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ARC CENTRE OF EXCELLENCE FOR ENGINEERED QUANTUM SYSTEMS

THE UNIVERSITY OF SYDNEY

Beyond the thermodynamic limit

A quantum information approach

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Outline

1. Background and motivation
2. Resource-theoretic framework
3. Overview of some interesting results
    A. Second laws of “quantum” thermodynamics
    B. Transition from macro- to nanoscale
    C. Thermodynamic processing of coherences (in energy basis)
4. Outlook

Background

Standard thermodynamics

- Wide applicability
- Statistical nature
- Thermodynamic limit
- Reversible cycles

Intermediate regime

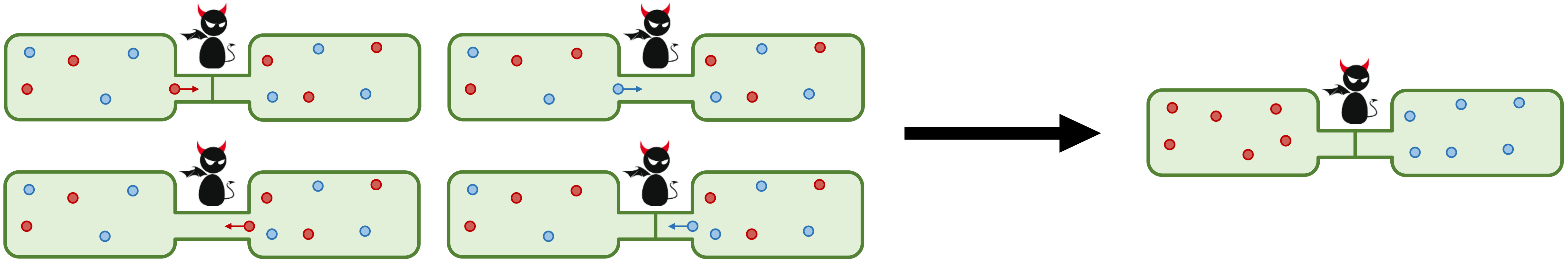
- Mixed nature
- Large but finite number of particles
- Irreversibility?

“Quantum” thermodynamics

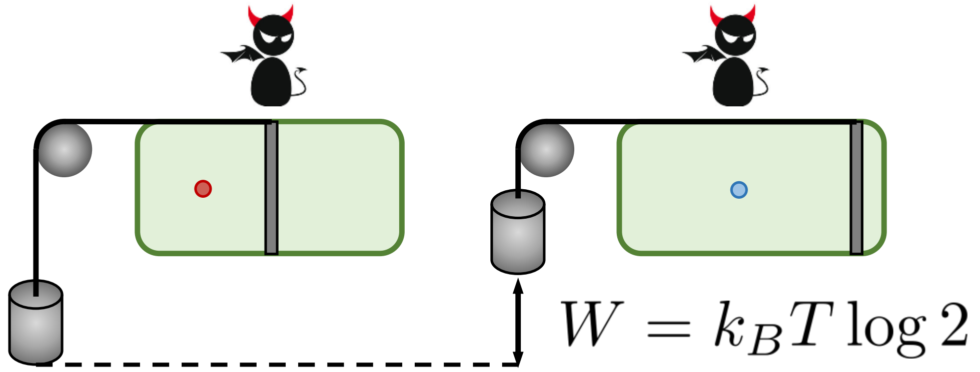
- Quantum regime
- Information-theoretic nature
- Single-shot processes
- Inherent irreversibility

Background

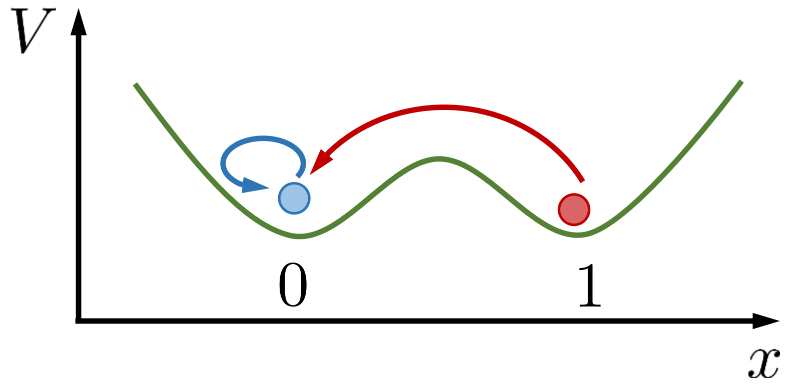
1874 - Maxwell's demon



1929 - Szilard engine



1961 – Landauer erasure



Motivation

Thermodynamic arrow of time for single quantum systems

Transition between macroscopic and nanoscale regime

Thermodynamic processing of coherences (in energy basis)

$$1 \text{ bit} = k_B T \log 2$$
$$1 \text{ qubit} = \ ?$$

Role of catalysis, correlations, entanglement, limitation of nanoscopic heat engines etc...

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Resource theory of thermodynamics

Free thermodynamic transformations modelled by *thermal operations:*

$$\mathcal{E}^{\beta}(\rho) = \mathrm{Tr}_B\left(U\left(\rho \otimes \gamma_B\right)U^{\dagger}\right) = \sigma$$

Thermal bath
at inverse temperature β

$$\begin{aligned} \gamma_B &= e^{-\beta H_B}/\mathcal{Z}_B \\ \mathcal{Z}_B &= \mathrm{Tr}\left(e^{-\beta H_B}\right) \end{aligned}$$

Hamiltonian: H_B

Energy-conserving
interaction U

$$[U, H \otimes \mathbb{1}_B + \mathbb{1} \otimes H_B] = 0$$

System
ρ

Hamiltonian: H

System
σ

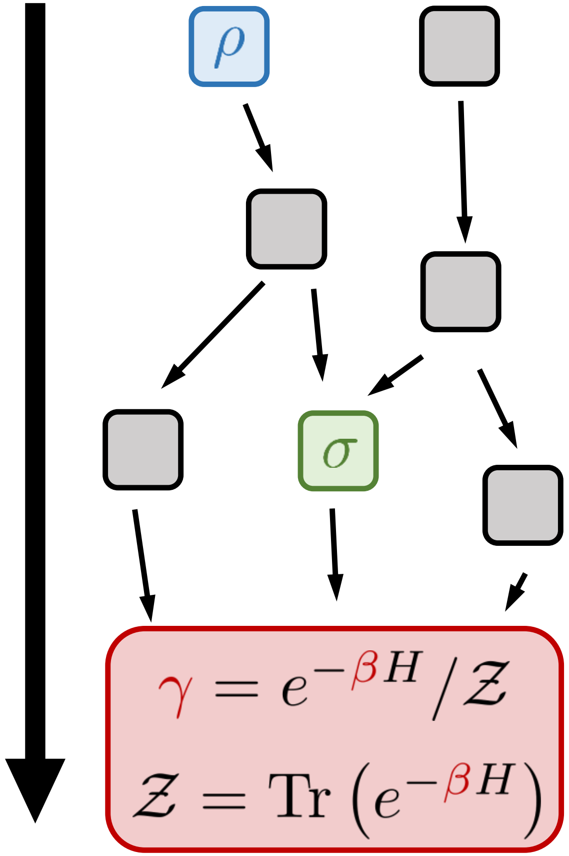
Hamiltonian: H

Resource theory of thermodynamics

General interconversion problem:

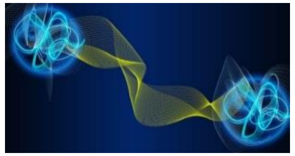
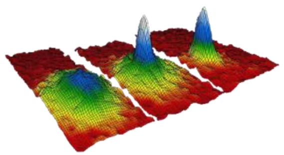
For initial and target states, ρ and σ, does there exist $\mathcal{E}^{\beta}$ such that $\mathcal{E}^{\beta}(\rho) = \sigma$?

Out of equilibrium



Equilibrium

Recently developed resource theories

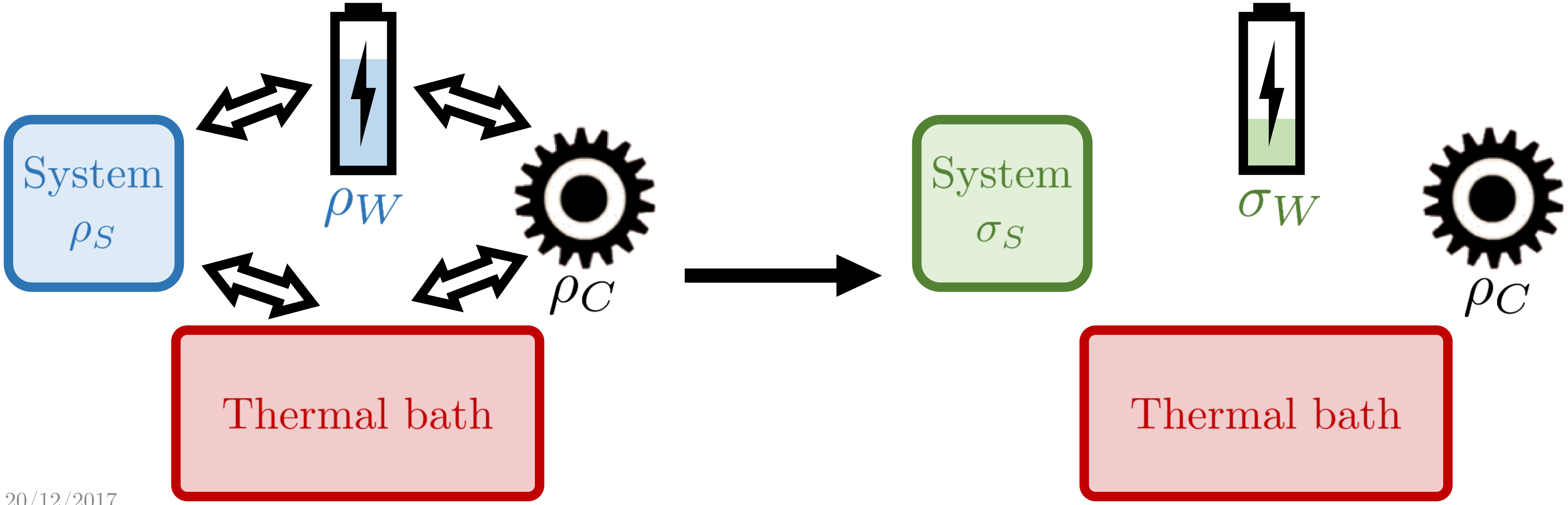




Entanglement	Coherence	Asymmetry
Non-local	Coherent	Asymmetric
↓	↓	↓
Separable	Incoherent	Symmetric

Resource theory of thermodynamics

Physical interpretation of the interconversion problem:

$$\underbrace{\mathcal{E}^{\beta}(\rho}_{\rho_S \otimes \rho_W \otimes \rho_C}) = \underbrace{\sigma}_{\sigma_S \otimes \sigma_W \otimes \rho_C}$$



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Second laws of "quantum" thermodynamics

Focus on initial and target *energy-incoherent* states:

$[\rho, H] = [\sigma, H] = 0 \quad \Longrightarrow \quad$ states represented by: $\boldsymbol{p} = \mathrm{eig}(\rho)$, $\boldsymbol{q} = \mathrm{eig}(\sigma)$, $\boldsymbol{\gamma} = \mathrm{eig}(\gamma)$.

Necessary and sufficient conditions for state interconversion:

$$\forall\, \alpha \in (-\infty, \infty): \quad F_\alpha(\boldsymbol{p}) \geq F_\alpha(\boldsymbol{q})$$

$$F_\alpha(\boldsymbol{p}) := \underbrace{-T \log \mathcal{Z}}_{\text{Free energy of the thermal state}} + \underbrace{T D_\alpha(\boldsymbol{p}||\boldsymbol{\gamma})}_{\text{Non-equilibrium contributions to free energy}}$$

$$D_\alpha(\boldsymbol{p}||\boldsymbol{\gamma}) := \frac{\mathrm{sgn}\alpha}{\alpha-1} \log \left(\sum_i {p_i}^\alpha {\gamma_i}^{1-\alpha}\right)$$

Note: all results with units such that $k_B = 1$.

Second laws of "quantum" thermodynamics

Interpretation of F_α for $\alpha = 1$:

$$F_1(\boldsymbol{p}) = \langle E \rangle_{\boldsymbol{p}} - TH(\boldsymbol{p})$$

Standard free energy

$$F = U - TS$$

Interpretation of inequality for $\alpha = 1$:

$$F_1(\boldsymbol{p}) \geq F_1(\boldsymbol{q})$$

2nd law of thermodynamics

Free energy decreases

Condition for $\alpha = 1$ involves only the average over $\boldsymbol{p}$:

$$\sum_{i=1}^{d} p_i \log \frac{p_i}{\gamma_i}$$

Conditions for $\alpha \neq 1$ involve other moments of $\boldsymbol{p}$:

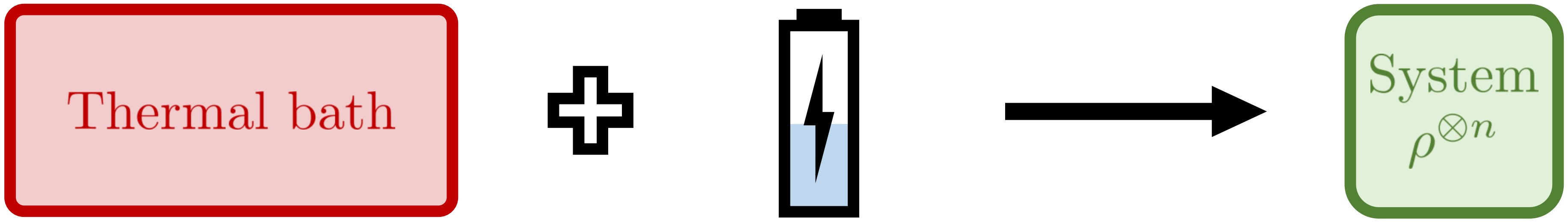
$$\sum_{i=1}^{d} p_i \left(\frac{p_i}{\gamma_i}\right)^{\alpha-1}$$

Asymptotic recovery of single 2nd law:

$$\forall_\alpha : D_\alpha^\epsilon(\boldsymbol{p}^{\otimes n} || \boldsymbol{\gamma}^{\otimes n}) \xrightarrow{n\to\infty} nD_1(\boldsymbol{p}||\boldsymbol{\gamma})$$

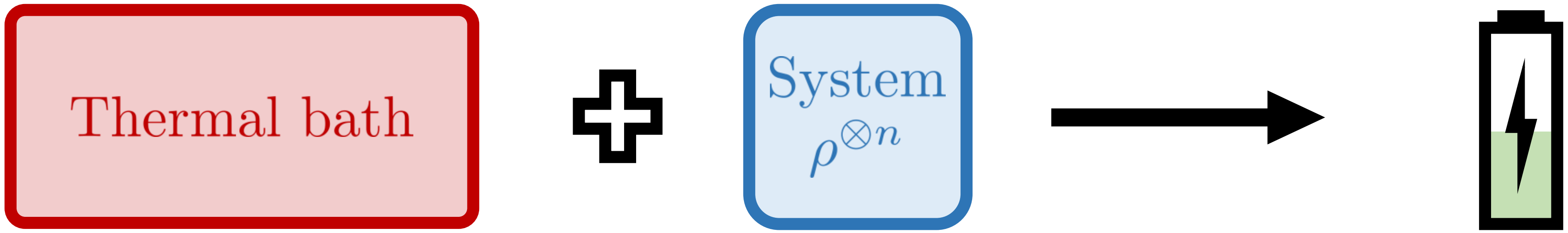
Work of formation and distillable work

Formation process:



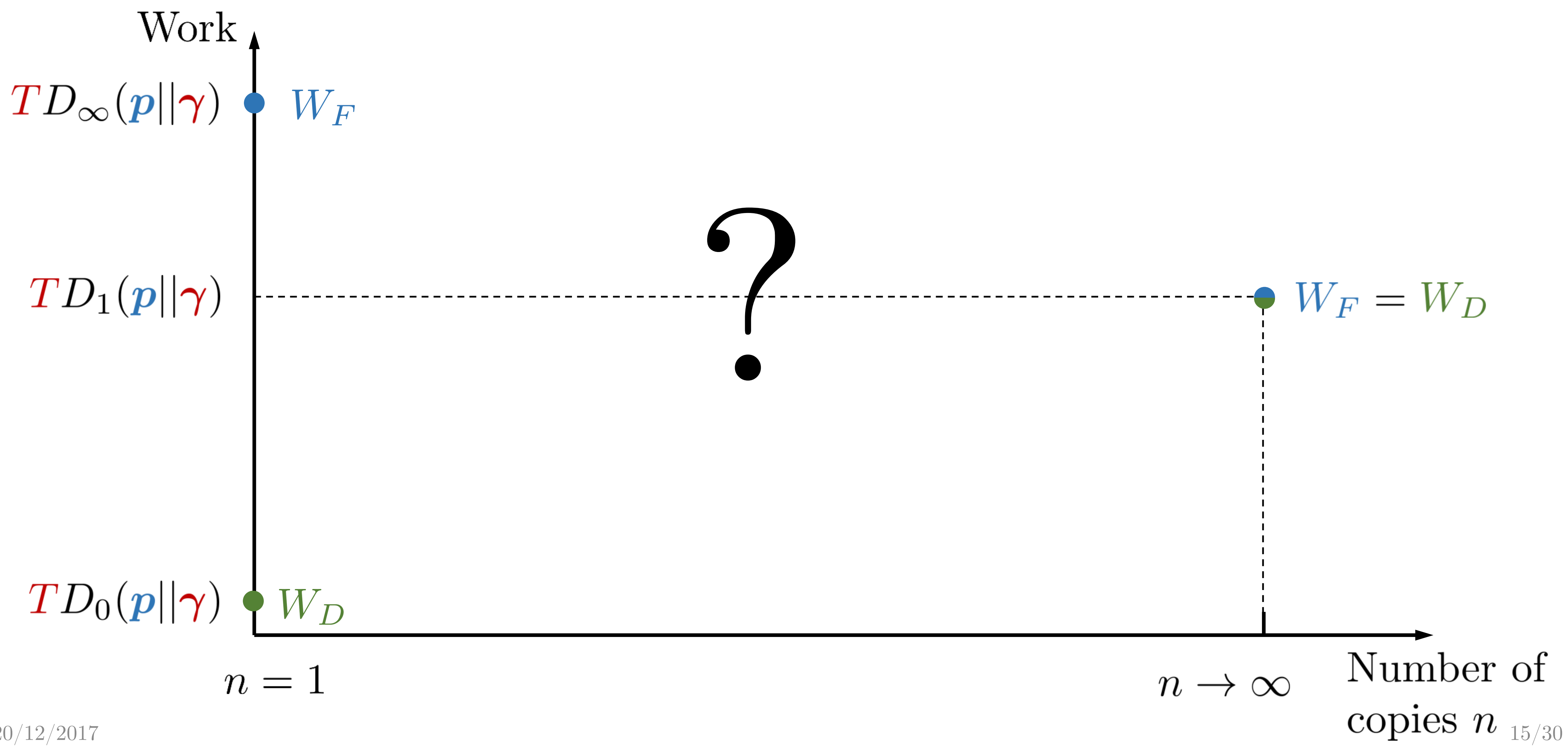
Work of formation: $n \cdot W_F$

Distillation process:



Distillable work: $n \cdot W_D$

Work of formation W_F and distillable work W_D



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Transition from macro- to nanoscale

General interconversion problem:

For initial and target states, ρ and σ, does there exist $\mathcal{E}^{\beta}$ such that $\mathcal{E}^{\beta}(\rho) = \sigma$?

Asymptotic interconversion problem:

For initial and target states, ρ and σ, does there exist $\mathcal{E}^{\beta}$ such that:

$$\mathcal{E}^{\beta}\left(\rho^{\otimes n} \otimes \gamma^{\otimes Rn}\right) \approx_{\epsilon} \sigma^{\otimes Rn} \otimes \gamma^{\otimes n}$$

What is the optimal interconversion rate R^{*} for ρ and σ, and error ϵ?

Error: $\sigma \approx_{\epsilon} \tilde{\sigma}$ means $1 - F(\sigma, \tilde{\sigma}) \leq \epsilon$ with F denoting fidelity.

Restrictions:

Focus on many copies (large but finite n) and *energy-incoherent* states:

$$[\rho, H] = [\sigma, H] = 0 \quad \Longrightarrow \quad \text{states represented by: } \boldsymbol{p} = \mathrm{eig}(\rho), \ \boldsymbol{q} = \mathrm{eig}(\sigma).$$

Transition from macro- to nanoscale

Relative entropy variance with the Gibbs state: $V(\boldsymbol{p}\|\boldsymbol{\gamma}) := \sum_{i=1}^{d} p_i \left(\log \frac{p_i}{\gamma_i} - D_1(\boldsymbol{p}\|\boldsymbol{\gamma})\right)^2$

Thermodynamic interpretation as generalised heat capacity:

If $\boldsymbol{p} = \boldsymbol{\gamma}'$, i.e., initial state is a Gibbs state at temperature T', then

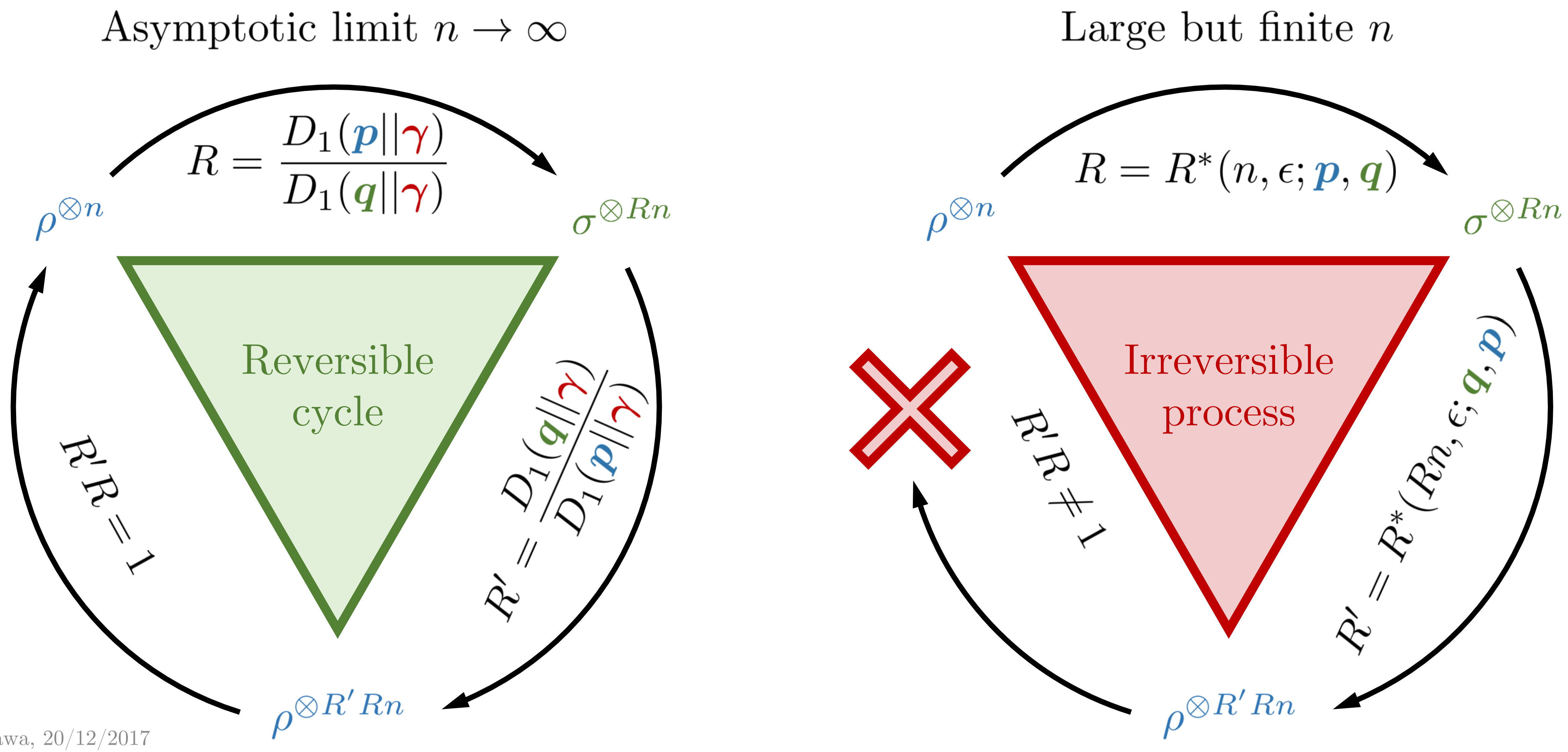
$$V(\boldsymbol{\gamma}'\|\boldsymbol{\gamma}) = \left(1 - \frac{T'}{T}\right)^2 \cdot c_{T'}, \qquad c_{T'} = \frac{\partial \langle E\rangle_{\boldsymbol{\gamma}'}}{\partial T'}$$

Specific heat capacity at temperature T'

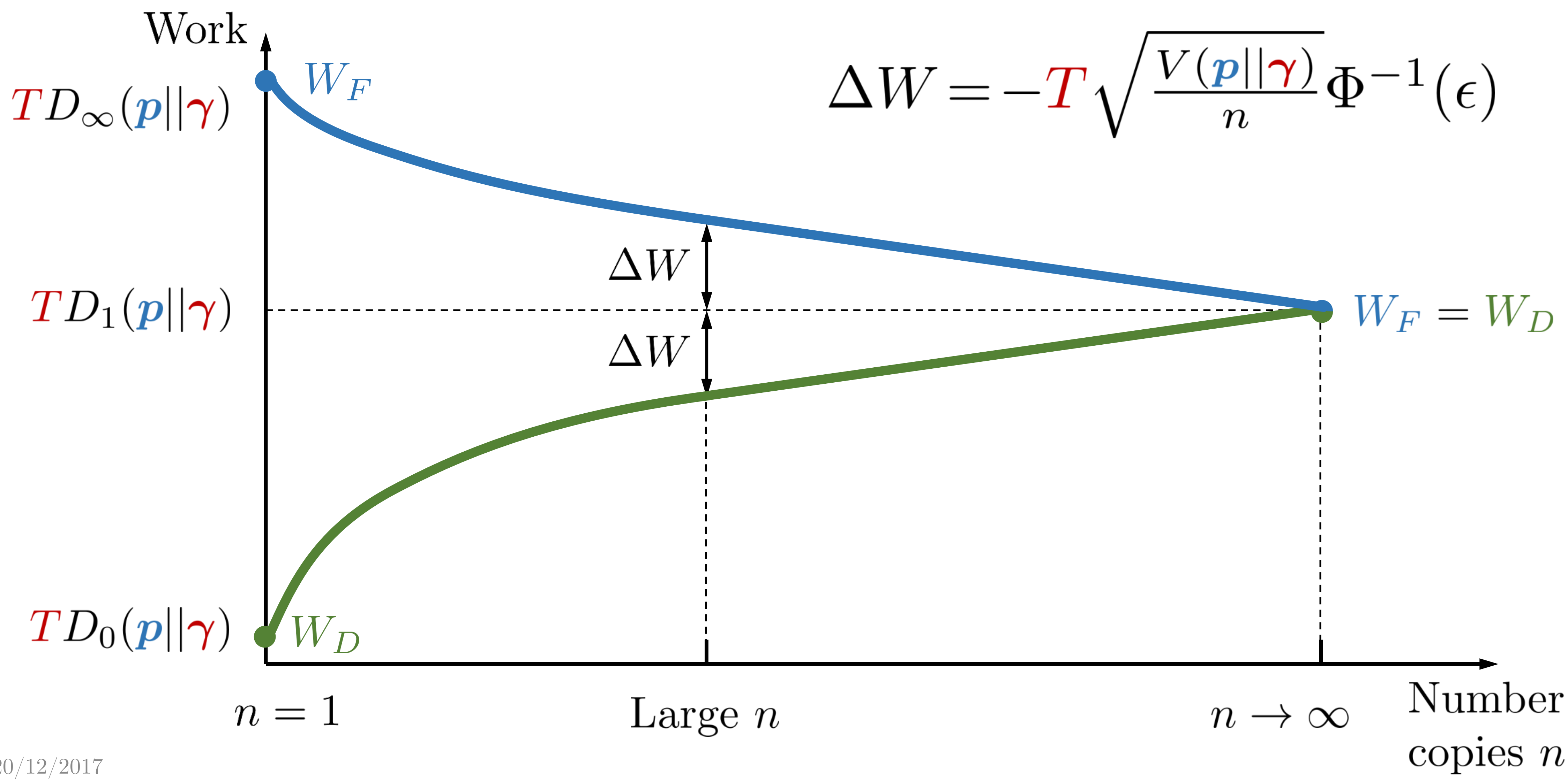
Optimal interconversion rate for $\rho \xrightarrow{\mathcal{E}^{\beta}} \sigma$:

$$R^*(n,\epsilon) \simeq \underbrace{\frac{D_1(\boldsymbol{p}\|\boldsymbol{\gamma})}{D_1(\boldsymbol{q}\|\boldsymbol{\gamma})}}_{\text{Asymptotic rate}} \left(1 + \underbrace{\sqrt{\frac{V(\boldsymbol{p}\|\boldsymbol{\gamma})}{n\, D_1(\boldsymbol{p}\|\boldsymbol{\gamma})^2}}\, Z_{\nu}^{-1}(\epsilon)}_{\text{Second-order correction}}\right)$$

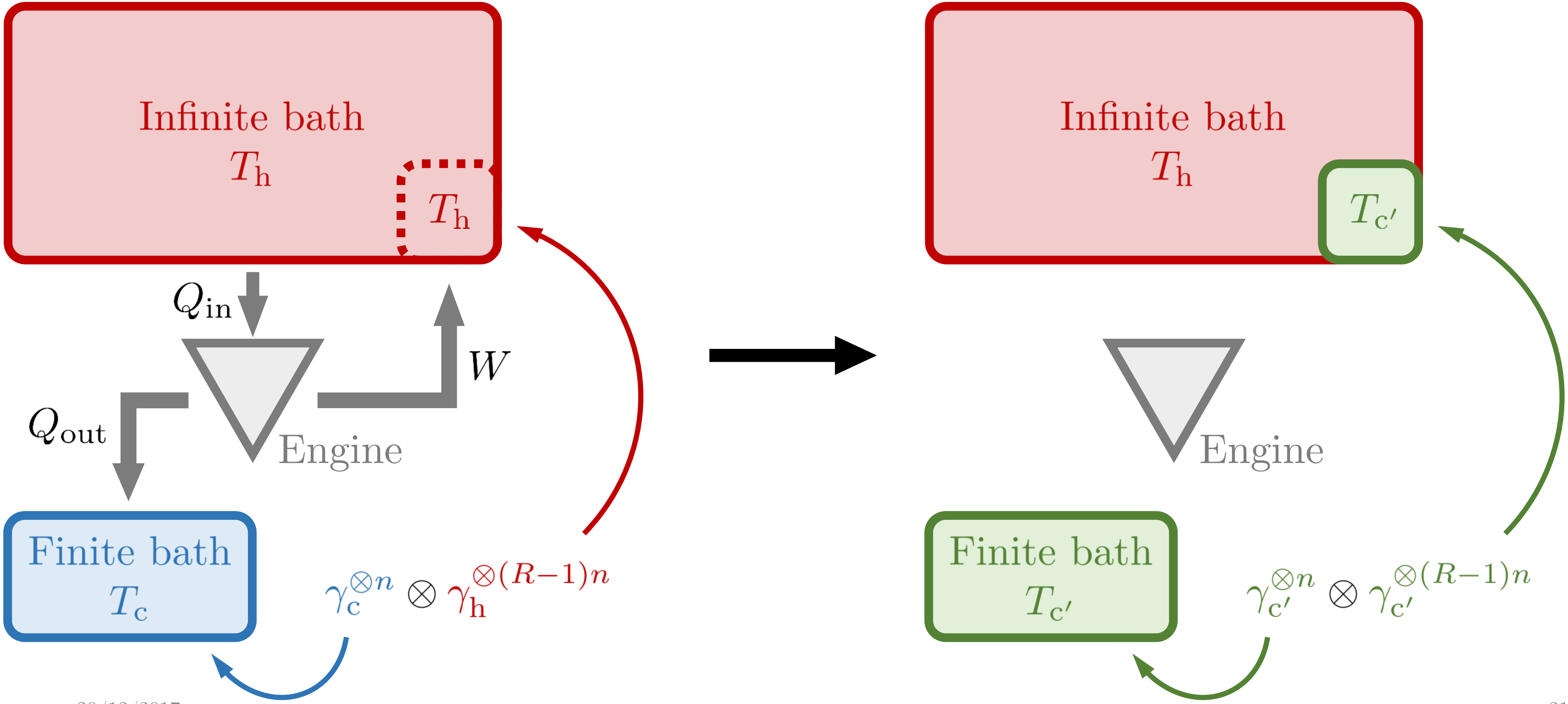
Finite-size irreversibility



Formation-distillation work gap



Heat engines and finite-size baths



Heat engines and finite-size baths

Efficiency of the process heating finite bath from T_{c} to $T_{\mathrm{c}'}$:

$$\eta(T_{\mathrm{c}} \to T_{\mathrm{c}'}) = \underbrace{\eta_C(T_{\mathrm{c}} \to T_{\mathrm{c}'})}_{\substack{\textit{Integrated} \\ \text{Carnot efficiency}}} + \underbrace{f(T_{\mathrm{c}}, T_{\mathrm{c}'}, T_{\mathrm{h}}) \cdot \frac{Z_\nu^{-1}(\epsilon)}{\sqrt{n}}}_{\substack{\text{Second-order correction} \\ \text{positive } (\epsilon > \epsilon_0) \text{ or negative } (\epsilon < \epsilon_0)}}$$

Allowing for imperfect work, one can achieve and even surpass Carnot efficiency.

Perfect work extraction at Carnot efficiency allowed for $\nu = 1$.

$\Rightarrow$ Possibility of engineering finite heat-baths in order to minimise undesirable dissipation of free energy.

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Thermodynamic processing of coherences

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$[\rho, H] \cancel{=} [\sigma, H] \cancel{=} 0 \quad \Longrightarrow \quad$ ~~states represented by: $\boldsymbol{p} = \text{eig}(\rho)$, $\boldsymbol{q} = \text{eig}(\sigma)$, $\boldsymbol{\gamma} = \text{eig}(\gamma)$.~~

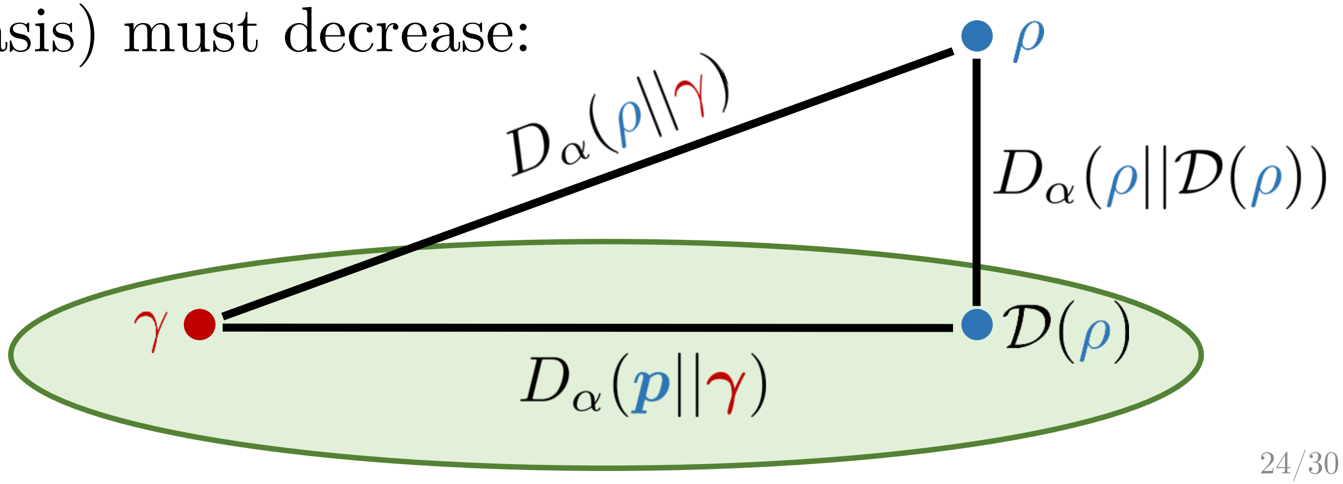
Time-translation covariance:

$$\mathcal{E}^{\beta}(e^{-iHt}\rho e^{iHt}) = e^{-iHt}\mathcal{E}^{\beta}(\rho)e^{iHt}$$

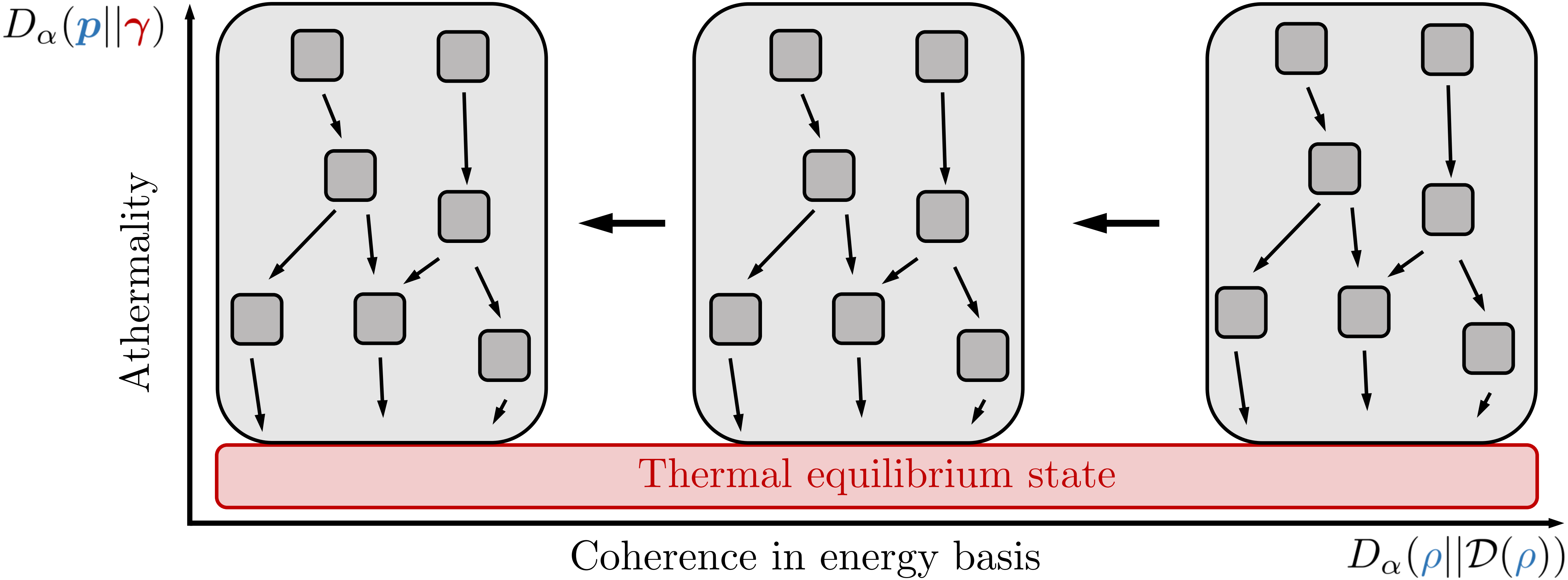
$$\mathcal{E}^{\beta}(\mathcal{D}(\rho)) = \mathcal{D}(\mathcal{E}^{\beta}(\rho)) \quad \text{with decohered state} \quad \mathcal{D}(\rho) = \sum_{i=1}^{d} \langle i|\rho|i\rangle \, |i\rangle\langle i|$$

All measures of coherence (in energy basis) must decrease:

$$\begin{aligned} D_\alpha(\rho||\mathcal{D}(\rho)) &\geq D_\alpha(\mathcal{E}^\beta(\rho)||\mathcal{E}^\beta(\mathcal{D}(\rho))) \\ &= D_\alpha(\mathcal{E}^\beta(\rho)||\mathcal{D}(\mathcal{E}^\beta(\rho))) \\ &= D_\alpha(\sigma||\mathcal{D}(\sigma)) \end{aligned}$$



Thermodynamic processing of coherences



Decreasing of all $D_\alpha(\boldsymbol{p}||\boldsymbol{\gamma})$ – necessary and sufficient for energy-incoherent states.

Decreasing of all $D_\alpha(\rho||\mathcal{D}(\rho))$ – necessary, but not sufficient, for general states.

Mode structure

For a Hamiltonian H and a state ρ,

$$H = \sum_{i=1}^{d} \hbar\omega_i \left|i\right\rangle\!\left\langle i\right| , \qquad \rho = \sum_{i,j=1}^{d} \rho_{ij} \left|i\right\rangle\!\left\langle j\right| .$$

Modes $\rho^{(\omega)}$ are defined by:

$$\rho^{(\omega)} := \sum_{\substack{i,j \\ \omega_i - \omega_j = \omega}} \rho_{ij} \left|i\right\rangle\!\left\langle j\right| = \sum_{i,j}^{(\omega)} \rho_{ij} \left|i\right\rangle\!\left\langle j\right| , \qquad \rho(0) = \sum_{\omega} \rho^{(\omega)}, \qquad \rho(t) = \sum_{\omega} \rho^{(\omega)} e^{-i\hbar\omega t}.$$

Each mode transforms independently and its *intensity* cannot increase:

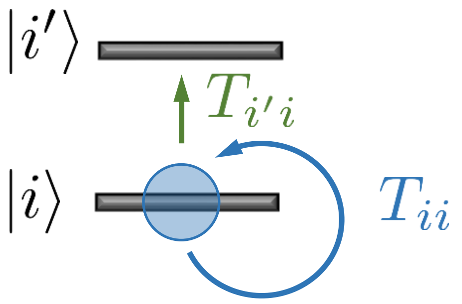
Given $\sigma = \mathcal{E}^{\beta}(\rho)$ we have $\sigma^{(\omega)} = \mathcal{E}^{\beta}(\rho^{(\omega)})$ and $\left\|\sigma^{(\omega)}\right\| \leq \left\|\rho^{(\omega)}\right\|$

Bounds on coherence transformations

Using mode structure one can bound the evolution of coherence in energy basis:

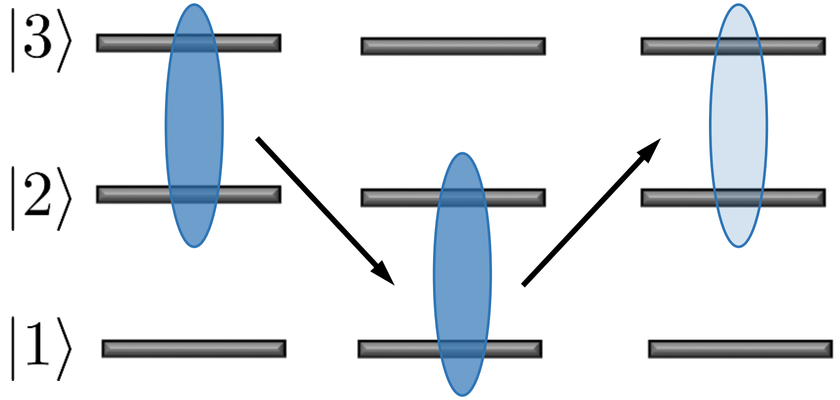
$$|\sigma_{i'j'}| \leq \sum_{i,j}^{(\omega_{i'j'})} \sqrt{T_{i'i}T_{j'j}}|\rho_{ij}|,$$

with transition matrix T:



One of the consequences – irreversibility of coherence transfer:

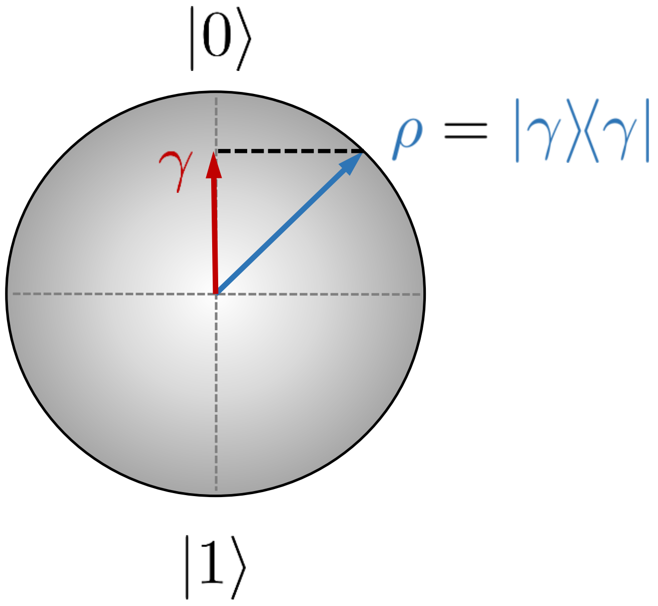
$$|\sigma_{i'j'}| \leq \sum_{i\geq i', j\geq j'}^{(\omega_{i'j'})} |\rho_{ij}| + \sum_{i<i', j<j'}^{(\omega_{i'j'})} |\rho_{ij}| e^{-\beta\hbar(\omega_{i'}-\omega_i)},$$



Work-locking

Non-equilibrium free energy composed of two parts:

$$D_1(\rho||\gamma) = \underbrace{D_1(\boldsymbol{p}||\boldsymbol{\gamma})}_{\text{Athermal part}} + \underbrace{D_1(\rho||\mathcal{D}(\rho))}_{\text{Coherent part}}$$



Coherent part of free energy is locked:

$$\mathcal{E}^{\beta}(\rho \otimes |0\rangle\langle 0|) = \gamma \otimes |w\rangle\langle w| \quad \Longleftrightarrow \quad \mathcal{E}^{\beta}(\mathcal{D}(\rho) \otimes |0\rangle\langle 0|) = \gamma \otimes |w\rangle\langle w|$$

Need to use "coherence catalysis" to unlock work...

Outlook

- Find necessary and sufficient conditions for single-shot transformations of states with coherence in energy basis.
- Study asymptotics for states with coherence in energy basis.
- Study the effects of finite-size baths on Landauer's erasure, fluctuation theorems, the third law of thermodynamics, etc.
- Clarify the notion of imperfect work.
- Investigate conditions for which Carnot efficiency can be achieved with finite-size baths (or with finite-size working body).
- Experimental verification?

Thank you!

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A. Second laws of “quantum” thermodynamics

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