On the existence of complete thermodynamic potentials for quantum systems

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Quantum Resources:

from mathematical foundations to operational characterisation

Singapore, 8 December 2022

Outline

- Introduction

- Part 1: Quantum thermodynamics of interacting *many-body* systems

Faist, Sagawa, Kato, Nagaoka, Brandao, Phys. Rev. Lett. **123**, 250601 (2019)
Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

- Part 2: Quantum thermodynamics of correlated-catalytic state conversion at *small-scale*

Shiraishi & Sagawa, Phys. Rev. Lett. **126**, 150502 (2021).

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- **Introduction**

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Thermodynamics

Entropy (or the free energy) provides the *complete* characterization of state convertibility between macroscopic equilibrium states.

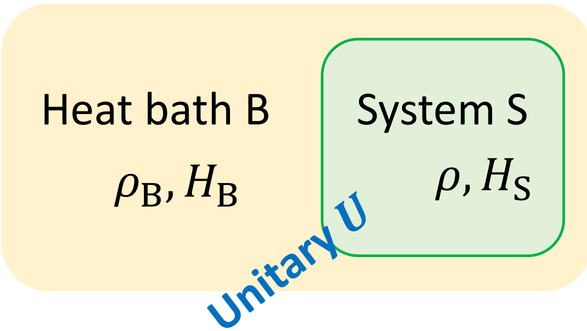
State conversion is possible,
if and only if $\Delta S \geq 0$ or $W \geq \Delta F$

Mathematically rigorous axiomatic formulation:
Lieb & Yngvason, Phys. Rep. (1999)

Watt steam engine (from Wikipedia)

Does such a *complete* thermodynamic potential exist in out-of-equilibrium and fully quantum situations?

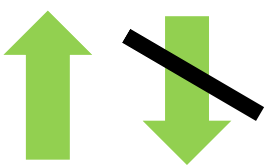
Resource theory of thermodynamics



Dynamics of S (CPTP map):

$$\boldsymbol{E}(\rho) = \mathrm{tr}_{\mathrm{B}}[U\rho \otimes \rho_{\mathrm{B}} U^{\dagger}]$$

Gibbs-preserving map (GPM): $\boldsymbol{E}(\rho^{\mathrm{G}}) = \rho^{\mathrm{G}}$ with $\rho^{\mathrm{G}} = e^{\beta(F_S - H_{\mathrm{S}})}$



Thermal operations cannot create coherence in the energy basis,
e.g., $|1\rangle \mapsto |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ Faist, Oppenheim, Renner, NJP (2015)

Thermal operation: $\rho_{\mathrm{B}} = e^{\beta(F_{\mathrm{B}} - H_{\mathrm{B}})}$ and $[U, H_{\mathrm{S}} + H_{\mathrm{B}}] = 0$

Conservation of the sum of the energies of S and B: **Energy is resource!**

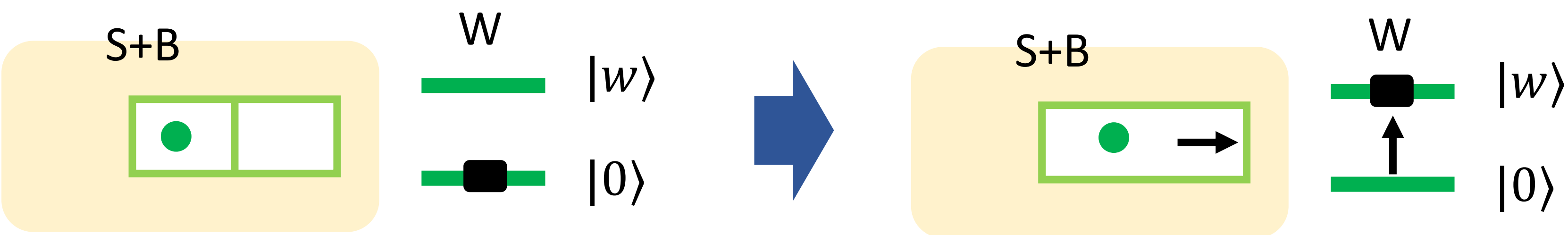
- ✓ Jaynes-Cummings model at the resonant condition
- ✓ Quantum master equation with the rotating wave approximation

Single-shot work bound

Idealized work storage (battery) W:

A two-level system with the initial and final states being pure.

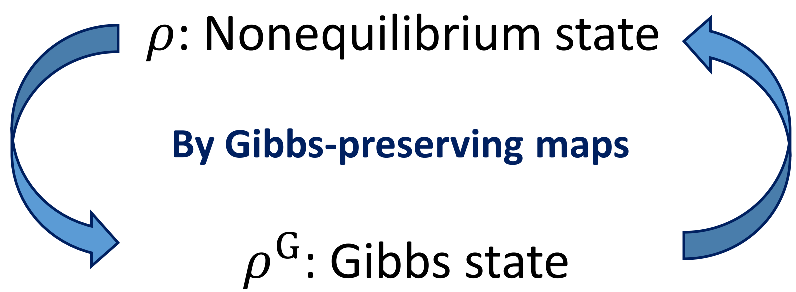
Work does not fluctuate, which excludes any entropic contribution of W.



The work bound is given by the min and max divergences

Horodecki & Oppenheim, Nature Commu. (2013);
Aberg, Nature Commu. (2013)

$\beta w \leq S_0(\rho||\rho^{\mathrm{G}})$

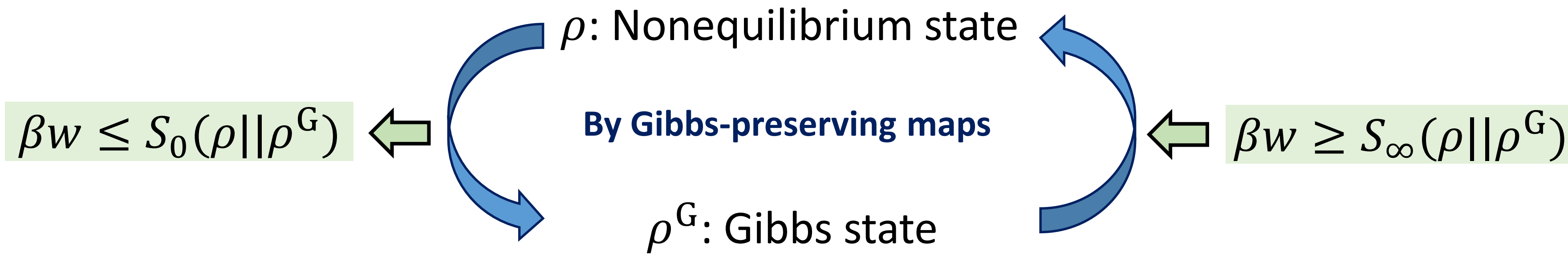


$\beta w \geq S_\infty(\rho||\rho^{\mathrm{G}})$

$S_0(\rho||\sigma) := -\ln(\mathrm{tr}[P_\rho \sigma])$

$S_\infty(\rho||\sigma) := \ln\left\|\sigma^{-1/2}\rho\sigma^{-1/2}\right\|_\infty$

Absence of reversibility in the single-shot case



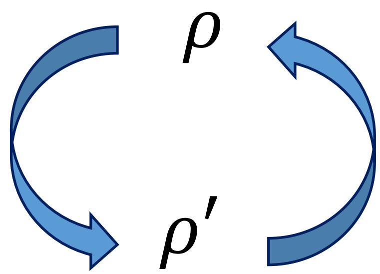
Analogy with the conventional case apparently fails;

- ✓ S_0 and S_∞ do not match in general; a mere cyclic operation requires work $S_\infty - S_0$.
- ✓ Thus, **a single *complete* thermodynamic potential does not exist,** except for equilibrium transitions.

Question and the results

Is it still possible to have a single thermodynamic potential $F_?$ that completely characterizes state convertibility, in out-of-equilibrium and fully quantum situations?

$w \leq F_?(\rho) - F_?(\rho')$ ⇐



⇐ $w \geq F_?(\rho) - F_?(\rho')$

Yes, if:

Take the asymptotic (*macroscopic*) limit, and if the state is spatially ergodic and the Hamiltonian is local and translation-invariant (**Part 1**);

or

Consider correlated-catalytic state conversion at *small-scale*, where an auxiliary system called *catalyst* is introduced and the system can be correlated with it (**Part 2**).

In both the cases, the thermodynamic potential is given by the KL divergence.

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- **Part 1: Quantum thermodynamics of interacting *many-body* systems**

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- Part 2: Quantum thermodynamics of correlated-catalytic state conversion at *small-scale*

  Shiraishi & Sagawa, Phys. Rev. Lett. **126**, 150502 (2021).

Collaborators

At *Caltech* (December 2018)

Kohtaro Kato

Philippe Faist

Fernando Brandao

… and Hiroshi Nagaoka

University of Electro-Communications

Faist, Sagawa, Kato, Nagaoka, Brandao, Phys. Rev. Lett. **123**, 250601 (2019)

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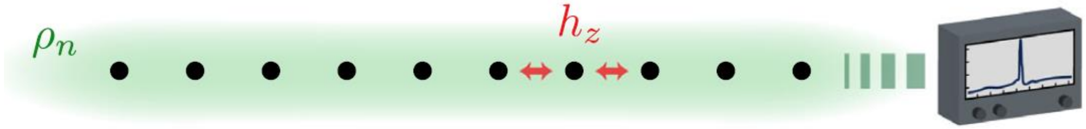
Main result: Quantum ergodic theorem

Consider a many-body spin system on a lattice **in any spatial dimension**.

State ρ: spatially ergodic

The fluctuation of any macroscopic observable (e.g., the total magnetization) vanishes in the macroscopic limit; any macroscopic observable has a definite value (no phase coexistence).



Hamiltonian: interaction is local and translation-invariant with Gibbs state ρ^{G}

Then, under a proper definition of the asymptotic limit given by **information spectrum**,

$$S_0(\rho||\rho^{\mathrm{G}}) \approx S_\infty(\rho||\rho^{\mathrm{G}}) \approx S_1(\rho||\rho^{\mathrm{G}})$$

where $S_1(\rho||\rho^G) := \mathrm{tr}[\rho \ln \rho - \rho \ln \rho^{\mathrm{G}}]$ is the Kullback-Leibler (KL) divergence.

Main result: Emergent thermodynamic potential

Under the foregoing setup,
$F_1(\rho) := S_1(\rho||\rho^{\mathrm{G}}) + F$ serves as the nonequilibrium free energy:

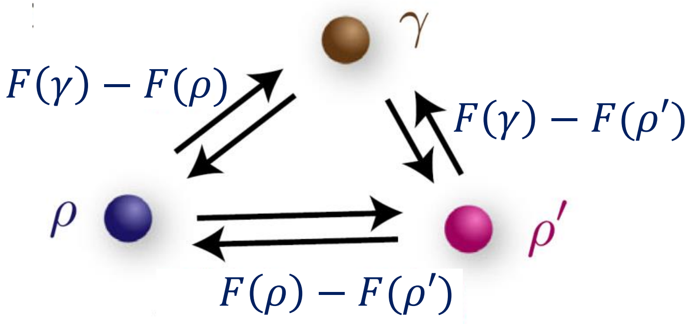
ρ can be asymptotically converted into ρ'
by a Gibbs-preserving map with the work cost w,

if and only if

$$w \geq F_1(\rho') - F_1(\rho)$$

Here, a Gibbs preserving map can be replaced by a thermal operation even in the fully quantum case, if the aid of a small amount of coherence is allowed.

Emergence of a thermodynamic potential for a complete characterization of state convertibility!



Smooth entropy and information spectrum

A proper way to take the asymptotic limit

Smooth divergences: Renner & Wolf (2004); Datta (2009)

$$S_\infty^\varepsilon(\rho||\sigma) := \min_{\tau : D(\tau,\rho)\le\varepsilon} S_\infty(\tau||\sigma)$$

$$S_0^\varepsilon(\rho||\sigma) := \max_{\tau : D(\tau,\rho)\le\varepsilon} S_0(\tau||\sigma)$$

Trace distance: $D(\rho,\sigma) := \frac{1}{2}\|\rho-\sigma\|_1$

Consider sequences of states $\hat{P} = \{\rho_n\}_{n=1}^\infty, \hat{\Sigma} = \{\sigma_n\}_{n=1}^\infty$ (not necessarily i.i.d.)

Information spectrum: Nagaoka & Hayashi (2007); Datta (2009)

Upper:

$$\overline{S}(\hat{P}||\hat{\Sigma}) := \lim_{\varepsilon\to+0} \limsup_{n\to\infty} \frac{1}{n} S_\infty^\varepsilon(\rho_n||\sigma_n)$$

Lower:

$$\underline{S}(\hat{P}||\hat{\Sigma}) := \lim_{\varepsilon\to+0} \liminf_{n\to\infty} \frac{1}{n} S_0^\varepsilon(\rho_n||\sigma_n)$$

Asymptotic state convertibility: Rigorous statement

Denote $(\hat{P}',\hat{\Sigma}') \prec^{\mathrm{a}} (\hat{P},\hat{\Sigma})$ if there exists a sequence of CPTP maps $\{\boldsymbol{E}_n\}_{n=1}^{\infty}$ s.t.

$$\lim_{n\to\infty} D(\boldsymbol{E}_n(\rho_n),\rho'_n) = 0 \quad \text{and} \quad \boldsymbol{E}_n(\sigma_n) = \sigma'_n$$

(Thermodynamically, GPM should preserve the Gibbs state exactly.)

Suppose that the upper and lower information spectrum collapse, i.e.,
$\underline{S}(\hat{P}||\hat{\Sigma}) = \overline{S}(\hat{P}||\hat{\Sigma}) =: S(\hat{P}||\hat{\Sigma})$ and $\underline{S}(\hat{P}'||\hat{\Sigma}') = \overline{S}(\hat{P}'||\hat{\Sigma}') =: S(\hat{P}'||\hat{\Sigma}')$.

Thm.

$(\hat{P}',\hat{\Sigma}') \prec^{\mathrm{a}} (\hat{P},\hat{\Sigma}) \;\Rightarrow\; S(\hat{P}'||\hat{\Sigma}') \leq S(\hat{P}||\hat{\Sigma})$

$(\hat{P}',\hat{\Sigma}') \prec^{\mathrm{a}} (\hat{P},\hat{\Sigma}) \;\Leftarrow\; S(\hat{P}'||\hat{\Sigma}') < S(\hat{P}||\hat{\Sigma})$

The (almost) necessary and sufficient condition is given by a single scalar potential S

Faist & Renner PRX (2018); Sagawa *et al.* JPhysA (2021);
Unital case: Gour et al., Phys. Rep. (2015); i.i.d. case: Matsumoto, arXiv (2010)

Quantum ergodic theorem: Rigorous statement

Infinite lattice $\mathbb{Z}^d$ in any spatial dimension $d = 1,2,3,\ldots$ Let $\Lambda \subset \mathbb{Z}^d$ with $|\Lambda| = n$.

Consider **spin systems**; Finite-dimensional local Hilbert spaces on individual sites

A translation-invariant state is **ergodic**, if the variance of any observable of the form $\frac{1}{|\Lambda|}\sum_{i\in\Lambda} T_i(A)$ vanishes in $\Lambda \to \mathbb{Z}^d$. Here, T_i is the shift operator on the lattice.

Let ρ_n be the reduced density operator on Λ of **an ergodic state**.

Let σ_n be the truncated Gibbs state on Λ of **a local and translation-invariant Hamiltonian** of the form $H_\Lambda = \sum_{i\in\Lambda} T_i(h_0)$.

Consider sequences $\hat{P} = \{\rho_n\}_{n=1}^{\infty}$ and $\hat{\Sigma} = \{\sigma_n\}_{n=1}^{\infty}$.

Thm.

$$\underline{S}(\hat{P}\|\hat{\Sigma}) = \overline{S}(\hat{P}\|\hat{\Sigma}) = S_1(\hat{P}\|\hat{\Sigma})$$

with the KL divergence rate $S_1(\hat{P}\|\hat{\Sigma}) := \lim_{n\to\infty} \frac{1}{n} S_1(\rho_n\|\sigma_n)$

Main idea: Quantum hypothesis testing

Task: Distinguish two states ρ and σ with σ being the false null hypothesis, and minimize the error probability of the second kind given by $\mathrm{tr}[\sigma Q]$ with $0 \leq Q \leq I$ while keeping $\mathrm{tr}[\rho Q] \geq \eta$ for $0 < \eta < 1$.

Hypothesis testing divergence: $$S_{\mathrm{H}}^{\eta}(\rho||\sigma) := -\ln\left(\frac{1}{\eta}\min_{0\leq Q\leq I, \mathrm{tr}[\rho Q]\geq\eta} \mathrm{tr}[\sigma Q]\right)$$

Determines the large deviation behavior: $\min \mathrm{tr}[\sigma Q] \simeq \eta e^{-S_H^{\eta}(\rho||\sigma)}$

It is known that $S_{\mathrm{H}}^{\eta\simeq 1}(\rho||\sigma) \simeq S_0^{\varepsilon\simeq 0}(\rho||\sigma)$ and $S_{\mathrm{H}}^{\eta\simeq 0}(\rho||\sigma) \simeq S_{\infty}^{\varepsilon\simeq 0}(\rho||\sigma)$ up to the system-size independent correction terms. Faist & Renner, PRX (2018)

Thus, the quantum ergodic theorem is equivalent to the **quantum Stein's lemma**:

For any $0 < \eta < 1$, $$\lim_{n\to\infty} \frac{1}{n} S_{\mathrm{H}}^{\eta}(\rho_n||\sigma_n) = S_1(\hat{P}||\hat{\Sigma})$$

Comparison with previous works

- **Classical case**: Stein's lemma, or asymptotic equipartition property (AEP)
  - i.i.d. case: well-known (see, e.g. Cover-Thomas)
  - p is ergodic and q is Markovian: e.g., Algoet & Cover, Annals of Prob. (1988)

- **Hiai & Petz,** CMP (1991)
  Partial proof for: ρ is completely ergodic and σ is i.i.d.

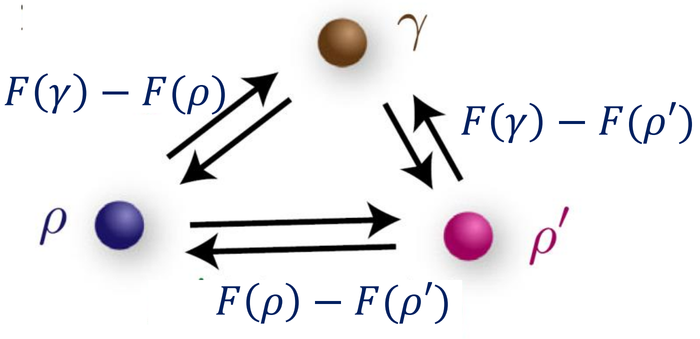
- **Ogawa & Nagaoka,** IEEE Trans. Info. Theory (2000)
  Proof for: ρ and σ are i.i.d.

- **Bjelakovic & Siegmund-Schultze,** CMP (2004)
  Proof for: ρ is ergodic and σ is i.i.d. **Non-interacting Hamiltonian**

- **The present work** (2019,2021)
  Proof for: ρ is ergodic and σ is the local Gibbs. **Interacting, many-body**

Summary of Part 1

- Proved the existence of a *complete* thermodynamic potential (a *complete* monotone) for a broad class of quantum spin systems out of equilibrium:
  - ✓ State is spatially ergodic
  - ✓ Hamiltonian is local and translation-invariant
  - ✓ In any spatial dimension



- The proof is based on:
  - ✓ Concept of information spectrum
  - ✓ Generalized quantum Stein's lemma beyond i.i.d.

- Towards resource theory of interacting, truly many-body systems

- **An open issue:** What does resource theory tell about the ergodicity breaking case (MBL, spin glass, etc.)?

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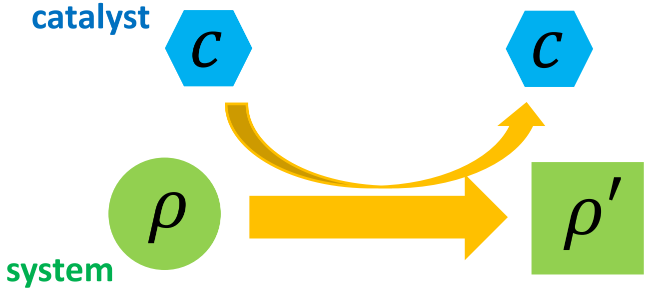
  Shiraishi & Sagawa, Phys. Rev. Lett. **126**, 150502 (2021).

Catalyst

- Catalyst assists state conversion while remaining its own state c unchanged:

$$\rho \otimes c \mapsto \rho' \otimes c$$



- The class of possible state conversions is extended

- Motivation from thermodynamics:
  It should be always allowed to add an auxiliary system "*without remaining any effect on the outside world.*"

Catalytic state conversion

Exact catalyst: No error is allowed in the catalyst state $\rho \otimes c \mapsto \rho' \otimes c$

In the classical case, the necessary and sufficient condition is given by the infinite family of the Renyi divergences $S_\alpha(\rho||\rho^{\mathrm{G}}), \alpha \in (-\infty, \infty)$

No single thermodynamic potential

Turgut, J. Phys. A (2007)
Klimesh, arXiv (2007)
Brandao et al., PNAS (2015)

In their intermediate regime, another nontrivial characterization of state convertibility emerges

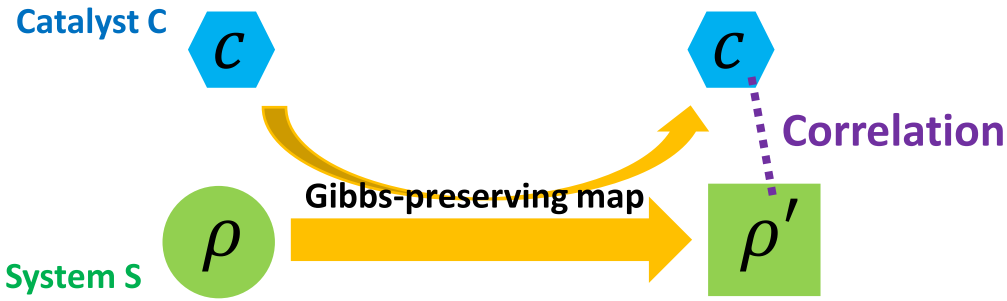
Embezzling phenomenon: If a finite (but arbitrarily small) error is allowed in the catalyst state, any states ρ, ρ' becomes convertible to each other

The resource theory becomes trivial

van Dam & Hayden,PRA (2003)
Brandao et al., PNAS (2015)

Correlated-catalytic state conversion

Catalyst returns to its initial state c exactly but with a negligibly small correlation



Conjecture: Wilming, Gallego, & Eisert, Entropy (2017); Lostaglio & Muller, PRL (2019)

The necessary and sufficient condition of state convertibility is given only by the KL divergence.

Proof for the **classical** case: Muller, PRX (2018)

Proof for the **quantum** case: Shiraishi & Sagawa, PRL (2021)

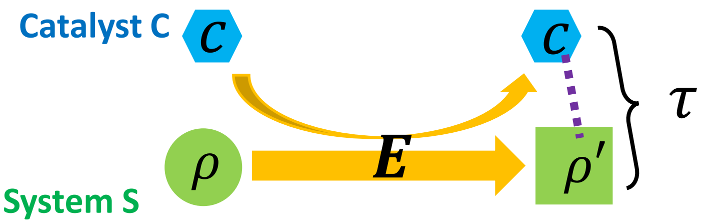
This talk

Main theorem

Theorem 1 of Shiraishi & Sagawa, PRL (2021)

Consider states ρ, ρ' of system S.

Let $F_1(\rho) := S_1(\rho||\rho^G) + F$ be the free energy.



$F_1(\rho) \geq F_1(\rho')$ is satisfied *if and only if*

there exist

- catalyst C and its state c,
- a Gibbs-preserving map $\boldsymbol{E}$ satisfying $E(\rho \otimes c) = \tau$

such that

- $\mathrm{tr}_S[\tau] = c$,
- $\mathrm{tr}_C[\tau]$ is arbitrarily close to ρ' (in the trace distance),
- the correlation (measured by mutual information) between S and C in τ is arbitrarily small.

Idea of the proof

Suppose that $F_1(\rho) \geq F_1(\rho')$. (Its converse is obvious from the monotonicity.)

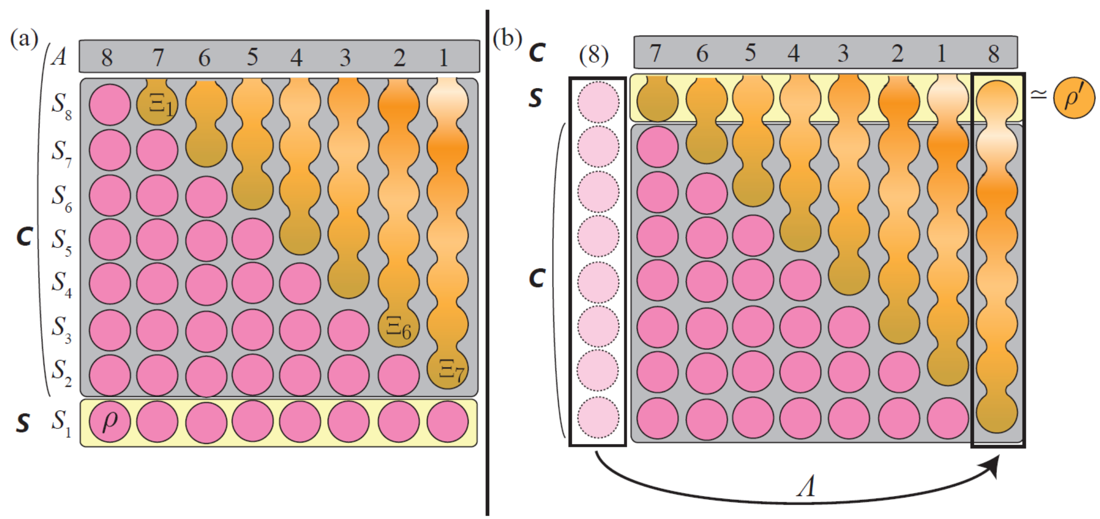
From the quantum Stein's lemma, $\rho^{\otimes n} \mapsto \rho'^{\otimes n}$ is asymptotically possible by a GPM.

Let Λ be the GPM such that $\Xi := \Lambda(\rho^{\otimes n}) \simeq \rho'^{\otimes n}$.

Prepare a (big) catalyst consisting of $(n-1)$-copies of S and A spanned by $\{|k\rangle\}_{k=1}^{n}$.

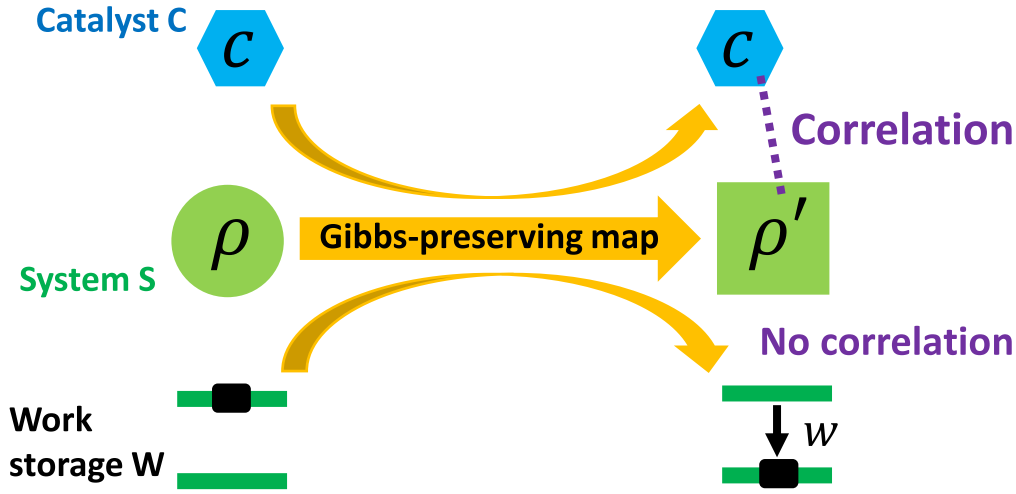
The catalyst state is $c := \frac{1}{n}\sum_{k=1}^{n} \rho^{\otimes(k-1)} \otimes \Xi_{n-k} \otimes |k\rangle\langle k|$,
where Ξ_i is the partial state of Ξ on the first i-copies of S.

Then consider the following operation on SC (for $n = 8$):



Work investment

Theorem 2 of Shiraishi & Sagawa, PRL (2021)



Consider single-shot work investment $w > 0$ without allowing correlation between W and SC.

(Thus this cannot be obtained from Theorem 1.)

Suppose that $F_1(\rho') > F_1(\rho)$.

The state conversion is possible *if and only if* $w \geq F_1(\rho') - F_1(\rho)$

Summary of Part 2

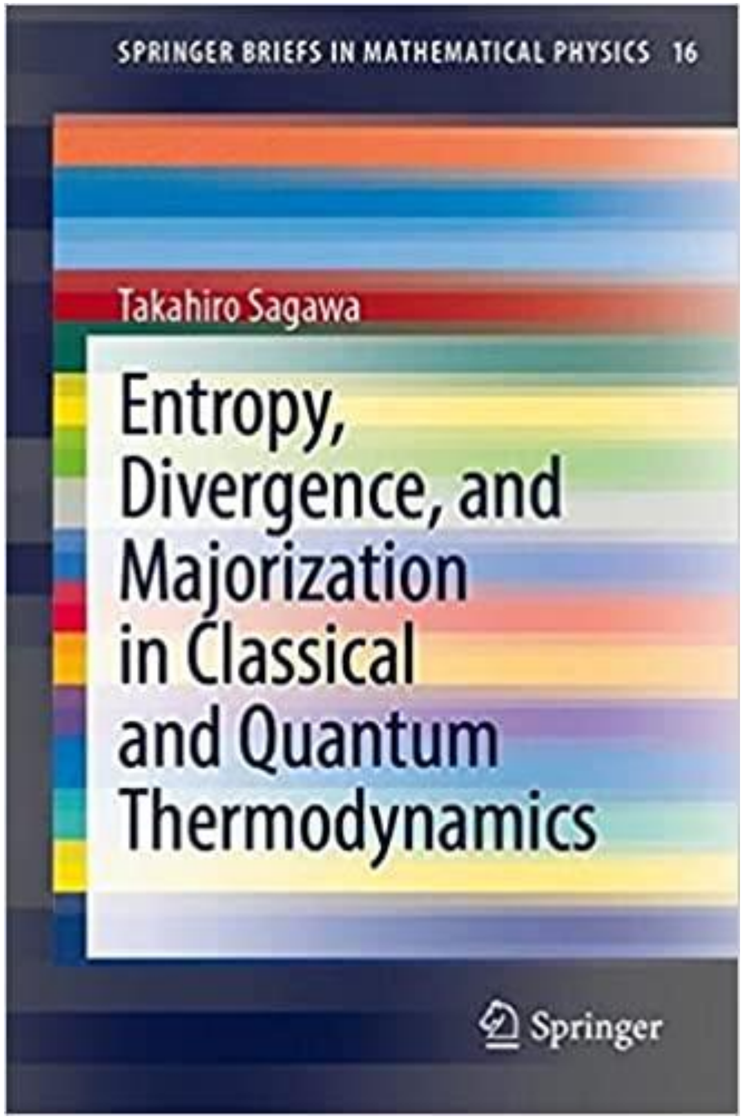
Shiraishi & Sagawa,
Phys. Rev. Lett. **126**, 150502 (2021).

- **Conjecture** [Wilming, Gallego, & Eisert, Entropy (2017); Lostaglio & Muller, PRL (2019)]:
  Catalytic state conversion is characterized by a single thermodynamic potential given by the KL divergence, $F_1(\rho) \coloneqq S_1(\rho || \rho^{\mathrm{G}}) + F$, if an arbitrarily small amount of **correlation** is allowed between the system and the catalyst.

- We proved the **quantum** case.
  - Based on the asymptotic theory, especially the quantum Stein's lemma, because the catalyst can be huge

- Our result is also applicable to:
  - More general state conversion $(\rho, \sigma) \mapsto (\rho', \sigma')$ (quantum d-majorization).
  - Various resource theories in which the KL divergence asymptotically emerges [cf. Brandao & Gour, PRL (2015)].

Thank you for your attention!



SpringerBriefs in Mathematical Physics

arXiv:2007.09974

Appendix of Part 1

Theorem I

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

Let $\Lambda \subset \mathbb{Z}^d$ with $|\Lambda| = n$.

Let ρ_n be the reduced density operator on Λ of **an ergodic state**.

Let σ_n be the truncated Gibbs state on Λ of **a local and translation-invariant Hamiltonian.**

Consider sequences $\hat{P} = \{\rho_n\}_{n=1}^{\infty}$ and $\hat{\Sigma} = \{\sigma_n\}_{n=1}^{\infty}$.

Then,

$$\underline{S}(\hat{P}\|\hat{\Sigma}) = \overline{S}(\hat{P}\|\hat{\Sigma}) = S_1(\hat{P}\|\hat{\Sigma})$$

with the KL divergence rate

$$S_1(\hat{P}\|\hat{\Sigma}) := \lim_{n\to\infty} \frac{1}{n} S_1(\rho_n\|\sigma_n)$$

Outline of the proof

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

Step 1 (Lemma 5):
Prove the quantum Stein's lemma under a very general sufficient condition that a sequence of "typical operators" W_n^ε exists.
The key idea: the *semidefinite programing*, which makes the converse part tractable.

This step is heavily inspired by Bjelakovic & Siegmund-Schultze, quant-ph/0307170.

Step 2 (Theorem 3):
Construct "relative typical projectors" for our setting:
$R_n^\varepsilon \coloneqq \mathrm{Proj}\left\{-\frac{1}{n}\ln\sigma_n \in [m-\varepsilon, m+\varepsilon]\right\}$ with $m \coloneqq -\lim_{n\to\infty}\frac{1}{n}\mathrm{tr}[\rho_n \ln\sigma_n]$;
consider typical projectors Π_n^ε of the quantum Shannon-McMillan theorem;
and show that $W_n^\varepsilon \coloneqq \Pi_n^\varepsilon R_n^\varepsilon$ satisfy the desired properties to apply Step 1,
by using the quantum Shannon-McMillan theorem
and the definition of ergodicity with observable h_0 in the local Hamiltonian.

Quantum Shannon-McMillan theorem: For ergodic states, there exist "typical projectors" with respect to the von Neumann entropy rate.

Bjelakovic, Krüger, Siegmund-Schultze, Szkoła, Inventiones mathematicae (2004)
Ogata, Letters in Mathematical Physics (2013)

A general condition for quantum Stein's lemma

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

Let $\hat{P} = \{\rho_n\}_{n=1}^{\infty}, \hat{\Sigma} = \{\sigma_n\}_{n=1}^{\infty}$ be any sequences of states.
Suppose that there exists $c \in \mathbb{R}$ such that
for any $\varepsilon > 0$, there exists a sequence of operators W_n^{ε} that satisfy,
for sufficiently large n,

$$W_n^{\varepsilon\dagger} W_n^{\varepsilon} \leq I;$$
$$\mathrm{tr}\left[W_n^{\varepsilon} \sigma_n W_n^{\varepsilon\dagger}\right] \leq e^{-n(c-2\varepsilon)};$$
$$W_n^{\varepsilon\dagger} \rho_n W_n^{\varepsilon} \leq e^{n(c+2\varepsilon)} \sigma_n;$$
$$\lim_n \mathrm{Re}(\mathrm{tr}[W_n^{\varepsilon} \rho_n]) = 1.$$

Then, for any $0 < \eta < 1$,

$$S_{\mathrm{H}}^{\eta}(\hat{P} \| \hat{\Sigma}) := \lim_{n\to\infty} \frac{1}{n} S_{\mathrm{H}}^{\eta}(\rho_n \| \sigma_n) = c.$$

Semidefinite programing: (**Primal** / **Dual**)

$$S_H^{\eta}(\rho\|\sigma) = -\ln \min_{\substack{0\leq Q\leq I \\ \mathrm{tr}[Q\rho]\geq\eta}} \frac{1}{\eta}\mathrm{tr}[Q\sigma] = -\ln \max_{\substack{\mu\geq 0, X\geq 0 \\ \mu\rho\leq\sigma+X}} \left(\mu - \frac{\mathrm{tr}[X]}{\eta}\right)$$

Primal: Choose $Q := W_n^{\varepsilon\dagger} W_n^{\varepsilon}$, then show $S_{\mathrm{H}}^{\eta}(\hat{P}\|\hat{\Sigma}) \geq c$.
Dual: Choose $X := 2\mu(I - W_n^{\varepsilon\dagger})\rho_n(I - W_n^{\varepsilon})$, then show $S_{\mathrm{H}}^{\eta}(\hat{P}\|\hat{\Sigma}) \leq c$.

Quantum Shannon-McMillan theorem

Suppose that $\hat{P} = \{\rho_n\}_{n=1}^{\infty}$ is ergodic.
Then, for any $\varepsilon > 0$, there exists a sequence of projectors Π_n^ε (typical projectors) that satisfy for sufficiently large n,

$$e^{-n(s+\varepsilon)}\Pi_n^\varepsilon \leq \Pi_n^\varepsilon \rho_n \Pi_n^\varepsilon \leq e^{-n(s-\varepsilon)}\Pi_n^\varepsilon,$$
$$e^{n(s-\varepsilon)} \leq \mathrm{tr}[\Pi_n^\varepsilon] \leq e^{n(s+\varepsilon)},$$
$$\lim_{n\to\infty} \mathrm{tr}[\Pi_n^\varepsilon \rho_n] = 1\,,$$

where $s := \lim_{n\to\infty} \frac{1}{n} S_1(\rho_n)$ is the von Neumann entropy rate.

Bjelakovic, Krüger, Siegmund-Schultze, Szkoła, Inventiones mathematicae (2004)
Ogata, Letters in Mathematical Physics (2013)

In the classical case,
this implies that $-\ln p_n$ converges to the Shannon entropy rate *in probability*.

Beyond ergodic states

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

$\hat{P}^{(k)}$: ergodic, $\hat{P}$: a mixture of $\hat{P}^{(k)}$'s with probability r_k $(k = 1, \ldots, K < \infty)$.

$\hat{\Sigma}$: local Gibbs

Then the upper and lower information spectrum split as

$$\underline{S}(\hat{P}||\hat{\Sigma}) = \min_k \{S_1(\hat{P}^{(k)}||\hat{\Sigma})\}$$

$$\overline{S}(\hat{P}||\hat{\Sigma}) = \max_k \{S_1(\hat{P}^{(k)}||\hat{\Sigma})\}$$

whereas $S_1(\hat{P}||\hat{\Sigma}) = \sum_k r_k S_1(\hat{P}^{(k)}||\hat{\Sigma})$

If $\hat{P}^{(k)}$'s have the same KL divergence rate,
the single-potential characterization still works.

Thermal operation (a general form)

Def.

A CP trace-nonincreasing map $\boldsymbol{E}$ is a **thermal operation** with the initial and final Hamiltonians H_{S} and $H_{\mathrm{S}}{}'$, if there exist a heat bath B with Hamiltonian H_{B} with the corresponding Gibbs state $\rho_{\mathrm{B}}^{\mathrm{G}}$ and a partial isometry V such that

$$\boldsymbol{E}(\rho) = \mathrm{tr}_{\mathrm{B}}[V\rho \otimes \rho_{\mathrm{B}}^{\mathrm{G}} V^{\dagger}]$$

and

$$V(H_{\mathrm{S}} + H_{\mathrm{B}}) - (H_{\mathrm{S}}' + H_{\mathrm{B}})V^{\dagger} = 0$$

- The trace-nonincreasing property reflects the possibility that the clock imperfect.
- Different Hilbert spaces for the input and output states are allowed.
- V is a partial isometry if $V^{\dagger}V$ and $VV^{\dagger}$ are projectors.

Thermal operation implies a Gibbs-sub-preserving map: $\boldsymbol{E}\left(e^{-\beta H_{\mathrm{S}}}\right) \leq e^{-\beta H_{\mathrm{S}}'}$

Aid of work and coherence

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

Def.

A CP trace-nonincreasing map $\boldsymbol{E}$ is a (w, η)-**work/coherence-assisted thermal operation** with the initial and final Hamiltonians H_{S} and $H_S{}'$, if there exist

a work storage W with Hamiltonians H_{W} and $H_{\mathrm{W}}{}'$
with energy eigenstates $|E\rangle$ and $|E'\rangle$ satisfying $E - E' = w$,

a coherence storage C with Hamiltonians H_{C} and $H_{\mathrm{C}}{}'$satisfying $\|H_{\mathrm{C}}\|_\infty \leq \eta$ and $\|H_{\mathrm{C}}{}'\|_\infty \leq \eta$ and pure states $|C\rangle$ and $|C'\rangle$ of C,

a thermal operation $\boldsymbol{E}_{\mathrm{SWC}}$ on SWC with Hamiltonian $H_{\mathrm{S}} + H_{\mathrm{W}} + H_{\mathrm{C}}$ and $H_{\mathrm{S}}{}' + H_{\mathrm{W}}{}' + H_{\mathrm{C}}{}'$

such that

$$\boldsymbol{E}(\rho) = \langle E'|\langle C'|\boldsymbol{E}_{\mathrm{SWC}}(\rho \otimes |E\rangle\langle E| \otimes |C\rangle\langle C|)|E'\rangle|C'\rangle$$

Again, the input and output Hilbert spaces can be different (for S, W, C).
An infinite-dimensional space is allowed for C (from a technical reason).

Asymptotic thermal operations

Consider sequences of states $\hat{P} = \{\rho_n\}_{n=1}^{\infty}$, $\hat{P}' = \{\rho_n'\}_{n=1}^{\infty}$ and Hamiltonians $\hat{H} = \{H_{S,n}\}_{n=1}^{\infty}$ and $\hat{H}' = \{H_{S,n}{}'\}_{n=1}^{\infty}$ and the corresponding Gibbs states $\hat{\Sigma}, \hat{\Sigma}'$.

Def.

$\hat{P}$ can be converted into $\hat{P}'$ by an **asymptotic thermal operation** with work cost w, if there exist sequences $\{w_n\}_{n=1}^{\infty}$, $\{\eta_n\}_{n=1}^{\infty}$, and $\{\varepsilon_n\}_{n=1}^{\infty}$, and a sequence of (w_n, η_n)-work/coherence assisted thermal operations $\{\boldsymbol{E}_n\}_{n=1}^{\infty}$ with Hamiltonians $H_{s,n}$ and $H_{S,n}{}'$ such that

$$D(\boldsymbol{E}_n(\rho_n), \rho_n') \leq \varepsilon_n$$

and $$\lim_{n\to\infty} \frac{w_n}{n} = w; \quad \lim_{n\to\infty} \frac{\eta_n}{n} = 0; \quad \lim_{n\to\infty} \varepsilon_n = 0.$$

The monotonicity of information spectrum still holds under the above (trace-nonincreasing) definition:

$$\underline{S}(\hat{P}||\hat{\Sigma}) + \beta w \geq \underline{S}(\hat{P}'||\hat{\Sigma}'); \quad \overline{S}(\hat{P}||\hat{\Sigma}) + \beta w \geq \overline{S}(\hat{P}'||\hat{\Sigma}')$$

Theorem II

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, J. Phys. A: Math. Theor. **54**, 495303 (2021).

Consider sequences of states $\hat{P} = \{\rho_n\}_{n=1}^{\infty}$, $\hat{P}' = \{\rho'_n\}_{n=1}^{\infty}$ and
Hamiltonians $\hat{H} = \{H_{S,n}\}_{n=1}^{\infty}$ and $\hat{H}' = \{H_{S,n}{}'\}_{n=1}^{\infty}$ and the corresponding Gibbs states $\hat{\Sigma}, \hat{\Sigma}'$.

Suppose that $\underline{S}(\hat{P}||\hat{\Sigma}) = \overline{S}(\hat{P}||\hat{\Sigma}) =: S(\hat{P}||\hat{\Sigma})$ and $\underline{S}(\hat{P}'||\hat{\Sigma}') = \overline{S}(\hat{P}'||\hat{\Sigma}') =: S(\hat{P}'||\hat{\Sigma}')$.

$\hat{P}$ can be converted into $\hat{P}'$ by an **asymptotic thermal operation**
with the initial and final Hamiltonians $\hat{H}$ and $\hat{H}'$ and with the work cost w,

if and only if

$$\beta w \geq S(\hat{P}'||\hat{\Sigma}') - S(\hat{P}||\hat{\Sigma})$$

This implies that **if the upper and lower information spectrum collapse, then thermal operations work in the fully quantum regime.**

The key lemma

Lemma 4 of
Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao,
J. Phys. A: Math. Theor. **54**, 495303 (2021).

If the lower and upper information spectrum collapse, then coherence is suppressed.

Let $H = \sum_k E_k P_k$ be the Hamiltonian with eigen-projector P_k.

Suppose that the exist $S \in \mathbb{R}$ and $\Delta > 0$ such that

$$S_\infty(\rho || e^{-\beta \mathrm{H}}) \leq S + \Delta\,; \quad S_{1/2}(\rho || e^{-\beta H}) \geq S - \Delta.$$

Then, for any k, k',

$$\|P_k \rho P_{k'}\|_1 \leq \exp(-\beta\,|E_k - E_{k'}|/2 + \Delta).$$

Here, $S_{1/2}(\rho||\sigma) := -\ln\left\|\rho^{1/2}\sigma^{1/2}\right\|_1^2$ plays a role of the min divergence, as
$S_{1/2}^{2\varepsilon}(\rho||\sigma) \geq S_0^{2\varepsilon}(\rho||\sigma) \geq S_{1/2}^{\varepsilon}(\rho||\sigma) - 6\ln(3/\varepsilon)$

Because the coherence in ρ is small in this case,
the aid of a small amount of coherence is enough to implement the thermal operation.

Theorem I + II

Consider a quantum spin system on lattice $\mathbb{Z}^d$ in any spatial dimension d.

Suppose that $\hat{P}$ and $\hat{P}'$ are ergodic, and Hamiltonians $\hat{H}$ and $\hat{H}'$ are local and translation-invariant with the Gibbs states $\hat{\Sigma}$ and $\hat{\Sigma}'$.

Then, $\hat{P}$ can be converted into $\hat{P}'$ by an asymptotic thermal operation with the work cost w (and with the aid of a small amount of coherence),

if and only if $$\beta w \geq S_1(\hat{P}' \| \hat{\Sigma}') - S_1(\hat{P} \| \hat{\Sigma})$$

with S_1 being the KL divergence rate.

The KL divergence is a (asymptotically) *complete* monotone.

The emergent thermodynamic potential is information spectrum in general, while it reduces to the KL divergence with an ergodic state and a local Hamiltonian.