The resource theory approach to quantum thermodynamics

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Outline

1. Quantum resource theories
2. Asymptotic analysis
3. Single-shot analysis
4. Catalysts
5. Work extraction in thermalisation
6. Discussion

Quantum resource theories

Quantum resource theories

- Paradigm for phrasing many scenarios of interest
- Three inter-related ingredients
  - Allowed operations: Things that can be done ‘easily’
  - Free states: States that can be prepared ‘easily’ – stable under allowed operations
  - Resource states: States that cannot be prepared ‘easily’ – cannot be prepared from free states by allowed operations

Example resource theories

Resource theory	Allowed operations	Free states	Resource states
Entanglement	local operations and classical communication	separable states	entangled states
Asymmetry	U representing group G	symmetric states	asymmetric states
Thermodynamics	energy conserving operations	thermal states	non-thermal states

Resource theory of thermodynamics[1]

- Free states
  - For any Hamiltonian H_b, can prepare thermal state

$$\tau_\beta(H_\mathrm{b}) = \frac{1}{Z_\mathrm{b}} \exp(-\beta H_\mathrm{b})$$

    at fixed background (inverse) temperature β, where $Z_\mathrm{b} = \mathrm{tr}[\exp(-\beta H_\mathrm{b})]$ partition function
  - "thermal bath"
- Allowed operations
  - Any unitary U such that $[U, H] = 0$, where H is the total Hamiltonian of all systems
  - "cyclic operations"

[1] F. G. S. L. Brandão, M. Horodecki, J. Oppenheim, J. M. Renes, R. W. Spekkens, Phys. Rev. Lett. **111**, 250404 (2013)

Transforming states

- Thermal Operation (TO): General transformation of ρ_s allowed by resource theory of thermodynamics

$$\mathcal{E}(\rho_\mathrm{s}) = \mathrm{tr}_\mathrm{b}[U(\rho_\mathrm{s} \otimes \tau_\beta(H_\mathrm{b}))U^\dagger]$$

  where $H = H_\mathrm{s} + H_\mathrm{b}$ and $[U, H] = 0$
- Transformation is possible

$$\rho_\mathrm{s} \xrightarrow{\mathrm{TO}} \sigma_\mathrm{s}$$

  if and only if $\sigma_\mathrm{s} = \mathcal{E}(\rho_\mathrm{s})$ for $\mathcal{E}(\cdot)$ some allowed transformation

Asymptotic analysis

Asymptotic state transformation

- Consider transformation

$$\rho_S^{\otimes n} \xrightarrow{\text{TO}} \sigma_S^{\otimes m}$$

- Interested in asymptotic rate of optimal transformation

$$R(\rho_S \to \sigma_S) = \max_{\text{TO}} \lim_{n \to \infty} \frac{m}{n}$$

Asymptotic state transformation[2]

- $$R(\rho_s \to \sigma_s) = \frac{D(\rho \,\|\, \tau_\beta(H_s))}{D(\sigma \,\|\, \tau_\beta(H_s))}$$
- $D(\cdot \,\|\, \cdot)$ is the quantum relative entropy

$$D(\rho \,\|\, \sigma) = \mathrm{tr}[\rho(\log \rho - \log \sigma)]$$

- Proof: Using ideas from quantum Shannon theory (e.g. typical subspaces)

[2] F. G. S. L. Brandão, M. Horodecki, J. Oppenheim, J. M. Renes, R. W. Spekkens, Phys. Rev. Lett. **111**, 250404 (2013)

Asymptotic state transformation

- Special form

$$D(\rho_s \,\|\, \tau_\beta(H_s)) = \beta(F(\rho_s) - F(\tau_\beta(H_s)))$$

- where $F(\cdot)$ is the generalised quantum free energy

$$\begin{aligned} F(\rho_s) &= \mathrm{tr}[H_s \rho_s] - TS(\rho_s) \\ &= \langle E \rangle_{\rho_s} - TS(\rho_s) \end{aligned}$$

  and $S(\rho) = -\mathrm{tr}[\rho \log \rho]$ von Neumann entropy
- Thermal state

$$F(\tau_\beta(H_s)) = -T \log Z_s$$

Asymptotic state transformation

- $$R(\rho_s \to \sigma_s) = \frac{F(\rho_s) - F(\tau_\beta(H_s))}{F(\sigma_s) - F(\tau_\beta(H_s))}$$
- Suggests interpretation in terms of work:
  - Extract work $W \leq n(F(\rho_s) - F(\tau_\beta(H_s)))$ from $\rho_s^{\otimes n}$
  - Invest work $W \geq m(F(\sigma_s) - F(\tau_\beta(H_s)))$ to prepare $\sigma_s^{\otimes m}$
  - $R(\rho_s \to \sigma_s)$ achievable if both are reversible

Single-shot analysis

Single-shot transformation

- Consider transformation

$$\rho_{\mathrm{S}} \xrightarrow{\mathrm{TO}} \sigma_{\mathrm{S}}$$

- Interested in characterising which transformations are possible
- e.g. guess $F(\rho_{\mathrm{S}}) \geq F(\sigma_{\mathrm{S}})$? Necessary but not sufficient
- Partial order $\rho_{\mathrm{S}} \succ_{\beta} \sigma_{\mathrm{S}}$ if and only if $\rho_{\mathrm{S}} \xrightarrow{\mathrm{TO}} \sigma_{\mathrm{S}}$

Thermo-majorisation[3]

- Necessary and sufficient conditions when ρ_s and σ_s diagonal in energy eigenbasis i.e. quasi-classical
-

$$\mathbf{p}_s = \mathrm{diag}(\rho_s) = (\langle E_1|\rho_s|E_1\rangle, \ldots, \langle E_d|\rho_s|E_d\rangle)$$

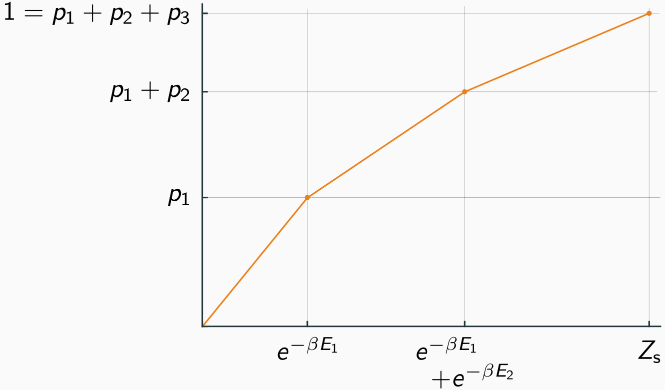
where $H_s = \sum_i E_i |E_i\rangle\langle E_i|$

- Assume β-ordered

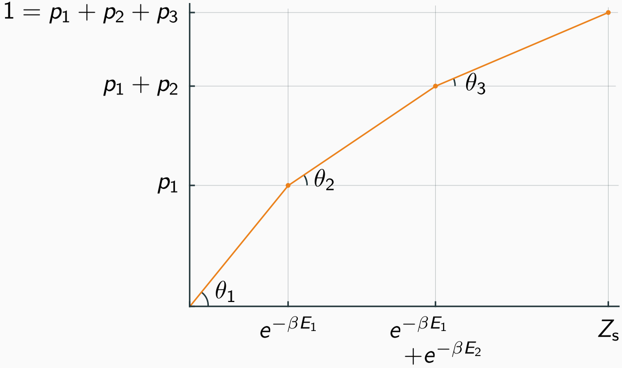
$$p_1 e^{+\beta E_1} \geq p_2 e^{+\beta E_2} \geq \ldots \geq p_d e^{+\beta E_d}$$

[3] M. Horodecki, J. Oppenheim, Nature Commun. **4**, 2059 (2013)

Thermo-majorisation curve

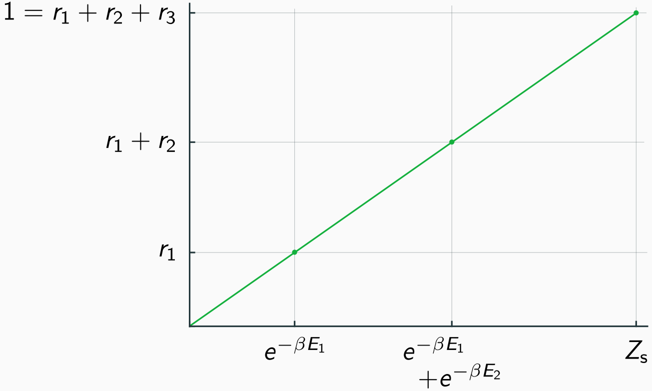


Thermo-majorisation curve



- β-order: $\theta_1 \geq \theta_2 \geq \theta_3$
- concave graph

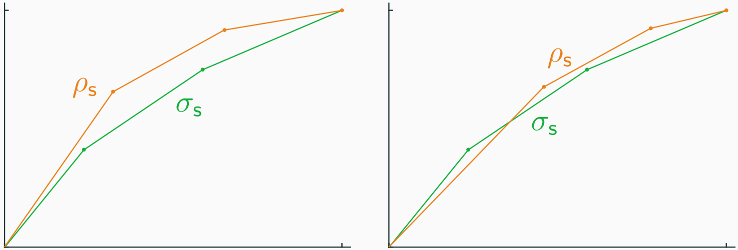
Thermo-majorisation curve of thermal state



- $\mathbf{r}_s = \mathrm{diag}(\tau_\beta(H_s)) = (e^{-\beta E_1}, \ldots, e^{-\beta E_d})/Z_s$
- straight line

Thermo-majorisation

- ρ_s thermo-majorises σ_s if and only if thermo-majorisation curve of ρ_s lies everywhere above the thermo-majorisation curve of σ_s.



$\rho_\mathrm{s} \succ_\beta \sigma_\mathrm{s}$ $\qquad$ $\rho_\mathrm{s} \not\succ_\beta \sigma_\mathrm{s}$ $\quad$ $\sigma_\mathrm{s} \not\succ_\beta \rho_\mathrm{s}$

- thermomajorised if "closer" to thermal

Catalysts

Catalytic transformation

- Consider transformation involving catalyst

$$\rho_{\mathrm{S}} \otimes \omega_{\mathrm{C}} \xrightarrow{\mathrm{TO}} \sigma_{\mathrm{S}} \otimes \omega_{\mathrm{C}}$$

- Catalyst remains in same state and uncorrelated from system
- Exist states such that $\rho_{\mathrm{S}} \not\xrightarrow{\mathrm{TO}} \sigma_{\mathrm{S}}$ but $\rho_{\mathrm{S}} \otimes \omega_{\mathrm{C}} \xrightarrow{\mathrm{TO}} \sigma_{\mathrm{S}} \otimes \omega_{\mathrm{C}}$ for appropriate ω_{C}
- Define

$$\rho_{\mathrm{S}} \xrightarrow{\mathrm{CTO}} \sigma_{\mathrm{S}}$$

  if there exists catalyst ω_{C} such that $\rho_{\mathrm{S}} \otimes \omega_{\mathrm{C}} \xrightarrow{\mathrm{TO}} \sigma_{\mathrm{S}} \otimes \omega_{\mathrm{C}}$
- Interested in characterising new partial order

α-free energies[4]

- Necessary and sufficient conditions when ρ_{S} and σ_{S} are quasi-classical given by α-free energies
- Quantum Renyi relative entropy

$$D_\alpha(\rho \,\|\, \sigma) = \frac{1}{\alpha - 1} \log \sum_i \lambda_i^\alpha \mu_i^{1-\alpha}$$

  where $\lambda = \mathrm{eig}(\rho)$ and $\mu = \mathrm{eig}(\sigma)$
- α-free energy

$$\begin{aligned} F_\alpha(\rho_{\mathrm{S}}) &= T D_\alpha(\rho_{\mathrm{S}} \,\|\, \tau_\beta(H_{\mathrm{S}})) - T \log Z_{\mathrm{S}} \\ &= \frac{T}{\alpha - 1} \log \sum_i p_i^\alpha e^{-\beta E_i (1-\alpha)} \end{aligned}$$

  if ρ is quasi-classical

[4] F.G.S.L. Brandão, M. Horodecki, N.H.Y. Ng, J. Oppenheim, S. Wehner, PNAS **112**, 3275 (2015)

α-free energies

$$F_\alpha(\rho_s) = \frac{T}{\alpha - 1} \log \sum_i p_i^\alpha e^{-\beta E_i(1-\alpha)}$$

- Non-increasing in α

$$F_\alpha(\cdot) \leq F_{\alpha'}(\cdot) \text{ if } \alpha \leq \alpha'$$

- $F_{\min}(\rho_s) = F_0(\rho_s) = -T \log \sum_{i:p_i \neq 0} e^{-\beta E_i}$
- $F_1(\rho_s) = F(\rho_s) = \langle E \rangle_{\rho_s} - TS(\rho_s)$
- $F_{\max}(\rho_s) = T \log \max_i p_i e^{\beta E_i}$

catalytic transformations

- Necessary and sufficient conditions for $\rho_{\mathsf{S}} \xrightarrow{\mathsf{CTO}} \sigma_{\mathsf{S}}$ when ρ_{S} and σ_{S} are quasi-classical

$$F_\alpha(\rho_{\mathsf{S}}) \geq F_\alpha(\sigma_{\mathsf{S}}) \quad \forall \alpha$$

- monotones under catalytic thermal operations – cannot increase

Work extraction in thermalisation

Work extraction

- How much work can be extracted from a system in the process of thermalisation?

$$\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}}) + W$$

- Second Law: $W \leq F(\rho_{\mathrm{s}}) - F(\tau_\beta(H_{\mathrm{s}}))$
- Need to store work somewhere
- Different answer depending on where and what you demand

Case 1: Deterministic work extraction[5]

- Work storage bit: two-level system, states $|0\rangle$ and $|1\rangle$ with Hamiltonian $H_\mathrm{w} = E_\mathrm{w} |1\rangle\langle 1|$
- Consider transformation

$$\rho_\mathrm{s} \otimes |0\rangle\langle 0|_\mathrm{w} \xrightarrow{\mathrm{TO}} \tau_\beta(H_\mathrm{s}) \otimes |1\rangle\langle 1|_\mathrm{w}$$

- System thermalised and work storage bit deterministically raised from $|0\rangle$ to $|1\rangle$
- Define

$$\begin{aligned} W_\mathrm{det}(\rho_\mathrm{s} \to \tau_\beta(H_\mathrm{s})) = \max \quad & E_\mathrm{w} \\ \text{such that} \quad & \rho_\mathrm{s} \otimes |0\rangle\langle 0|_\mathrm{w} \xrightarrow{\mathrm{TO}} \tau_\beta(H_\mathrm{s}) \otimes |1\rangle\langle 1|_\mathrm{w} \end{aligned}$$

- i.e. largest energy that can be put into work storage bit

[5] M. Horodecki, J. Oppenheim, Nature Commun. **4**, 2059 (2013)

Case 1: Deterministic work extraction

- For quasi-classical states

$$W_{\mathrm{det}}(\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}})) = F_{\min}(\rho_{\mathrm{s}}) - F_{\min}(\tau_\beta(H_{\mathrm{s}}))$$

  where $F_{\min}(\rho_{\mathrm{s}}) = -T \log \sum_{i:p_i \neq 0} e^{-\beta E_i}$
- Result independent of catalyst: inclusion of catalyst doesn't change the amount of deterministic work that can be extracted
- Generally less than $F(\rho_{\mathrm{s}}) - F(\tau_\beta(H_{\mathrm{s}}))$

Case 2: Average work extraction[6]

- Weight system: infinite ladder, states $|x\rangle$ with Hamiltonian

$$H_{\mathrm{w}} = mg \int dx x \, |x\rangle \langle x|$$

- Consider transformation

$$\rho_{\mathrm{s}} \otimes \rho_{\mathrm{w}} \xrightarrow{\mathrm{TO}} \tau_\beta(H_{\mathrm{s}}) \otimes \sigma_{\mathrm{w}}$$

  and identify change in average energy of weight

$$\mathrm{tr}[H_{\mathrm{w}}\sigma_{\mathrm{w}}] - \mathrm{tr}[H_{\mathrm{w}}\rho_{\mathrm{w}}] = \langle E\rangle_{\sigma_{\mathrm{w}}} - \langle E\rangle_{\rho_{\mathrm{w}}}$$

  as form of average work
- Extractable average work

$$\begin{aligned} W_{\mathrm{av}}(\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}})) = \max \quad & \langle E\rangle_{\sigma_{\mathrm{w}}} - \langle E\rangle_{\rho_{\mathrm{w}}} \\ \text{such that} \quad & \rho_{\mathrm{s}} \otimes \rho_{\mathrm{w}} \xrightarrow{\mathrm{TO}} \tau_\beta(H_{\mathrm{s}}) \otimes \sigma_{\mathrm{w}} \end{aligned}$$

- i.e. largest change in average energy of the weight

[6] P.S., A.J. Short, S. Popescu, Nature Commun. 5, 4185 (2014)

Case 2: Average work extraction

- Problem: $W_{\mathrm{av}}(\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}})) = \infty$
- Weight is non-equilibrium system – in particular infinite entropy dump
- Solution: Restrict TO to special class

$$U_{\mathrm{sbw}} = \sum_{i,j} \left|E_j\right\rangle \langle E_i| \otimes \Gamma_{E_j - E_i}$$

where $(H_{\mathrm{s}} + H_{\mathrm{b}}) |E_i\rangle = E_i |E_i\rangle$ and

$$\Gamma_a |x\rangle = |x + a\rangle$$

shift operator on weight

Case 2: Average work extraction

- Intuitive idea: Weight responds independent of its state
- Can show that $W_{\mathrm{av}}(\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}}))$ now independent of ρ_{w}
- For all states

$$W_{\mathrm{av}}(\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}})) \leq F(\rho_{\mathrm{s}}) - F(\tau_\beta(H_{\mathrm{s}}))$$

- i.e. 'standard' second law holds
- For quasi-classical states can achieve

$$W_{\mathrm{av}}(\rho_{\mathrm{s}} \to \tau_\beta(H_{\mathrm{s}})) = F(\rho_{\mathrm{s}}) - F(\tau_\beta(H_{\mathrm{s}}))$$

Discussion

Other results

- Approximate transformations
- Additional constraints from coherences
- Third law of thermodynamics
- Fluctuation relations
- Multiple conserved quantities

Summary

- Resource theory approach provides powerful framework to study the ultimate limits to thermodynamics in the quantum regime
- Provides generalisations to the second law for state transformations
- Different paradigms for work extraction in the thermalisation process

Thank you