

# Shortcut to Equilibration enabled by the Inertial Theorem

Quantum Thermodynamics – Espoo 2019

Roie Dann<sup>1</sup>

Ander Tobalina<sup>2</sup>

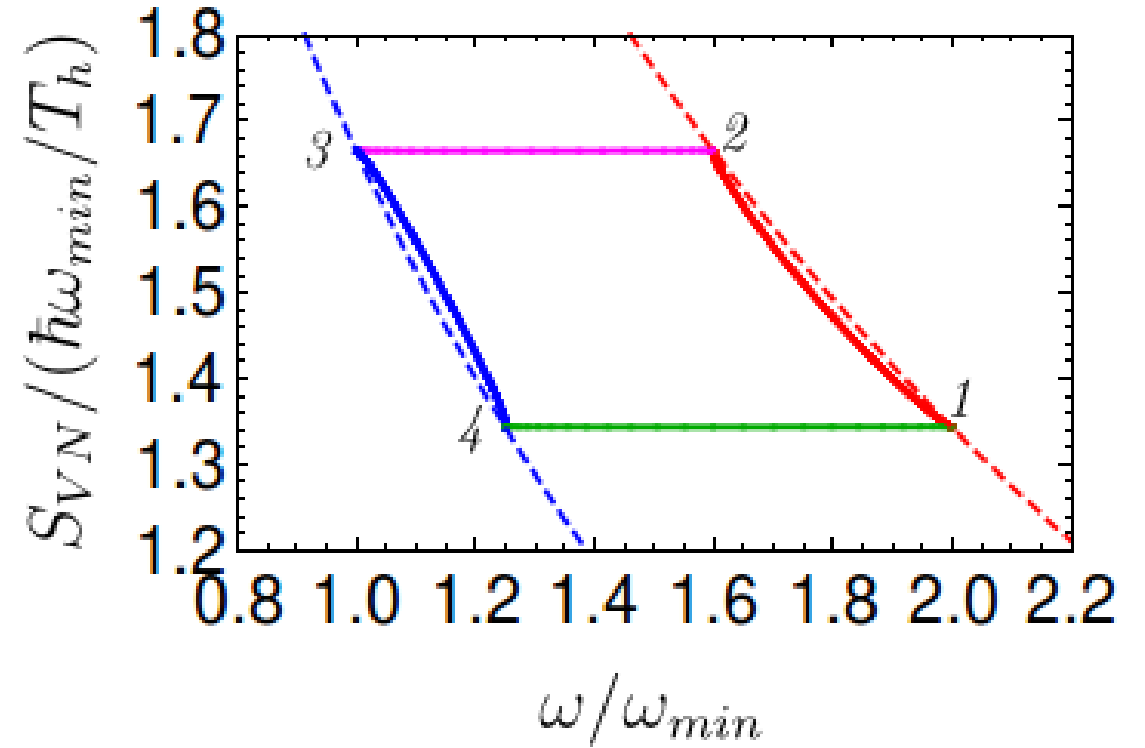
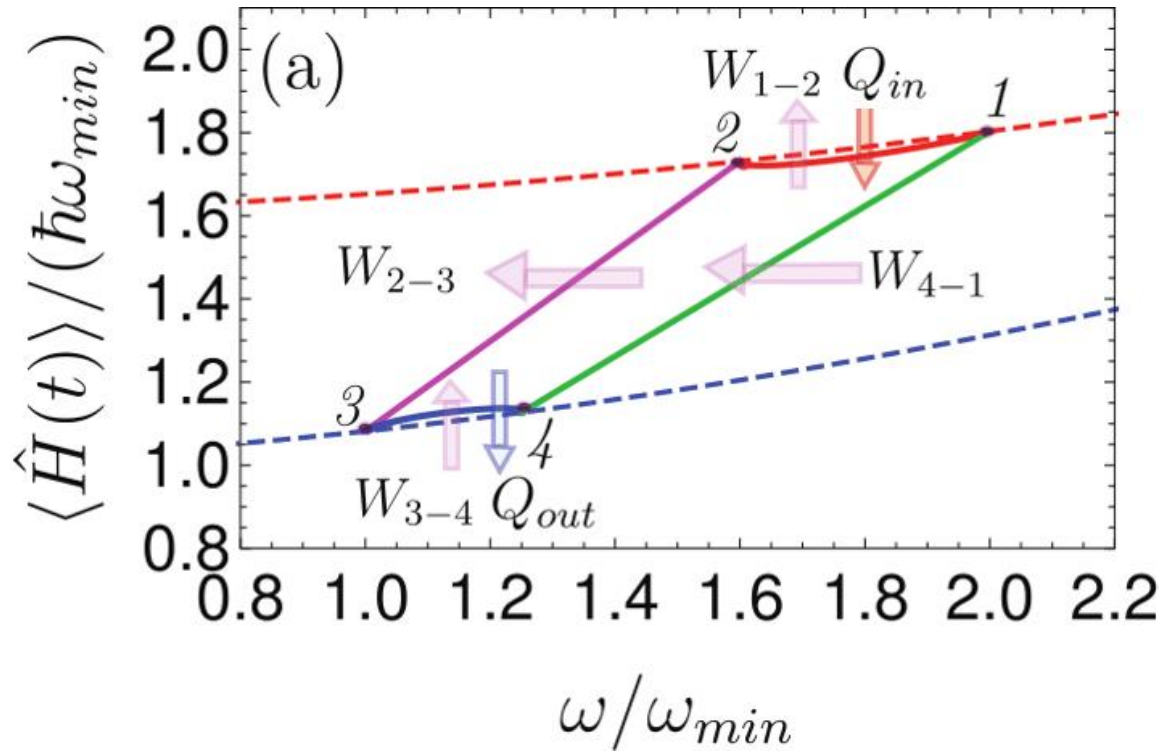
Ronnie Kosloff<sup>1</sup>

<sup>1</sup> Institute of Chemistry Hebrew University Jerusalem, Israel  
The Fritz Haber Center for Molecular Dynamics

<sup>2</sup> Department of Physical Chemistry, University of Basque Country, Bilbao, Spain

# Motivation – Quantum Carnot cycle

**Work and Heat simultaneously**



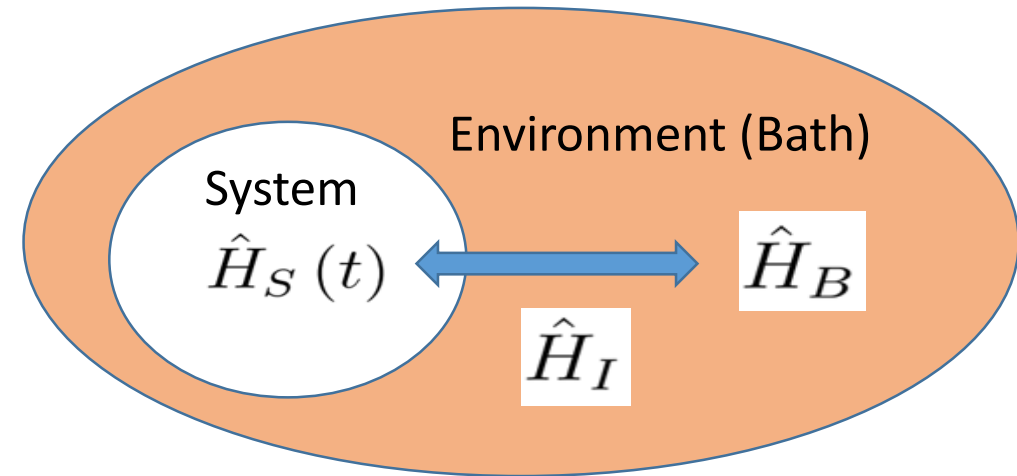
Open dynamics including **non-adiabatic driving**

# Motivation – Quantum Carnot cycle

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_I$$

Open dynamics with **non-adiabatic driving**

Complete description including both **coherence** and **energy**



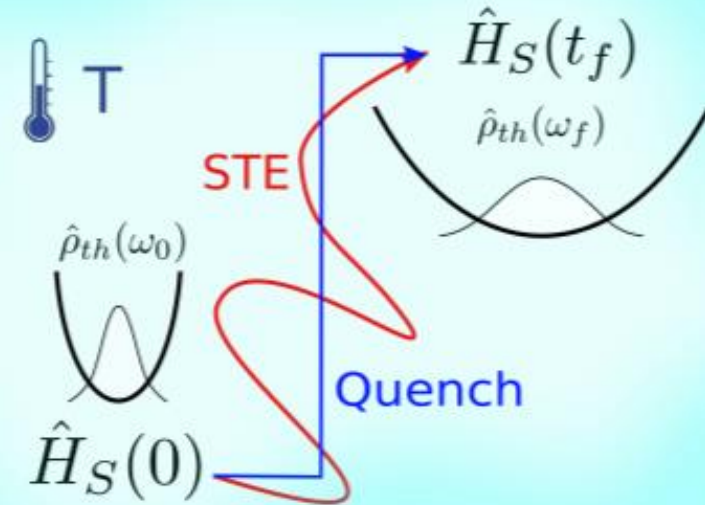
# Motivation II – Increase the **power** output of a Carnot-analog cycle

➔ **Shortcut  
to  
equilibration**

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_I$$

Open system control problem:

How to control a state to state transformation  
in an open system?



Entropy change

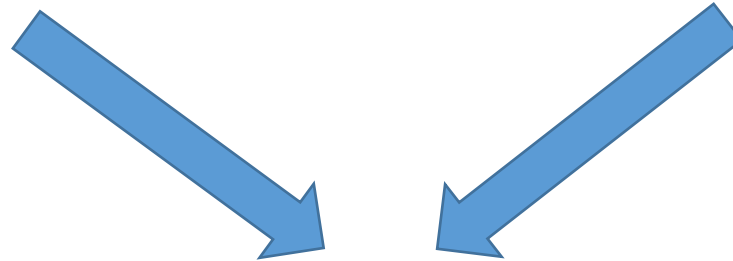
# How can we obtain the Master equation?

Analytic tools:

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_I$$

Non-Adiabatic Master Equation (NAME)

Inertial theorem



Non-adiabatic open system dynamics

Time-dependent Markovian Master Eq., R. Dann, A. Levy, and R. Kosloff, *Phys. Rev. A* 98, 052129 (2018).  
The Inertial Theorem, R. Dann and R. Kosloff, *arXiv:1810.12094* (2018).

# NAME – Time dependent non-adiabatic process

Separation of timescales between system and bath allows reduced system dynamics

$$\frac{d}{dt}\hat{\rho}_S = \mathcal{L}_S(t)\hat{\rho}_S$$

$$\frac{d}{dt}\hat{\rho}_S(t) = \sum_k c_k(t) \left( \hat{L}_k(t) \hat{\rho}_S(t) \hat{L}_k^\dagger(t) + \frac{1}{2} \{ \hat{L}_k^\dagger(t) \hat{L}_k(t), \hat{\rho}_S(t) \} \right)$$

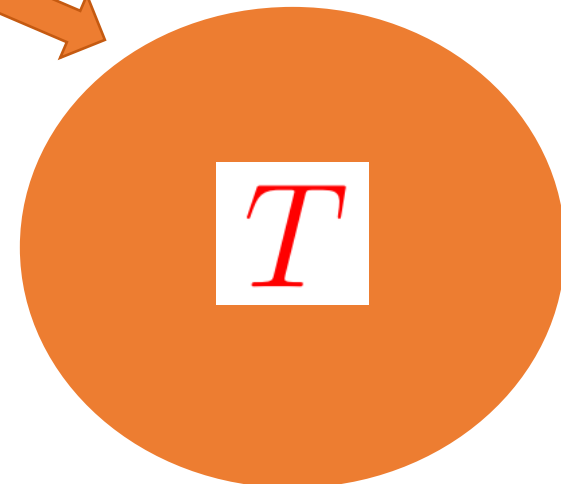
Lindblad Jump Operators:  $\hat{L}_k(t)$

Where  $\mathcal{L}_S$  depends on the bath implicitly.

Not necessarily periodic!

$$\hat{H}_S(0)$$

$$\hat{H}_S(t_f)$$



# Non Adiabatic Master Equation (NAME)

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_I$$

$$\hat{H}_I = \sum_k g_k \hat{A}_k \otimes \hat{B}_k$$

- Following Davies's derivation, the first step is a transformation to the Interaction picture:

$$\tilde{A}_k(t) = \hat{U}_S^\dagger(t) \hat{A}_k \hat{U}_S(t) \quad \tilde{B}_k(t) = e^{i\hat{H}_B t} \hat{B}_k e^{-i\hat{H}_B t}$$

Where the system evolution operator is given by,

$$i \frac{\partial \hat{U}_S(t)}{\partial t} = \hat{H}_S(t) \hat{U}_S(t) \quad \hat{U}_S(0) = I \quad \hbar = 1$$

# How do we find the jump operators ?

## Liouville space representation:

Operator Hilbert space with an inner product:  $(\hat{X}_i, \hat{X}_j) \equiv \text{tr}(\hat{X}_i^\dagger \hat{X}_j)$

**Time-dependent Hamiltonian:**  $\hat{H}_S(t)$

$$\mathcal{U}_S(t) = \mathcal{T} e^{i \int_0^t ([\hat{H}_S(t'), \cdot] + \frac{\partial}{\partial t'}) dt'}$$

$$\mathcal{U}_S(t) \hat{F}_j(0) = \lambda(t) \hat{F}_j(0)$$

## Wave-function representation:

$$\tilde{F}_j(t) = \hat{U}^\dagger(t) \hat{F}_j(0) \hat{U}_S(t) = \lambda_j(t) \hat{F}_j(0)$$

**Stationary Hamiltonian:**  $\hat{H}_S = \sum_i \epsilon_i |i\rangle \langle i|$

$$\mathcal{U}_S(t) = e^{i[\hat{H}_S, \cdot]t}$$

$$\mathcal{U}_S(t) |n\rangle \langle m| = e^{i(\epsilon_n - \epsilon_m)t} |n\rangle \langle m|$$

**Excitations**

  $\{\hat{F}_j\}$  **Eigenoperators**



# Derivation of the NAME

Transformation to the Interaction picture:  $\tilde{\rho}(t) = \hat{U}_B^\dagger \hat{U}_S^\dagger(t) \hat{\rho}(t) \hat{U}_S(t) \hat{U}_B$

$$\longrightarrow \frac{d}{dt} \tilde{\rho}(t) = -i \left[ \tilde{H}_I(t), \tilde{\rho}(t) \right]$$

If  $\hat{H}_I = \sum_k g_k \hat{A}_k \otimes \hat{B}_k$  then we can expand in  $\hat{A}_k$

the **eigeneoperator** basis  $\{\hat{F}_j\} \longrightarrow \tilde{A}_k(t) = \sum_j \xi_j^k(t) e^{i\theta_j(t)} \hat{F}_j$

Interaction  
representation

$$\longrightarrow \tilde{H}_I(t) = \sum_j \xi_j^k(t) e^{i\theta_j(t)} \hat{F}_j \otimes \tilde{B}_k$$

$$\hat{F}_j \equiv \hat{F}_j(0)$$

$\hat{F}_j$

become the jump operators

**Time independent!**

# Non Adiabatic Master Equation (NAME)

$$\tau_S = \left( \frac{1}{\omega_i(t)} \right) \quad \tau_B \sim \frac{1}{\Delta\nu} \quad \tau_R \propto (g^2)^{-1} \quad \tau_d$$

1. Weak coupling
2. Born- Markov approximation
3. Fast bath dynamics relative to the external driving

$$\tilde{\rho}(t) = \tilde{\rho}_S(t) \otimes \tilde{\rho}_B$$

$$1. \tau_B \ll \tau_R \quad 2. \tau_B \ll \tau_S \quad 3. \tau_B \ll \tau_d$$

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}_S(t) = & -i \left[ \tilde{H}_{LS}(t), \tilde{\rho}_S(t) \right] \\ & + \sum_{k,j} \left( \xi_j^k(t) \right)^2 g_k^2 \gamma_{kk} \left( \alpha_j^k(t) \right) \left( \hat{F}_j \tilde{\rho}_S(t) \hat{F}_j^\dagger - \frac{1}{2} \{ \hat{F}_j^\dagger \hat{F}_j, \tilde{\rho}_S(t) \} \right) \end{aligned}$$

$$\hat{F}_j \equiv \hat{F}_j(0)$$

**Lamb-shift**  $\tilde{H}_{LS}(t) = \sum_{k,j} \hbar S_{kk} \left( \alpha_j^k(t) \right) \hat{F}_j^\dagger \hat{F}_j$

# How to solve the free dynamics with driving ?

## Inertial Theorem



The **inertial theorem** approximates the evolution of a quantum system, driven by an external field. The theorem is valid for fast driving provided the acceleration rate is small.

**Liouville space representation:** Elements  $\{\hat{X}\}$  with inner product  $(\hat{X}_i, \hat{X}_j) \equiv \text{tr}(\hat{X}_i^\dagger \hat{X}_j)$

Operator basis:  $\vec{v}(t) = \{\hat{X}_1(t), \dots, \hat{X}_N(t)\}$

$$\frac{d}{dt} \vec{v}(t) = \left( i [\hat{H}_S(t), \bullet] + \frac{\partial}{\partial t} \right) \vec{v}(t) \xrightarrow{\text{Closed Algebra}} \frac{d}{dt} \vec{v}(t) = -i \mathcal{M}(t) \vec{v}(t)$$

For the appropriate driving protocol and operator basis,  
we can **factorize the generator**

$$\mathcal{M}(t) = \Omega(t) \mathcal{B}(\vec{\chi})$$

$$\vec{\chi} = \{\chi_1, \dots, \chi_r\}$$

The Inertial Theorem, R. Dann and R. Kosloff, *arXiv:1810.12094* (2018).

# Inertial Theorem: For slowly varying $\vec{\chi}$ :

Inertial  
solution

Geometric  
phase

$$\vec{v}(\chi, \theta) = \sum_k c_k e^{-i \int_{\theta_0}^{\theta} d\theta' \lambda_k} e^{i \phi_k} \vec{F}_k(\vec{\chi}(\theta))$$

$$\phi_k(\theta) = i \int_{\vec{\chi}(\theta_0)}^{\vec{\chi}(\theta)} d\vec{\chi} \left( \vec{G}_k | \nabla_{\vec{\chi}} \vec{F}_k \right)$$

$$\mathcal{M}(t) = \Omega(t) \mathcal{B}(\vec{\chi})$$

$$\theta(t) = \int_0^t \Omega(t') dt'$$

$\vec{G}_k$  - bi-orthogonal partners of  $\vec{F}_k$

Inertial condition

$$\Upsilon \ll 1$$

Inertial parameter

$$\Upsilon = \max_{\vec{\chi}} \left[ \frac{\left( \vec{G}_k, \nabla_{\vec{\chi}} \mathcal{B} \vec{F}_n \right)}{(\lambda_n - \lambda_k)^2} \left( \frac{d\vec{\chi}}{d\theta} \right)^2 \right] \ll 1$$

The Inertial Theorem, R. Dann and R. Kosloff, *arXiv:1810.12094* (2018).

Experimental Verification of the Inertial Theorem, C.K.Hu, R.Dann, *et al.* , *arXiv:1903.00404*

# Explicit example – quantum Harmonic oscillator

$$\hat{H}_S = \frac{\hat{P}^2}{2m} + \frac{1}{2}m\omega^2(t) \hat{Q}^2$$

Liouville time-dependent operator basis

$$\vec{v}(t) = \{\hat{H}_S, \hat{L}, \hat{C}, \hat{K}, \hat{J}, \hat{I}\}^T$$

$$\hat{L} = \frac{\hat{P}^2}{2m} - \frac{1}{2}m\omega^2(t) \hat{Q}^2 \quad \hat{C} = \frac{\omega(t)}{2} (\hat{P}\hat{Q} + \hat{Q}\hat{P})$$

$$\hat{K} = \sqrt{\omega(t)} \hat{Q} \quad \hat{J} = \frac{\hat{P}}{m\sqrt{\omega(t)}}$$

Closed Algebra

Heisenberg equation

$$\frac{d\vec{v}(t)}{dt} = \mathcal{M}(t) \vec{v}(t) = -i\omega(t) \mathcal{B} \vec{v}(t)$$

**Protocol:**  $\omega(t) = \frac{\omega(0)}{1 - \mu\omega(0)t}$

$$\vec{\chi} = \mu = \frac{\dot{\omega}}{\omega^2}$$

$$\mathcal{B} = i \begin{bmatrix} \mu & -\mu & 0 & 0 & 0 & 0 \\ -\mu & \mu & -2 & 0 & 0 & 0 \\ 0 & 2 & \mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\mu}{2} & 1 & 0 \\ 0 & 0 & 0 & -1 & -\frac{\mu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

# Inertial solution – quantum Harmonic oscillator

$$\frac{d\vec{v}(t)}{dt} = -i\omega(t) \mathcal{B}(\mu) \vec{v}(t)$$

**Inertial solution**

$$\vec{v}(t) = \sum_k c_k e^{-i \int_{\theta(0)}^{\theta(t)} d\theta' \lambda_k} e^{i\phi_k} \vec{b}_k(\mu(t))$$

**Geometric phase**

$$\phi_k(\theta(t)) = i \int_{\mu(\theta(0))}^{\mu(\theta(t))} d\mu \left( \vec{g}_k | \nabla_{\mu} \vec{b}_k \right)$$

$$\hat{U}_S(t)$$

**Eigenvectors of  $\mathcal{B}(\mu)$  = Eigen operators  $\hat{b}_k$**

**Inertial condition**

$$\Upsilon \sim \frac{1}{(2\kappa)^2 \omega(t)} \frac{d\mu}{dt} \ll 1$$

$$\kappa = \sqrt{4 - \mu^2} \quad \theta(t) = \int_0^t \omega(t') dt'$$

In comparison, Adiabatic condition for HO:  $\mu \ll 1$

The Inertial Theorem, R. Dann and R. Kosloff, *arXiv:1810.12094* (2018).

# Reduced driven system dynamics – incorporating the NAME and the Inertial Theorem

Transforming variables in the interaction picture:

$$[\tilde{b}, \tilde{b}^\dagger] = 1$$

$$\frac{d}{dt} \tilde{\rho}_S(t) = k_\downarrow(t) \left( \hat{b} \tilde{\rho}_S(t) \hat{b}^\dagger - \frac{1}{2} \{ \hat{b}^\dagger \hat{b}, \tilde{\rho}_S(t) \} \right) + k_\uparrow(t) \left( \hat{b}^\dagger \tilde{\rho}_S(t) \hat{b} - \frac{1}{2} \{ \hat{b} \hat{b}^\dagger, \tilde{\rho}_S(t) \} \right)$$

$$k_\downarrow(t) = k_\uparrow(t) e^{\alpha(t)/k_B T} = \frac{\alpha(t) |\vec{d}|^2}{8\pi\epsilon_0 \hbar c} (1 + N(\alpha(t)))$$

$$\alpha(t) = \sqrt{1 - \frac{1}{4} \left( \frac{\dot{\omega}(t)}{\omega^2(t)} \right)^2} \omega(t)$$

$$\hat{b} \equiv \hat{b}(0) = \sqrt{\frac{m\omega(0)}{2\hbar}} \frac{(\kappa + i\mu)}{\kappa} \left( \hat{Q}(0) + \frac{\mu + i\kappa}{2m\omega(0)} \hat{P}(0) \right)$$

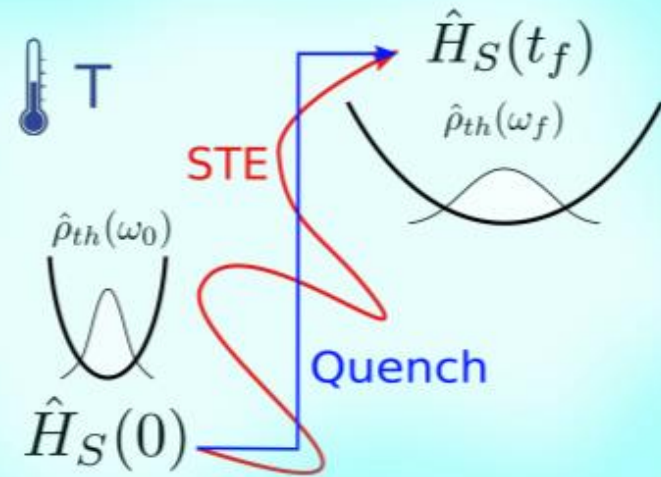
$$\kappa = \sqrt{4 - \mu^2}$$

# Shortcut to Equilibration

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_B + \hat{H}_I$$

$$\hat{\rho}_S^{th}(\omega_0) \longrightarrow \hat{\rho}_S^{th}(\omega_f)$$

**Entropy change**





# Engineering the shortcut to equilibration protocol

Guessing a **solution** of the Generalized Canonical form

$$\tilde{\rho}_S(t) = (Z(t))^{-1} e^{\gamma(t)\tilde{b}^2} e^{\beta(t)\tilde{b}^\dagger\tilde{b}} e^{\gamma^*(t)(\tilde{b}^\dagger)^2}$$

$$\dot{\beta} = k_\downarrow (e^\beta - 1) + k_\uparrow (e^{-\beta} - 1 + 4e^\beta |\gamma|^2)$$

$$\dot{\gamma} = (k_\downarrow + k_\uparrow) \gamma - 2k_\uparrow \gamma e^{-\beta}$$

$$\dot{\beta} = k_\downarrow (\alpha(t)) (e^\beta - 1) + k_\uparrow (\alpha(t)) (e^{-\beta} - 1)$$

For an initial thermal state

$$\beta(0) = -\frac{\hbar\omega(0)}{k_B T} \quad \beta(t_f) = -\frac{\hbar\omega(t_f)}{k_B T}$$

$$\mu(0) = \mu(t_f) = 0$$

$$y = e^\beta$$

$$y(s) = y(0) + c_3 s^3 + c_4 s^4 + c_5 s^5$$

$$s = t/t_f$$

$$\alpha(t) = \sqrt{1 - \frac{1}{4} \left( \frac{\dot{\omega}(t)}{\omega^2(t)} \right)^2} \omega(t)$$

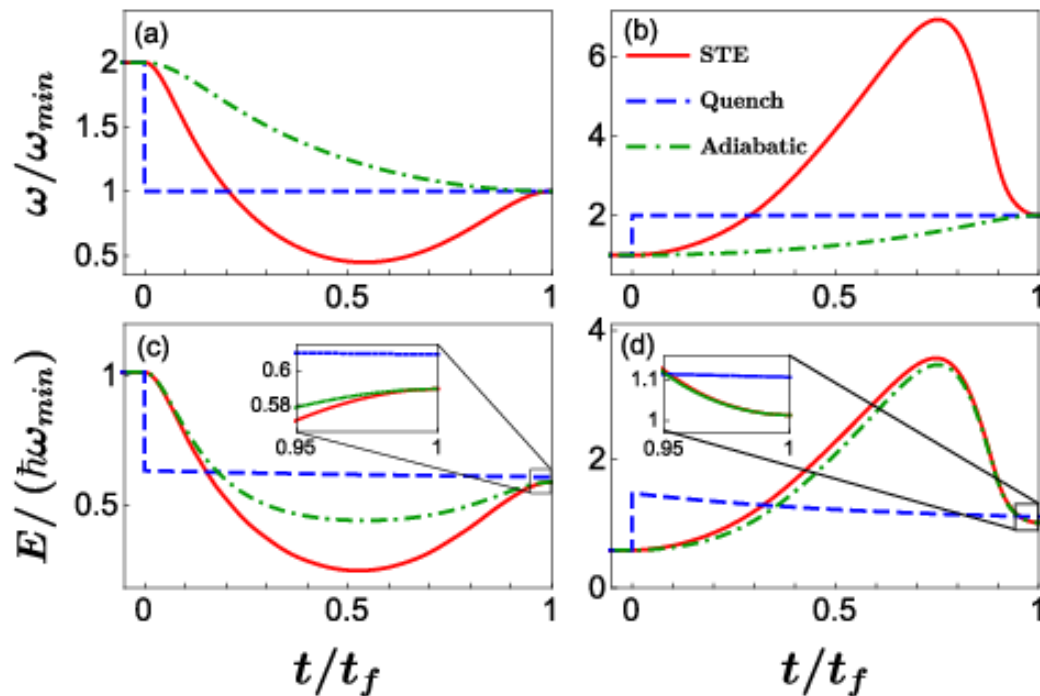
$$\frac{d}{dt} \tilde{\rho}_S(t) \rightarrow \dot{\beta} \rightarrow \beta(t) \rightarrow \alpha(t) \rightarrow \omega(t)$$

$$\hat{H}_S = \frac{\hat{P}^2}{2m} + \frac{1}{2} m \omega^2(t) \hat{Q}^2$$

# STE - Results

Expansion

Compression



STE

Quench

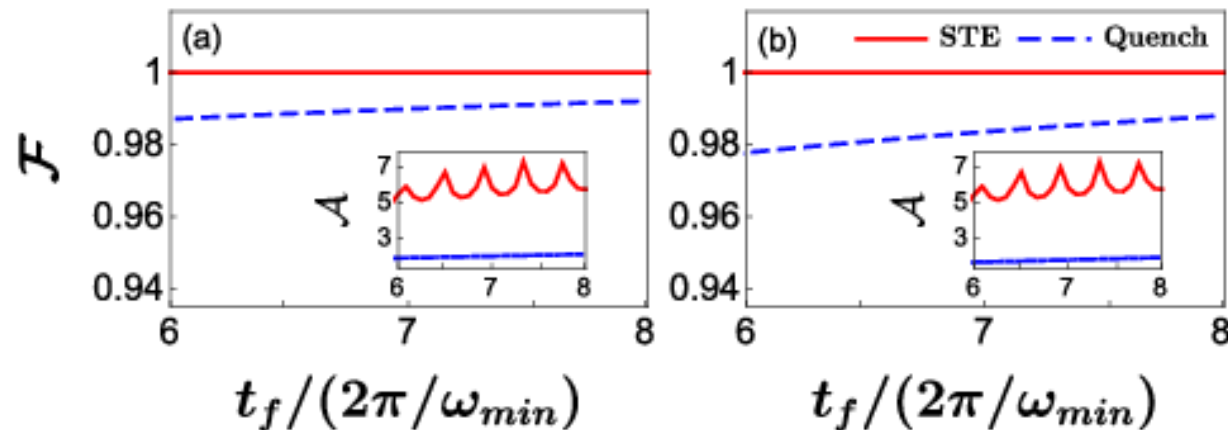
Adiabatic

$$Coh \equiv \omega^{-1} \sqrt{\langle \hat{L} \rangle^2 + \langle \hat{C} \rangle^2}$$

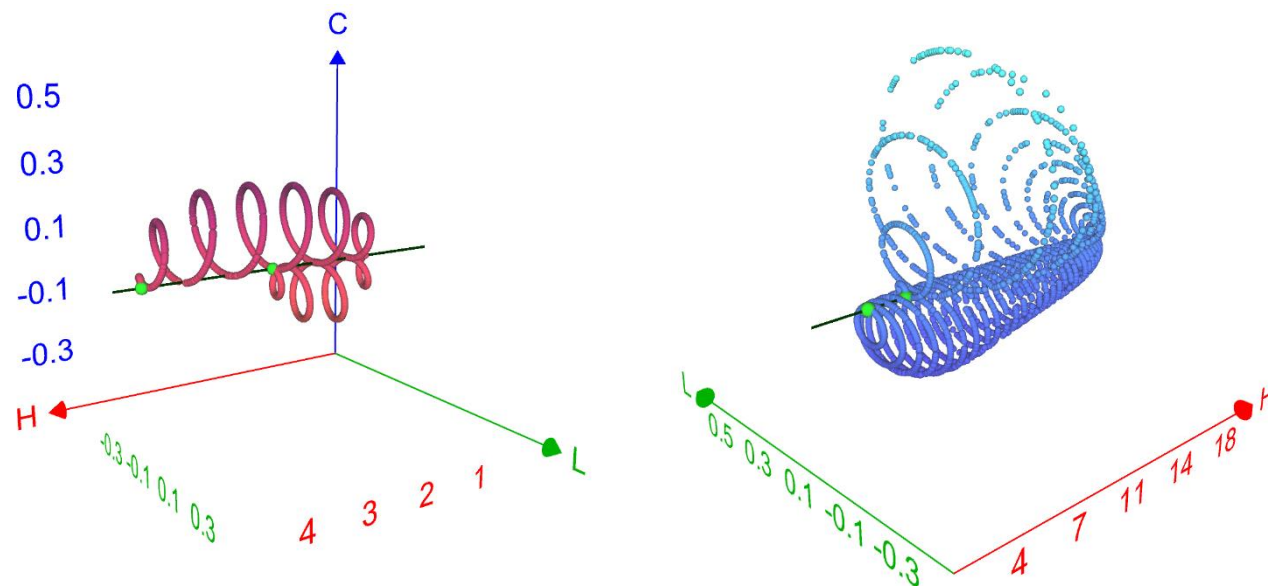
Expansion

Compression

$$\mathcal{A} = -\log_{10}(1 - \mathcal{F})$$



**3 fold improvement in time**



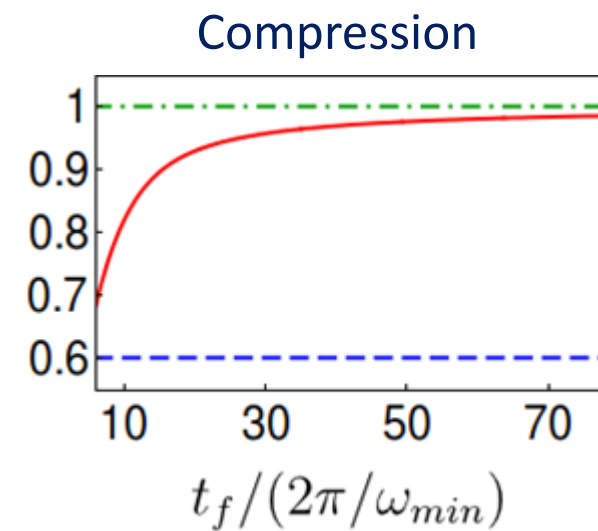
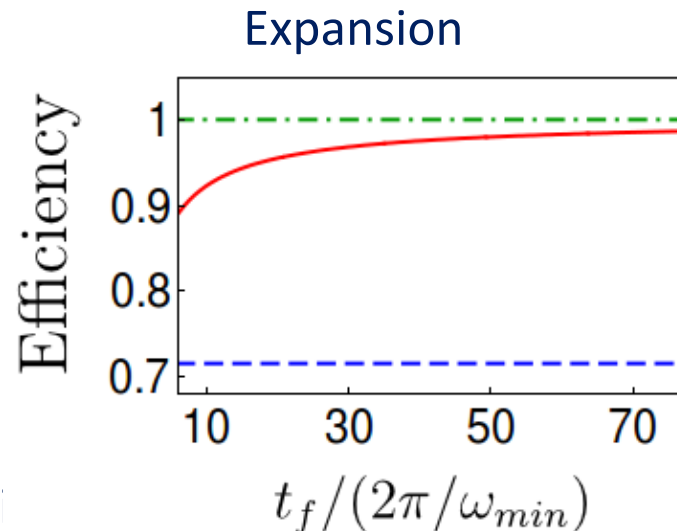
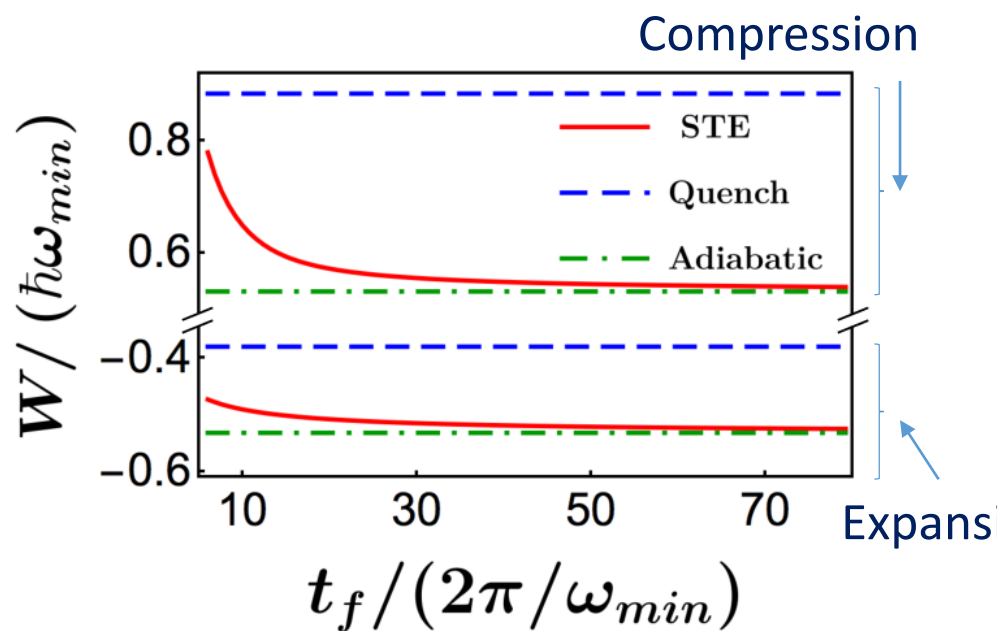
# STE- How much does it cost?

STE

Quench

Adiabatic

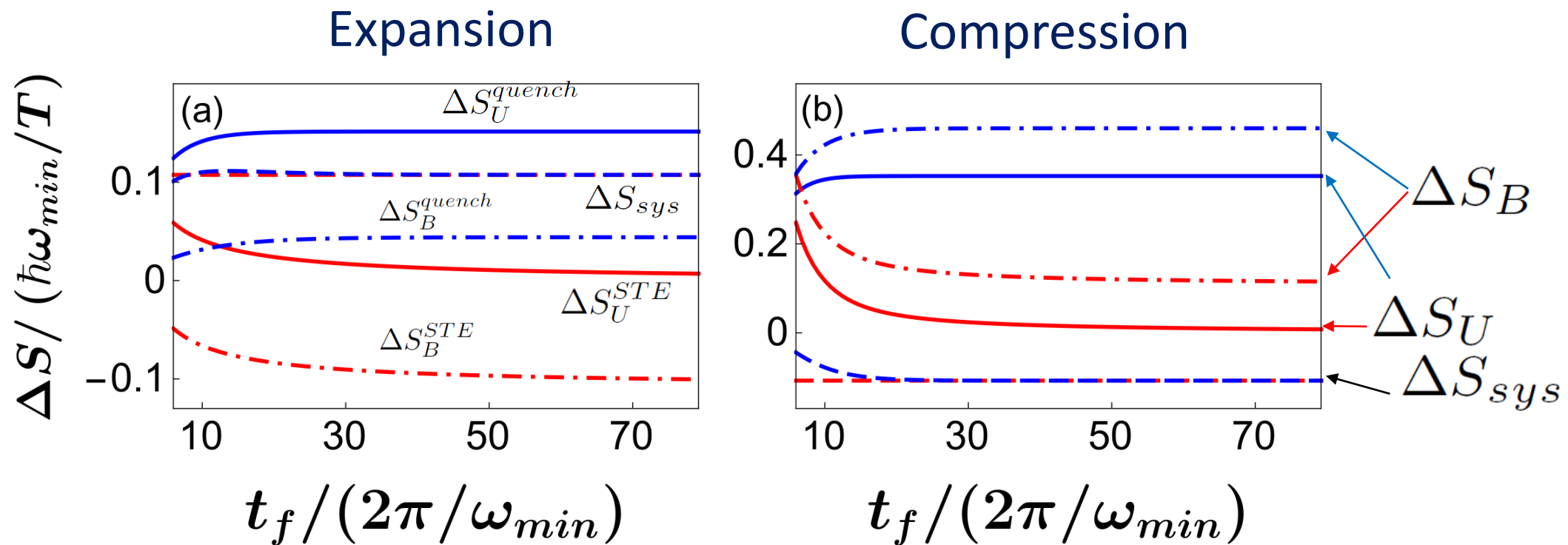
**Rapid driving costs!**



$$W = \int_0^t dt' \operatorname{tr} \left( \frac{\partial \hat{H}(t')}{\partial t'} \hat{\rho}_S(t') \right)$$

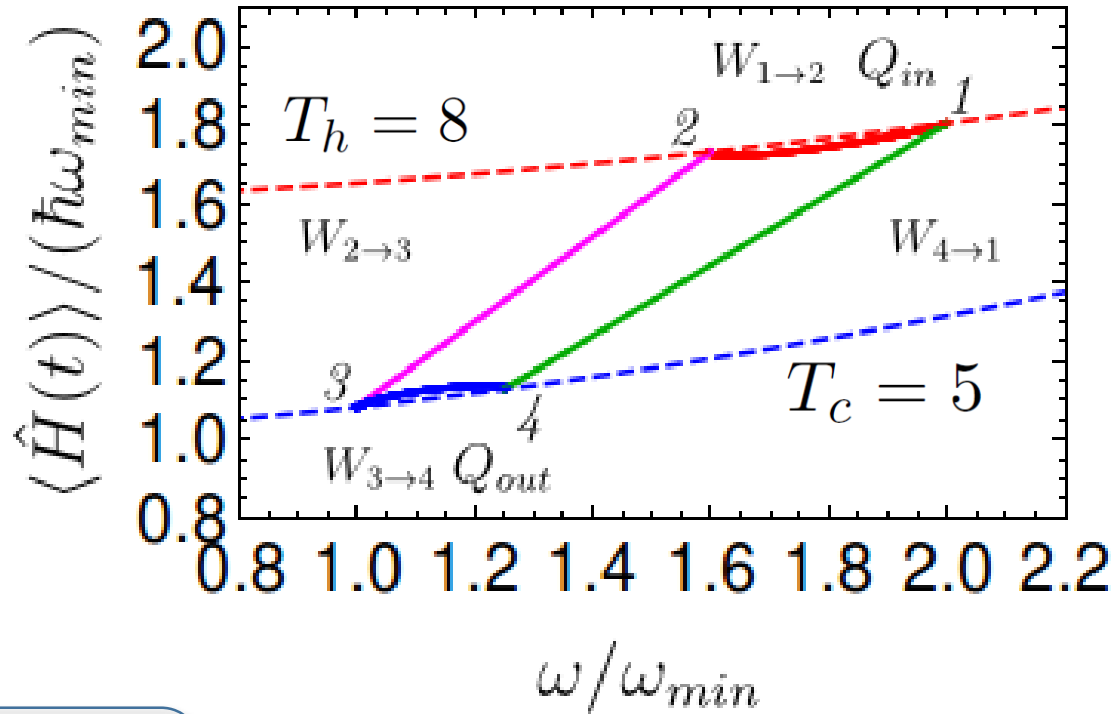
Efficiency:  $\frac{W}{W_{ideal}}$

# STE – Thermodynamic analysis



# Quantum Carnot-analog cycle

$$\tau_{cycle} = 250 / (2\pi / \omega_{min})$$

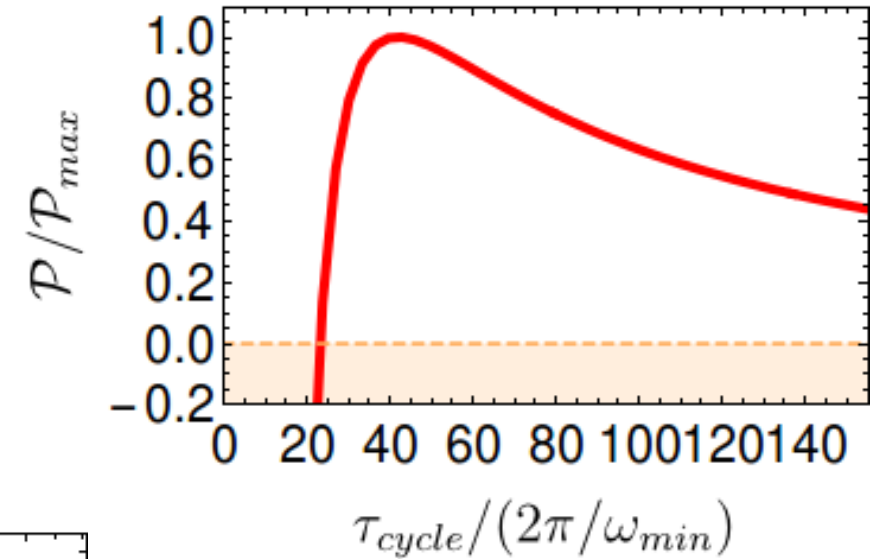
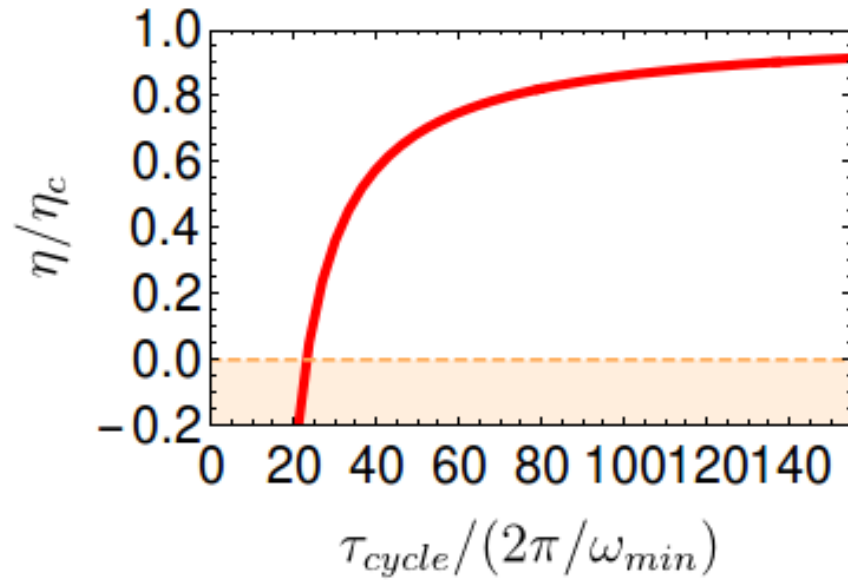


- Open expansion
- Adiabatic expansion
- Open compression
- Adiabatic compression

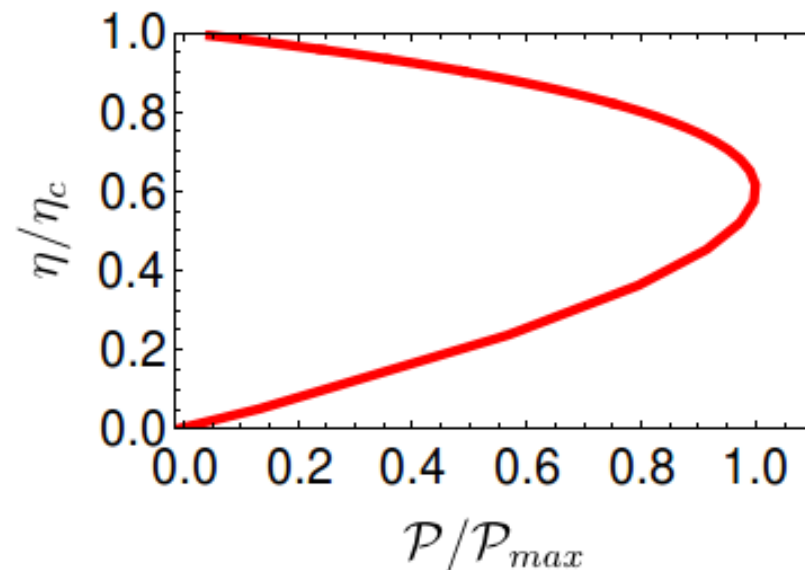
$$\eta_c = 0.375$$

$$\omega_{min} = 5$$

# Quantum Carnot-analog cycle

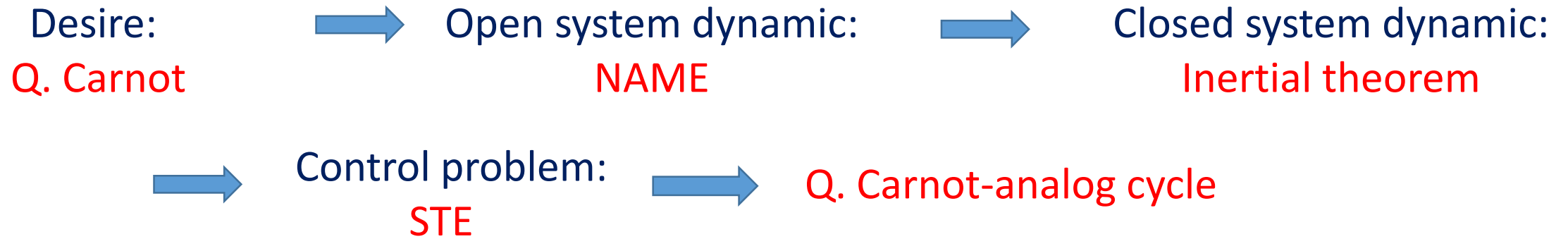


$$\eta_{CA} = 0.56\eta_C$$



**Efficiency vs Power  
tradeoff**

# The Journey we took:



## Shortcut to Equilibration - Study implications

- Quantum Carnot-Analog cycle
- Open quantum system control – rapid change of the system entropy
- Cooling

