ARC CENTRE OF EXCELLENCE FOR
ENGINEERED QUANTUM SYSTEMS

THE UNIVERSITY OF SYDNEY

Beyond the thermodynamic limit

An information-theoretic perspective

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Outline

1. Background and motivation
2. Thermodynamic setting
3. Main result
4. Discussion and applications
5. Mathematical framework and technical details
6. Outlook

Background and motivation

Standard thermodynamics

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

Our work

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

Quantum thermodynamics

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

Outline

Resource theory of thermodynamics

Free thermodynamic transformations modelled by *thermal operations:*

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

Thermal bath
at inverse temperature β

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

Hamiltonian: H_B

Energy-conserving
interaction U

$[U, H + H_B] = 0$

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 $\mathcal{E}^{\beta}(\rho)=\sigma$?

Studied interconversion problem:

For initial and target states, ρ and σ, does there exist $\mathcal{E}^{\beta}$ such that $\mathcal{E}^{\beta}\left(\rho^{\otimes n}\right)\approx_{\epsilon}\sigma^{\otimes Rn}$?

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

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

Restrictions:

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

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

Relevant information-theoretic notions

Gibbs state γ of the system at inverse temperature β:

$$\gamma = e^{-\beta H}/\mathcal{Z}, \;\; \mathcal{Z} = \mathrm{Tr}\left(e^{-\beta H}\right); \qquad [\gamma, H] = 0 \Rightarrow \text{state represented by } \boldsymbol{\gamma} = \mathrm{eig}(\gamma)$$

Relative entropy with the Gibbs state: $D(\boldsymbol{p}\|\boldsymbol{\gamma}) := \sum_{i=1}^{d} p_i \log \frac{p_i}{\gamma_i}$

Thermodynamic interpretation as generalised free energy:

$$T D(\boldsymbol{p}\|\boldsymbol{\gamma}) = \underbrace{\left(\langle E\rangle_{\boldsymbol{p}} - T H(\boldsymbol{p})\right)}_{\substack{\text{Free energy} \\ F = U - TS}} - \underbrace{\left(-T \log \mathcal{Z}\right)}_{\substack{\text{Free energy of} \\ \text{the thermal state} \\ -T\log\mathcal{Z}}}$$

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

Relevant information-theoretic notions

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

Thermodynamic interpretation as generalised heat capacity:

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

$$V(\boldsymbol{\gamma}'\|\boldsymbol{\gamma}) = \underbrace{\left(1 - \frac{T'}{T}\right)^2}_{\text{Carnot-like factor}} \cdot c_{T'}$$

Specific heat capacity at temperature T'

$$c_{T'} = \frac{\partial \langle E \rangle_{\gamma'}}{\partial T'}$$

Note: $V(\boldsymbol{p}\|\boldsymbol{\gamma}) = 0$ when $\boldsymbol{p}$ is sharp (ρ is an energy eigenstate).

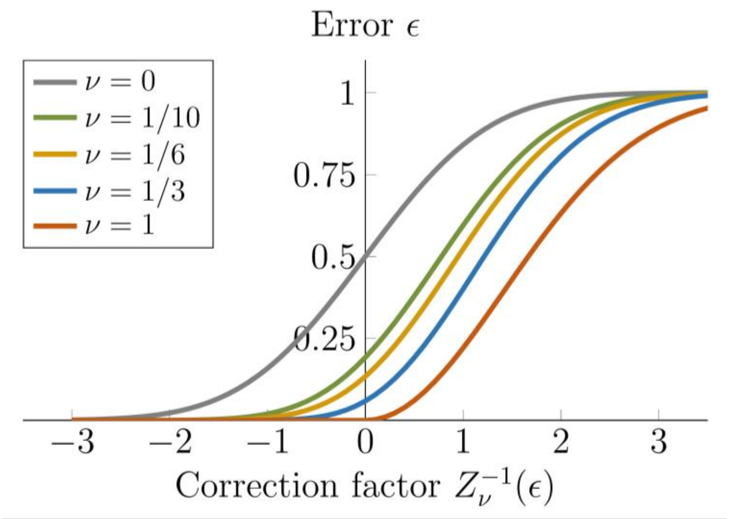
Outline

Main result

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

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

Rayleigh-normal distribution Z_ν:



Z_0 - standard normal distribution Φ

Z_1 - Rayleigh distribution ($Z_1(x) = 0$ for $x \leq 0$)

Irreversibility parameter: $\nu = \dfrac{V(\boldsymbol{q}\|\boldsymbol{\gamma})/D(\boldsymbol{q}\|\boldsymbol{\gamma})}{V(\boldsymbol{p}\|\boldsymbol{\gamma})/D(\boldsymbol{p}\|\boldsymbol{\gamma})}$

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   - Formation-distillation work gap
   - Performance of heat engines
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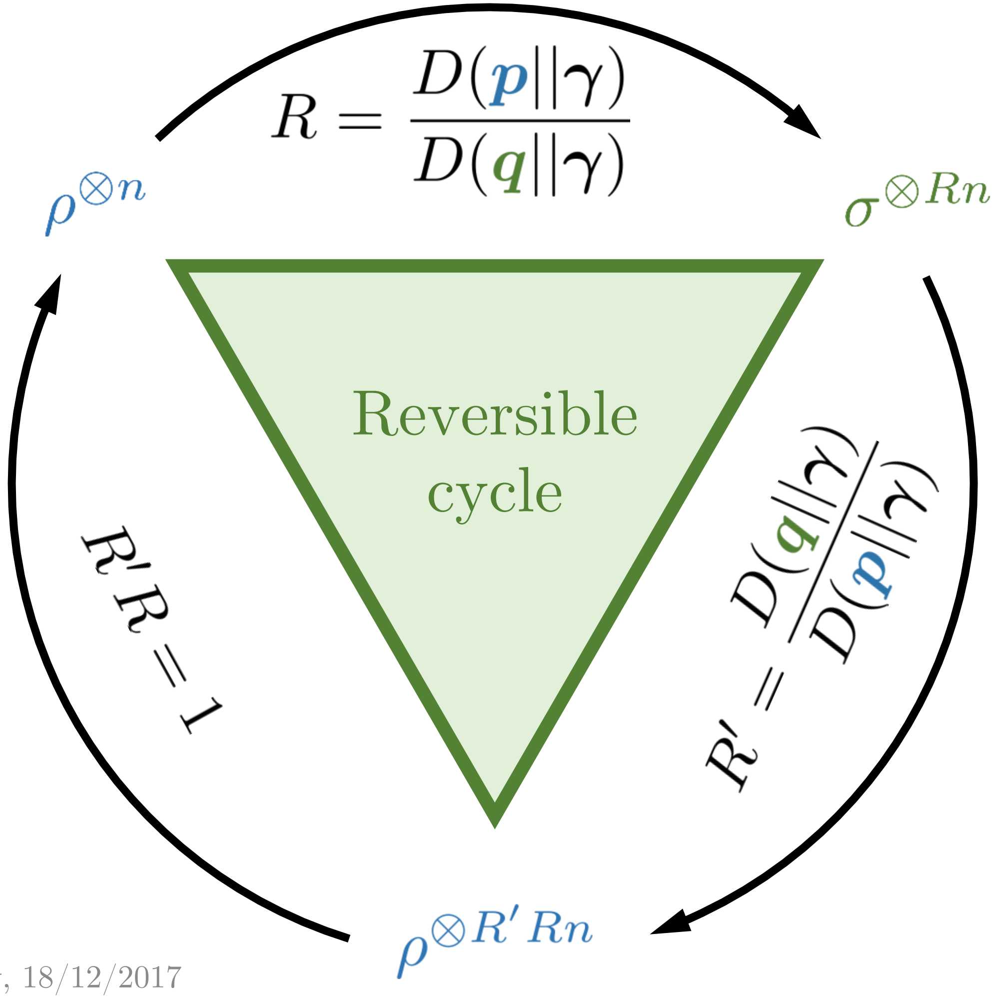
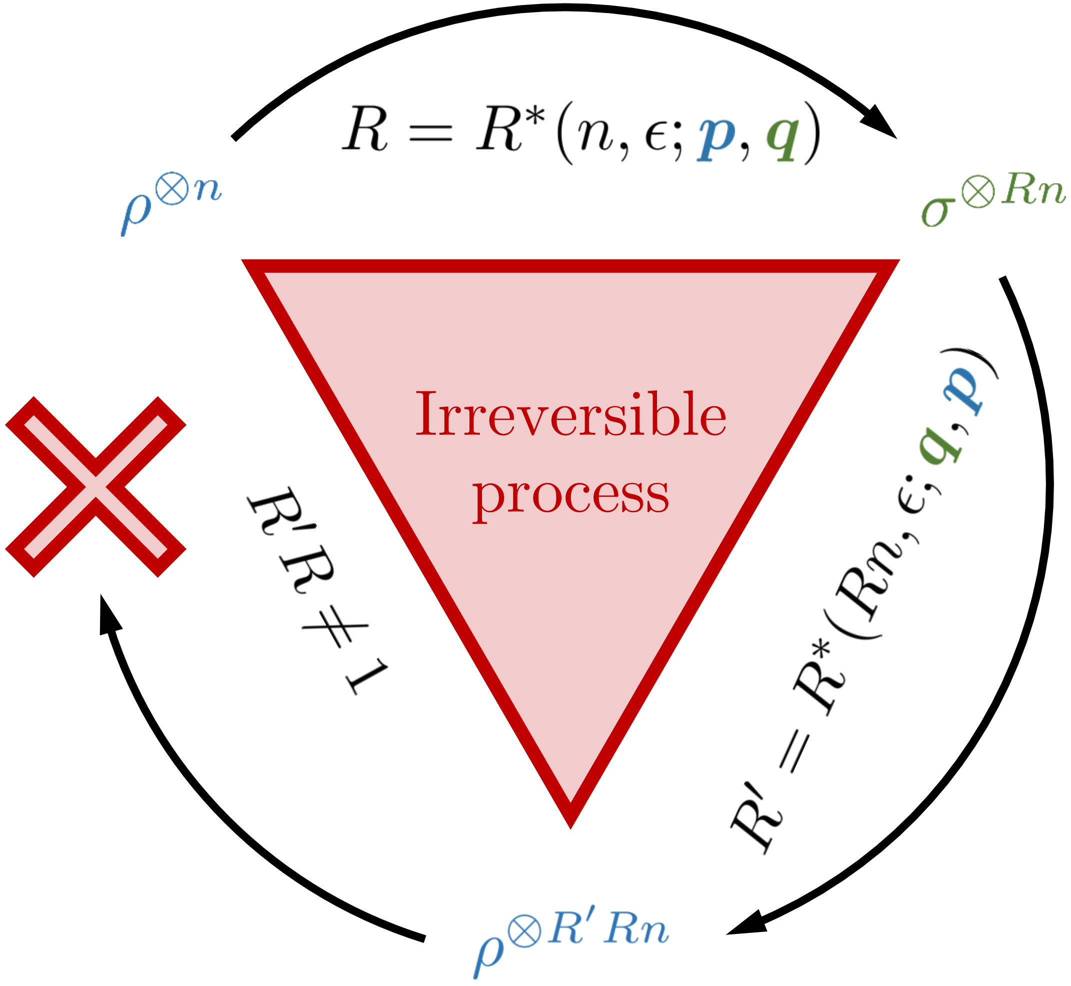
Finite-size irreversibility

Asymptotic limit $n \to \infty$



Large but finite n



Finite-size irreversibility

Optimal *reversibility rate* (transformation $\rho \xrightarrow{\mathcal{E}^\beta} \sigma \xrightarrow{\mathcal{E}^\beta} \rho$):

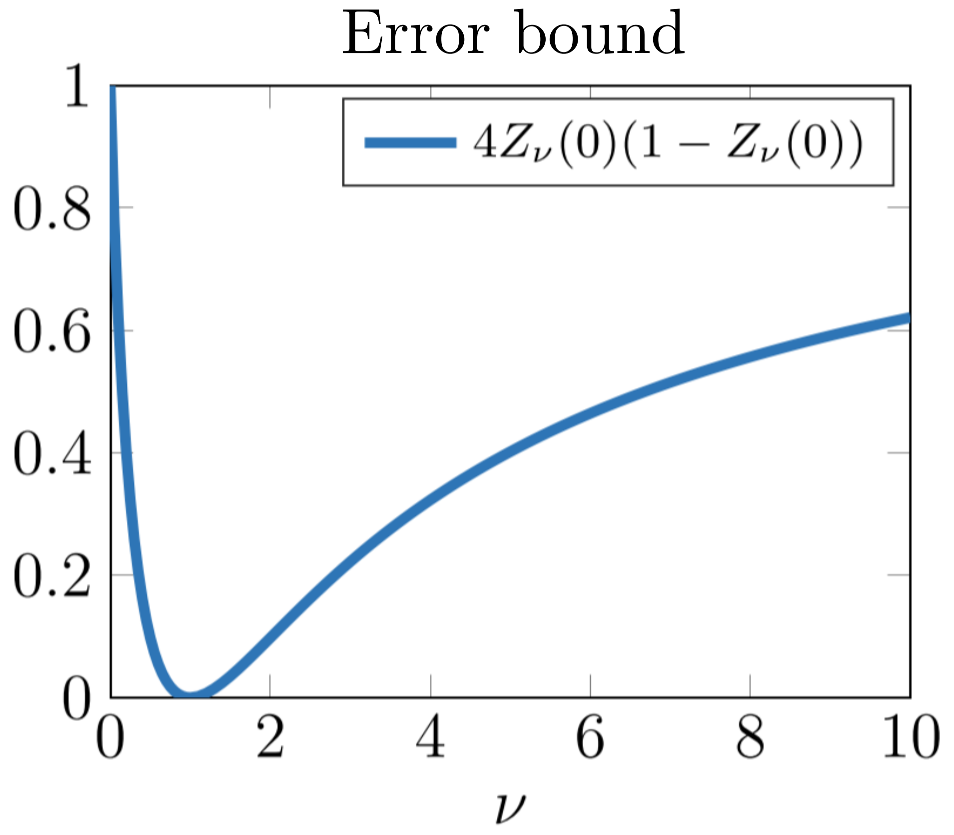
$$R_r^* \simeq 1 + \sqrt{\frac{V(\boldsymbol{p}||\boldsymbol{\gamma})}{nD(\boldsymbol{p}||\boldsymbol{\gamma})^2}}\left(Z_\nu^{-1}(\epsilon_1) + Z_\nu^{-1}(\epsilon_2)\right)$$

Threshold error: $\epsilon_0 := Z_\nu(0)$

Demanding reversibility, $R_r^* = 1$, means:

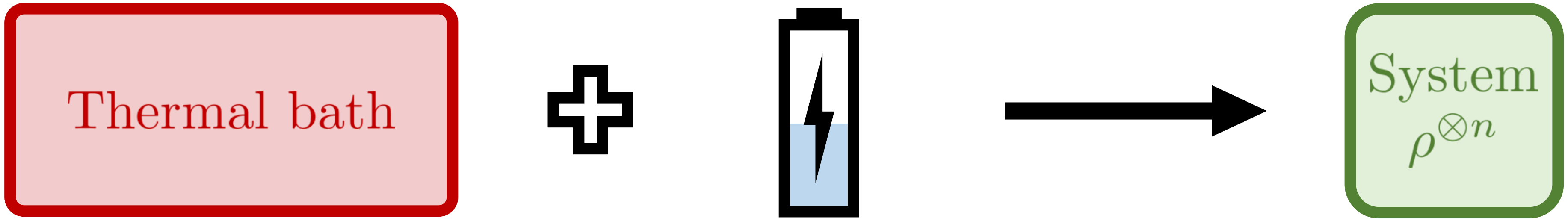
$$\epsilon \leq 4\epsilon_0(1-\epsilon_0) = 4Z_\nu(0)\left(1 - Z_\nu(0)\right)$$

Perfect reversibility, with $\epsilon = 0$, possible if $\nu = 1$.



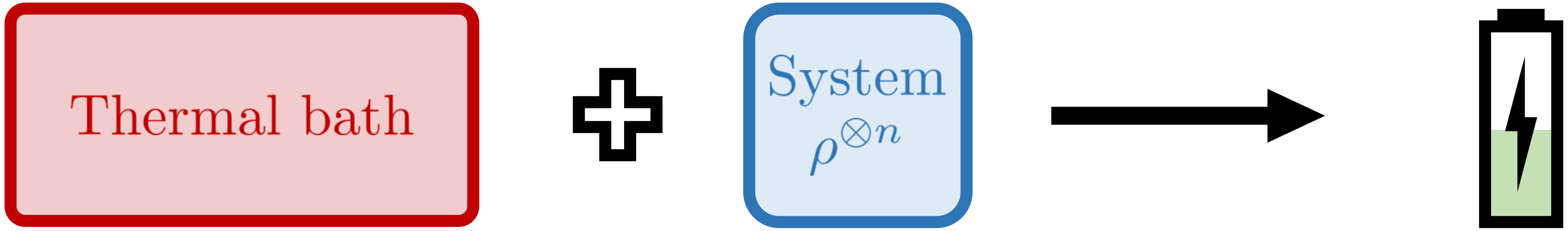
Formation-distillation work gap

Formation process:



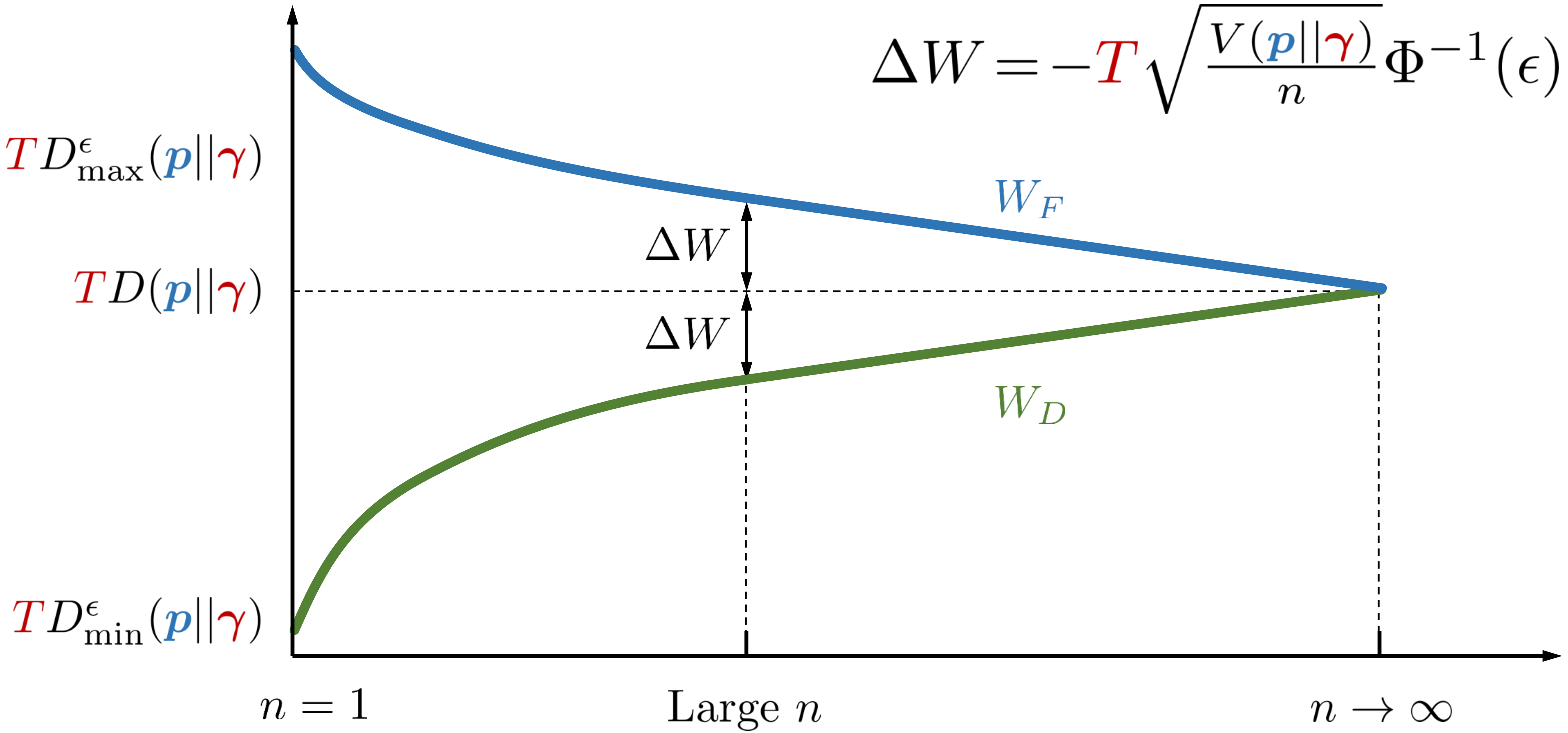
Work of formation: $n \cdot W_F$

Distillation process:

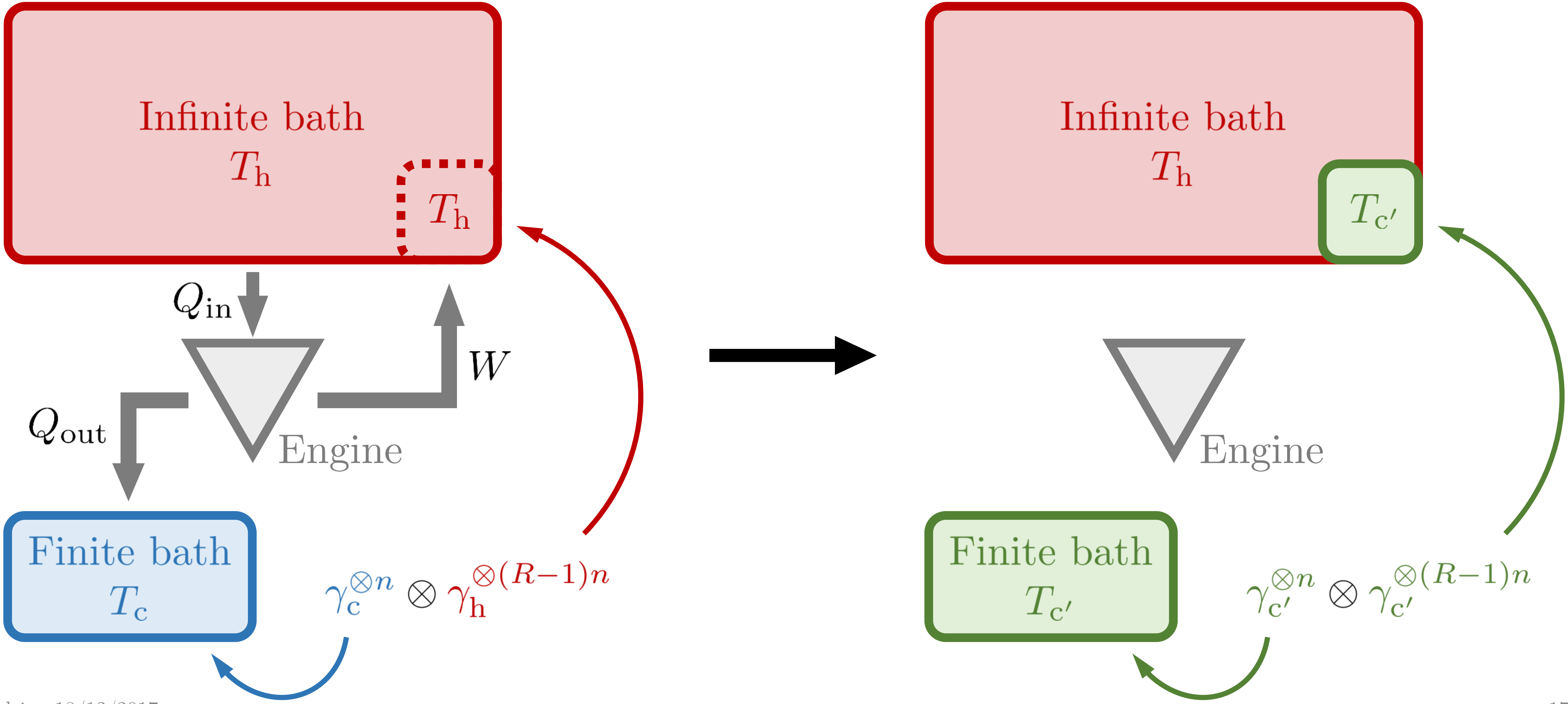


Distillable work: $n \cdot W_D$

Formation-distillation work gap



Performance of heat engines



Performance of heat engines

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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    - Approximate (thermo)majorisation
    - Sketch of the proof
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Thermal operations and (thermo)majorisation

Notation:

Λ^β - *Gibbs-preserving* (GP) stochastic matrix, $\Lambda^\beta \boldsymbol{\gamma} = \boldsymbol{\gamma}$.

Λ^0 - *bistochastic* matrix, $\Lambda^0 \boldsymbol{\eta} = \boldsymbol{\eta}$, where $\boldsymbol{\eta} := [1/d, \ldots, 1/d]$.

Γ^β - *embedding* matrix mapping between canonical and microcanonical pictures:

$$\text{For } \boldsymbol{\gamma} = \left[\frac{D_1}{D}, \ldots, \frac{D_d}{D}\right] \text{ we have } \hat{\boldsymbol{p}} = \Gamma^\beta \boldsymbol{p} = \Bigg[\underbrace{\frac{p_1}{D_1}, \ldots, \frac{p_1}{D_1}}_{D_1 \text{ times}}, \ldots, \underbrace{\frac{p_d}{D_d}, \ldots, \frac{p_d}{D_d}}_{D_d \text{ times}}\Bigg].$$

Note: $\hat{\boldsymbol{\gamma}} = \boldsymbol{\eta}$ and $\hat{\Lambda}^\beta := \Gamma^\beta \Lambda^\beta (\Gamma^\beta)^{-1}$ is bistochastic.

$\boldsymbol{p} \succ \boldsymbol{q}$ - *majorisation* relation, i.e., $\sum_{i=1}^k p_i^\downarrow \geq \sum_{i=1}^k q_i^\downarrow$ for all k.

Thermal operations and (thermo)majorisation

1. Equivalence between thermal and GP interconversion (energy-incoherent states):

$$\mathcal{E}^{\beta}(\rho) = \sigma \quad \iff \quad \Lambda^{\beta}\boldsymbol{p} = \boldsymbol{q}$$

2. Equivalence between GP and embedded bistochastic interconversion:

$$\Lambda^{\beta}\boldsymbol{p} = \boldsymbol{q} \quad \iff \quad \Lambda^{0}\hat{\boldsymbol{p}} = \hat{\boldsymbol{q}}$$

3. Equivalence between embedded bistochastic interconversion and majorisation:

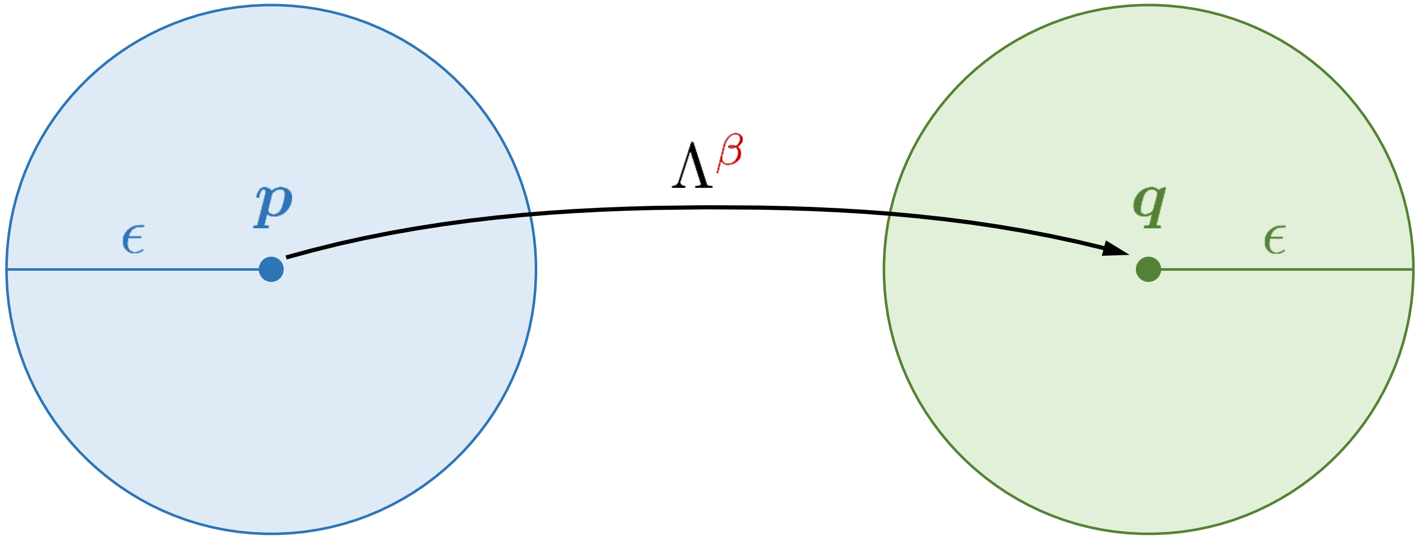
$$\Lambda^{0}\hat{\boldsymbol{p}} = \hat{\boldsymbol{q}} \quad \iff \quad \hat{\boldsymbol{p}} \succ \hat{\boldsymbol{q}}$$

4. Equivalence between embedded majorisation and thermomajorisation:

$$\hat{\boldsymbol{p}} \succ \hat{\boldsymbol{q}} \quad \iff \quad \boldsymbol{p} \succ^{\beta} \boldsymbol{q}$$

Approximate (thermo)majorisation

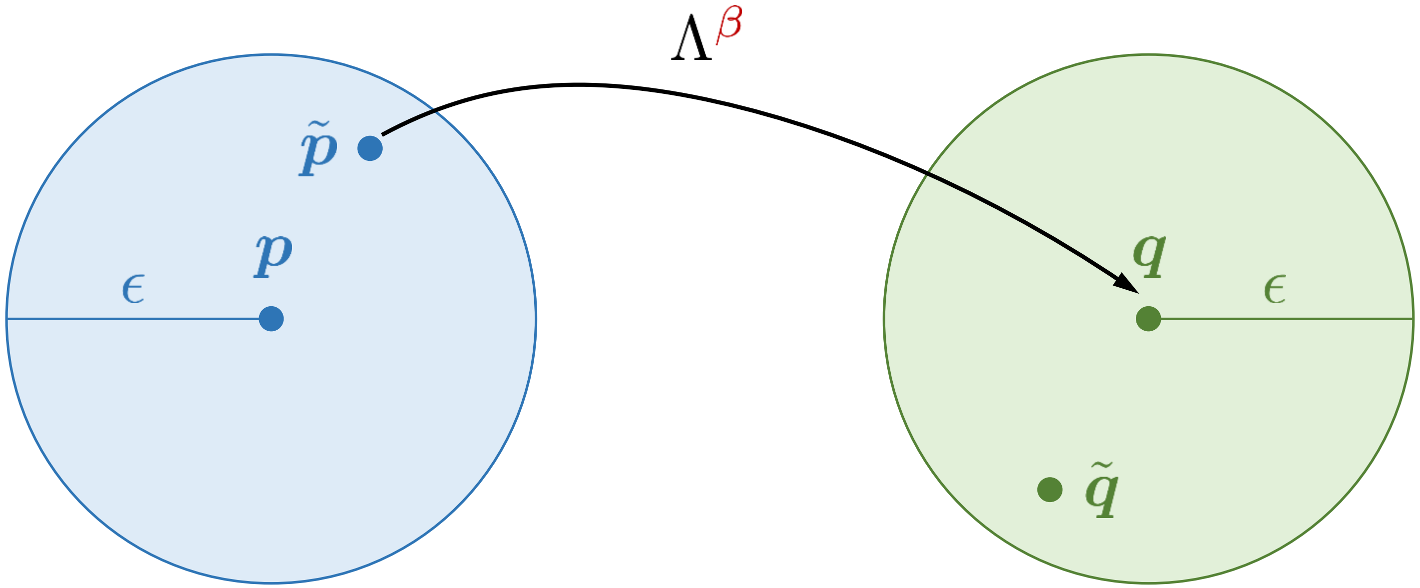
Distance between distributions: $\delta(\boldsymbol{p}, \tilde{\boldsymbol{p}}) := 1 - F(\boldsymbol{p}, \tilde{\boldsymbol{p}})$



Thermomajorisation: $\boldsymbol{p} \succ^{\beta} \boldsymbol{q}$

Approximate (thermo)majorisation

Distance between distributions: $\delta(\boldsymbol{p},\tilde{\boldsymbol{p}}) := 1 - F(\boldsymbol{p},\tilde{\boldsymbol{p}})$

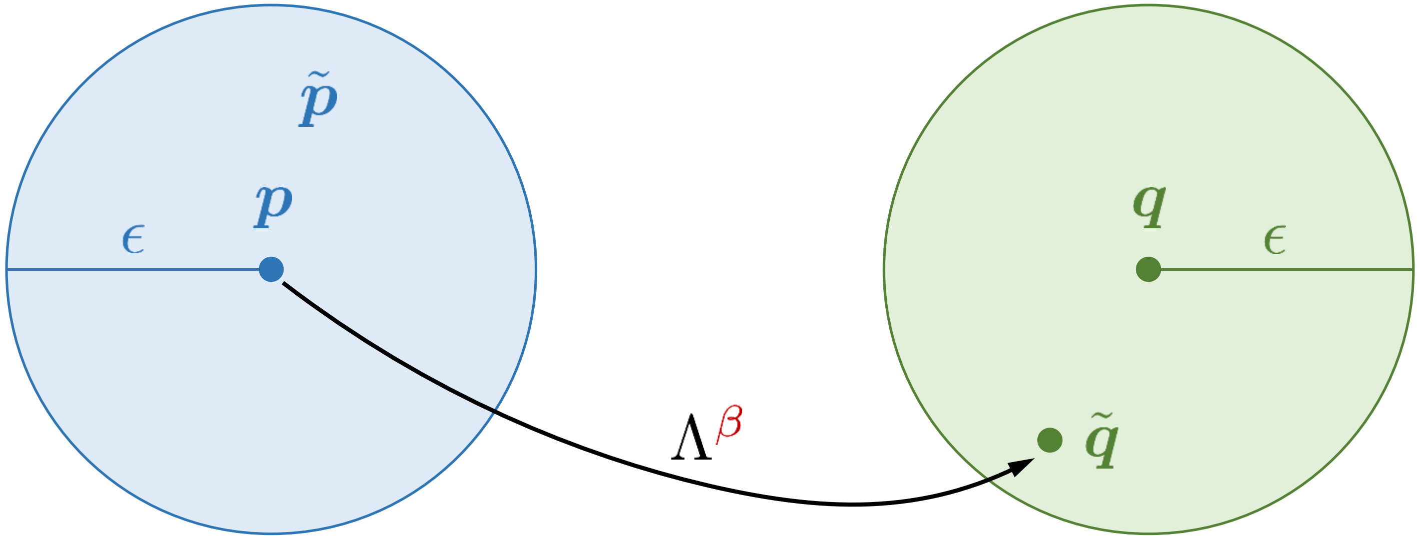


ϵ-pre-thermomajorisation: $\boldsymbol{p} \;{}_{\epsilon}\!\succ^{\beta} \boldsymbol{q}$

$$\tilde{\boldsymbol{p}} \succ^{\beta} \boldsymbol{q} \quad \text{and} \quad \delta(\boldsymbol{p},\tilde{\boldsymbol{p}}) \leq \epsilon.$$

Approximate (thermo)majorisation

Distance between distributions: $\delta(\boldsymbol{p}, \tilde{\boldsymbol{p}}) := 1 - F(\boldsymbol{p}, \tilde{\boldsymbol{p}})$



ϵ-post-thermomajorisation: $\boldsymbol{p} \succ_{\epsilon}^{\beta} \boldsymbol{q}$

$$\boldsymbol{p} \succ^{\beta} \tilde{\boldsymbol{q}} \quad \text{and} \quad \delta(\boldsymbol{q}, \tilde{\boldsymbol{q}}) \leq \epsilon.$$

Approximate (thermo)majorisation

Relations between different notions of approximate majorisation

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
\hat{\boldsymbol{p}} \succ_\epsilon \hat{\boldsymbol{q}} \arrow[r, Leftrightarrow] \arrow[d, Leftrightarrow] & \boldsymbol{p} \succ^\beta_\epsilon \boldsymbol{q} \arrow[d, Rightarrow, shift left, "/" marking] \\
\hat{\boldsymbol{p}}\; {}_\epsilon\!\succ \hat{\boldsymbol{q}} \arrow[r, Rightarrow, shift right, "/" marking] & \boldsymbol{p}\; {}_\epsilon\!\succ^\beta \boldsymbol{q} \arrow[l, Rightarrow, shift right] \arrow[u, Rightarrow, shift left]
\end{tikzcd}
$$

Sketch of the proof

Our goal is to find optimal $R^*(n,\epsilon)$ such that: $\mathcal{E}^\beta(\rho^{\otimes n}) \approx_\epsilon \sigma^{\otimes Rn}$

Adding Gibbs states is free, so equivalently: $\mathcal{E}^\beta(\rho^{\otimes n} \otimes \gamma^{\otimes Rn}) \approx_\epsilon \sigma^{\otimes Rn} \otimes \gamma^{\otimes n}$

Introducing: $P^n := \boldsymbol{p}^{\otimes n} \otimes \boldsymbol{\gamma}^{\otimes Rn}, \quad Q^n := \boldsymbol{q}^{\otimes Rn} \otimes \boldsymbol{\gamma}^{\otimes n}$

$\hat{P}^n := \hat{\boldsymbol{p}}^{\otimes n} \otimes \boldsymbol{\eta}^{\otimes Rn}, \quad \hat{Q}^n := \hat{\boldsymbol{q}}^{\otimes Rn} \otimes \boldsymbol{\eta}^{\otimes n}$

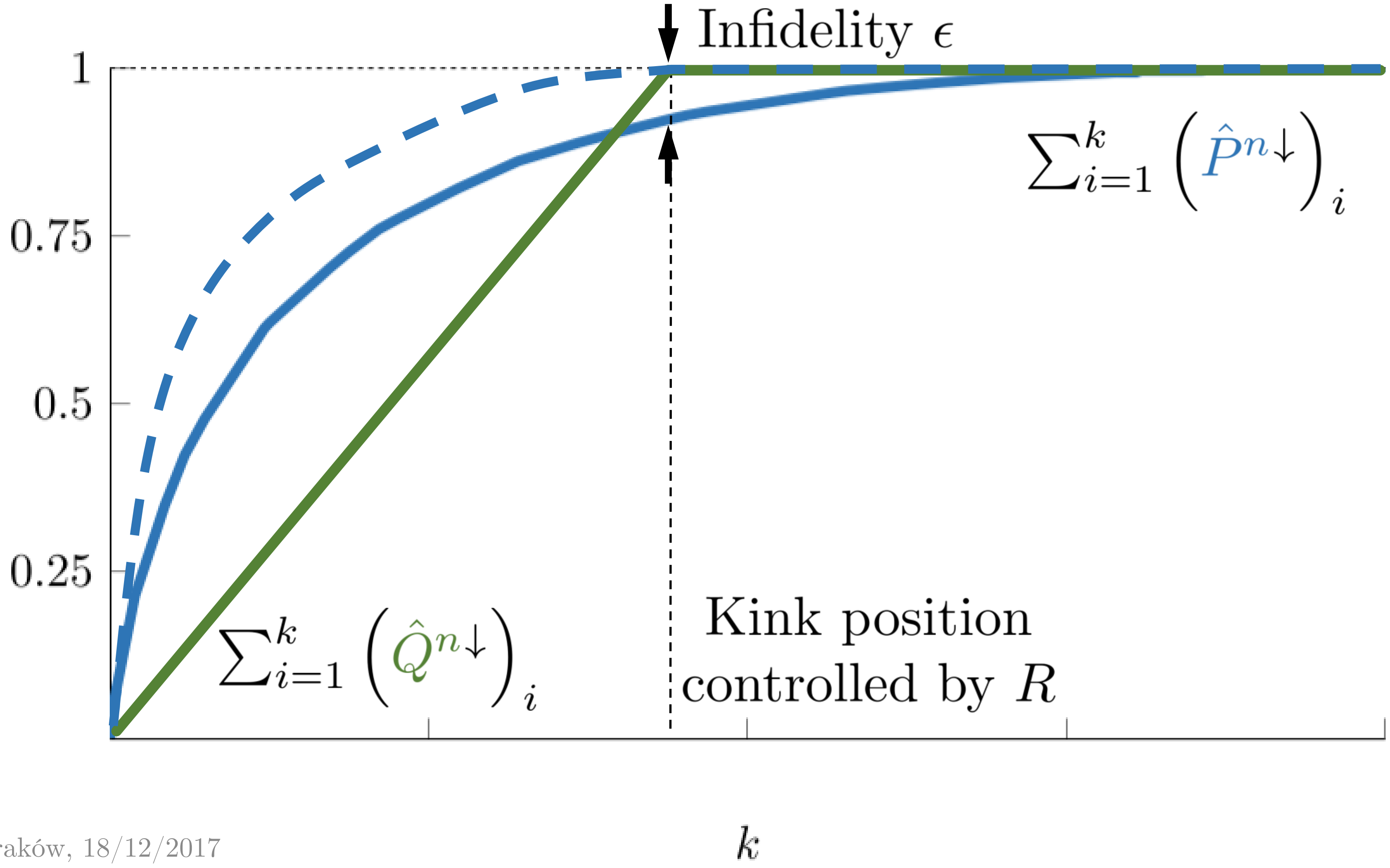
For energy-incoherent states the condition is: $P^n \succ_\epsilon^\beta Q^n$

Embedded post-majorisation $\Leftrightarrow$ post-thermo-majorisation, so: $\hat{P}^n \succ_\epsilon \hat{Q}^n$

Post-majorisation $\Leftrightarrow$ pre-majorisation, so: $\hat{P}^n \, {}_\epsilon\!\succ \hat{Q}^n$

Sketch of the proof

We need to look at majorisation curves of $\hat{P}^n$ and $\hat{Q}^n$.



Recall:

$$\hat{P}^n = \hat{\boldsymbol{p}}^{\otimes n} \otimes \boldsymbol{\eta}^{\otimes Rn}$$
$$\hat{Q}^n = \hat{\boldsymbol{q}}^{\otimes Rn} \otimes \boldsymbol{\eta}^{\otimes n}$$

Focus on distillation:

$$\boldsymbol{q} = [1, 0, \ldots, 0]$$

Optimal majorising curve:
cut tail and rescale

Sketch of the proof

For general $\boldsymbol{q}$ majorisation curve of $\hat{Q}^n$ is piece-wise linear.

Idea: divide the support into boxes and construct a distribution $\tilde{\hat{P}}^n$ with the same shape as $\hat{P}^n$ (so that it is close to $\tilde{\hat{P}}^n$) and the same mass as $\hat{Q}^n$ (so that it majorises $\hat{Q}^n$) within each box.

Tools: Variations of central limit theorem used to obtain majorisation curves for $\hat{P}^n$ and $\hat{Q}^n$ when $n \to \infty$.

Final step: unembed the solution, obtained in terms of $D(\hat{\cdot}\|\boldsymbol{\eta})$ and $V(\hat{\cdot}\|\boldsymbol{\eta})$, to express it using $D(\cdot\|\boldsymbol{\gamma})$ and $V(\cdot\|\boldsymbol{\gamma})$.

Outlook

- Apply the results to other thermodynamic problems involving finite-size baths, e.g. Landauer's erasure, fluctuation theorems, the third law of thermodynamics.
- Clarify the notion of imperfect work (construct a comparison platform to continuously distinguish between work-like and heat-like forms of energy).
- Investigate conditions for which Carnot efficiency can be achieved with finite-size baths (or with finite-size working body).
- Extend to general quantum states with coherence.

Details: arXiv:1711.01193

Thank you!