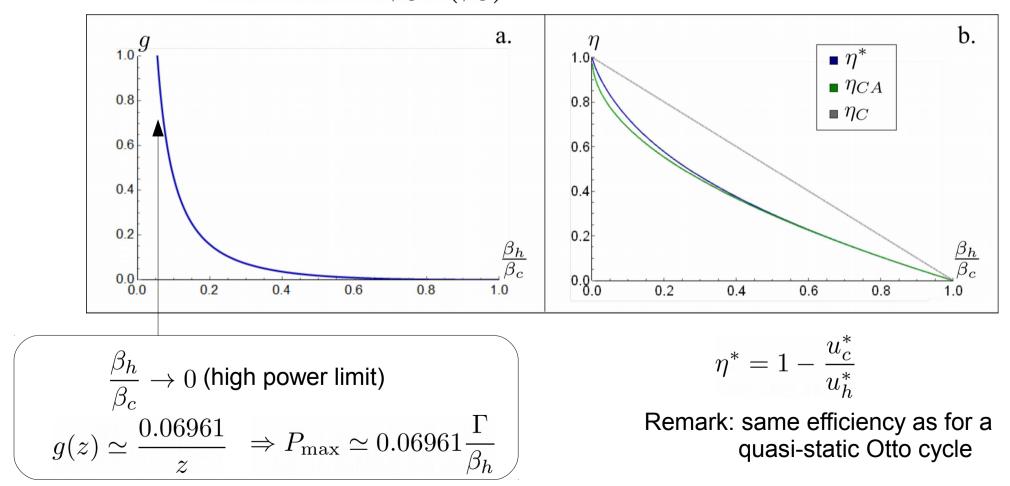
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## Maximum power cycle for a 2-level system

$$\hat{H}(t) = u(t)|1\rangle\langle 1]$$
  
$$\hat{\rho}(t) = p(t)|1\rangle\langle 1| + [1 - p(t)]|0\rangle\langle 0|$$

Maximum power 
$$P_{\max} = -\mathcal{K}^* = \frac{\Gamma}{\beta_c} g\left(\frac{\beta_h}{\beta_c}\right)$$



## Conclusions



### **1.** Slow driving of quantum thermal machines [1]

- Perturbation theory of slowly driven master equations
- Universal formula for the efficiency at maximum power



## 2. Optimal driving of quantum thermal machines [2]

- Optimal control theory approach (*Pontryagin's minimum principle*)
- Optimal processes are finite-time Carnot cycles
- Maximum power = conserved quantity of the control problem:  $-\mathcal{K}$
- Full solution for a two-level system heat engine

[1] Cavina, AM, Giovannetti, Phys. Rev. Lett. (2017).[2] Cavina, AM, Carlini, Giovannetti, arXiv: (2017).