On the existence of a complete thermodynamic potential for quantum many-body systems

Takahiro Sagawa

Department of Applied Physics, University of Tokyo

CSH Online Workshop “Stochastic thermodynamics of complex systems”
May 27, 2020 @Zoom

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)

Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, arXiv:1907.05650

Accepted by QIP 2020

Outline

- Introduction
- Preliminaries
- Main result
- Technical details
- Summary

Outline

- **Introduction**
- Preliminaries
- Main result
- Technical details
- Summary

Complete thermodynamic potential

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 $W \geq \Delta F$

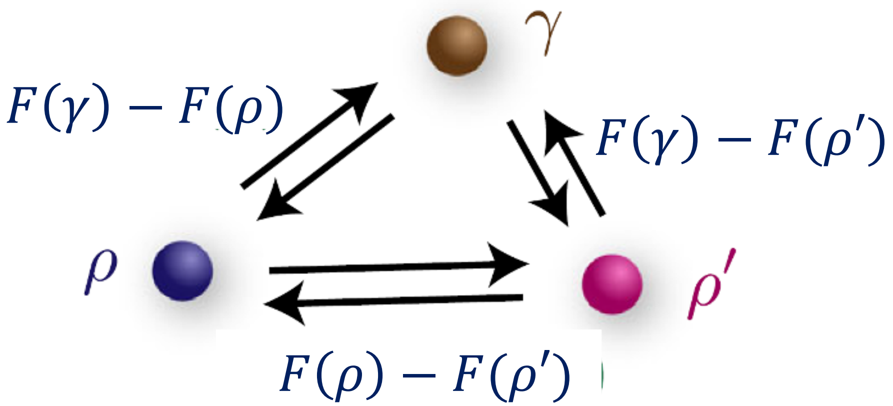
Mathematically rigorous axiomatic formulation:
Lieb & Yngvason, Phys. Rep. (1999)

Watt steam engine (from Wikipedia)

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

Our result

Proved **the existence of a thermodynamic potential**
that completely characterizes state convertibility
of a broad class of interacting quantum many-body systems
with some physically reasonable assumptions,
even for out-of-equilibrium and fully quantum situations.

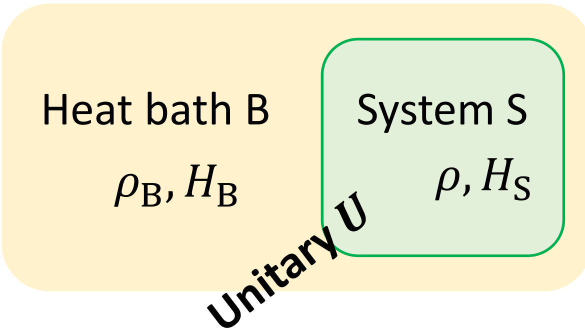


A methodology:
Resource theory of thermodynamics

Outline

- Introduction
- **Preliminaries**
- Main result
- Technical details
- Summary

Thermodynamic operations

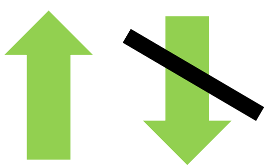


Dynamics of S:

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

Completely-positive and trace-preserving (CPTP) map

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



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!**

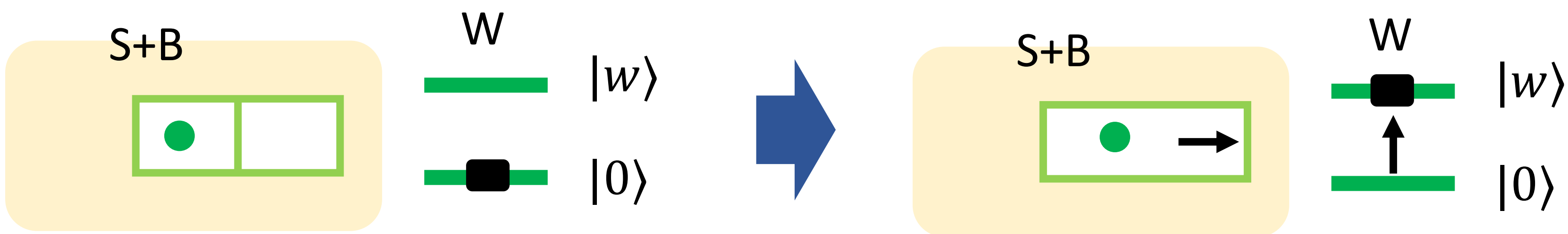
- ✓ Jaynes-Cummings model at the resonant condition
- ✓ Quantum master equation with the rotating wave approximation

Single-shot work bound: a resource-theoretic view

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 (2013); Aberg (2013)

ρ: Nonequilibrium state

By Gibbs-preserving maps

ρ^{G}: Gibbs state

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

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

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

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

Outline

- Introduction
- Preliminaries
- **Main result**
- Technical details
- Summary

Reversibility in equilibrium thermodynamics

Equilibrium 1

$w \leq F(1) - F(2)$ $w \geq F(1) - F(2)$

Equilibrium 2

- ✓ The equality is achieved in the quasi-static limit, where the work costs exactly cancel in the cyclic opeation; *"without remaining any effect on the outside world…"*

- ✓ This implies that state conversion is completely characterized by **a single thermodynamic potential, equilibrium free energy $\boldsymbol{F}$.**

Reversibility in the single-shot case

ρ: Nonequilibrium state

$\beta w \leq S_0(\rho||\rho^{\mathrm{G}})$ $\Leftarrow$ **By Gibbs-preserving maps** $\Leftarrow$ $\beta w \geq S_\infty(\rho||\rho^{\mathrm{G}})$

ρ^{G}: Gibbs state

Analogy with the conventional case apparently fails;

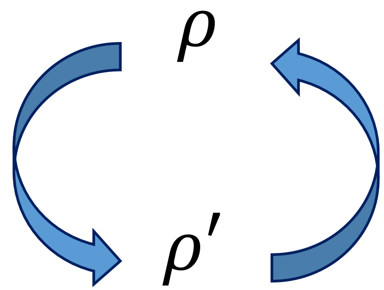
- ✓ S_0 and S_∞ do not match in general; a mere cyclic operation requires work $S_\infty - S_0$.
- ✓ Thus, **a single *complete* thermodynamic potential does not exist,** except for equilibrium transitions.
- ✓ Moreover, the above inequalities cannot apply for thermal operations in the fully quantum regime.

Question and the result

Q1: Is it still possible to have a single thermodynamic potential $F_?$ that completely characterizes state convertibility, in out-of-equilibrium and fully quantum situations?

Q2: If Yes, does the potential work not only for the Gibbs-preserving maps, but also for thermal operations?

$$w \leq F_?(\rho) - F_?(\rho') \Leftarrow$$



$$\Leftarrow w \geq F_?(\rho) - F_?(\rho')$$

A1: Yes, if taking the asymptotic (macroscopic) limit, and
if the state is spatially ergodic and the Hamiltonian is local and translation-invariant.

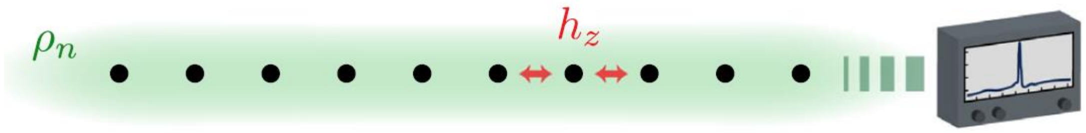
A2: Yes, with the aid of a small amount of quantum coherence.

Main result (1/2)

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 ,

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

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

This is equivalent to a generalization of the quantum Stein's lemma for quantum hypothesis testing, beyond independent and identically distributed (i.i.d.) situations.

Main result (2/2)

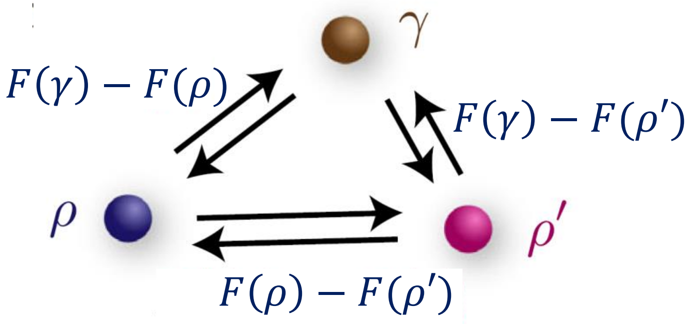
Under the foregoing setup,
$F_1(\rho) := S_1(\rho || \rho^{\mathrm{G}}) + F$ serves as the nonequilibrium free energy:

ρ can be asymptotically converted into ρ'
by a thermal operation with the work cost w
and with the aid of a small amount of quantum coherence,

if and only if $$\boxed{w \geq F_1(\rho') - F_1(\rho)}$$

Here, thermal operation asymptotically works in the fully quantum case;
The key is the fact that any ergodic state has a small amount of coherence.

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



Outline

- Introduction
- Preliminaries
- Main result
- **Technical details**
- Summary

Smooth entropy and information spectrum

A proper way to take the asymptotic limit

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

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

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

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:

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

Our quantum ergodic theorem

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

Main methodology: 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:

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

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 $0 < \eta < 1$,

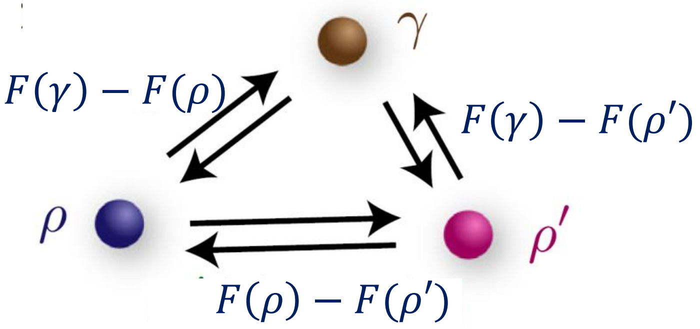
$$\lim_{n\to\infty}\frac{1}{n}S_{\mathrm{H}}^{\eta}(\rho_n||\sigma_n) = S_1(\hat{P}||\hat{\Sigma})$$

Outline

- Introduction
- Preliminaries
- Main result
- Technical details
- **Summary**

Summary and outlook

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



- The proof consists of:
  - ✓ Generalized quantum Stein's lemma beyond i.i.d.
  - ✓ Construct asymptotic thermal operations in the fully quantum regime

- 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.)?

Thank you for your attention!

Faist, Sagawa, Kato, Nagaoka, Brandao, Phys. Rev. Lett. **123**, 250601 (2019)
Sagawa, Faist, Kato, Matsumoto, Nagaoka, Brandao, arXiv:1907.05650

Appendix

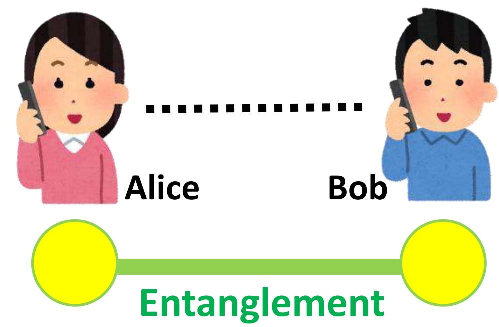
What is resource theory?

An information theoretic framework to quantify "useful resources"

It is crucial to identify what are **free** states and **free** operations.

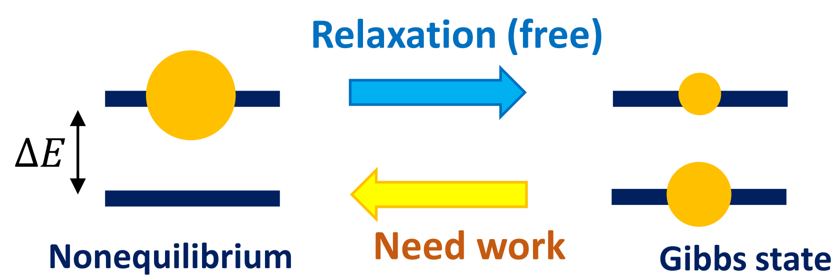
Resource theory of entanglement

Resource: entanglement
Free states: separable states
Free operations: local operation and classical communication (LOCC)



Resource theory of thermodynamics

Resource: work / free energy
Free states: Gibbs states (thermal equilibrium)
Free operations: Relaxation processes



Note: Resource theory of entanglement $\cong$ Resource theory of thermodynamics at $T = \infty$

Various resource theories

Resource theory of **entanglement**

Free state: separable state**;** **Free operation:** LOCC

Horodecki, Horodecki, Horodecki, & Horodecki, RMP (2009)

Resource theory of **thermodynamics**

Free state: Gibbs state; **Free operation:** Gibbs-preserving map or thermal operation

Horodecki & Oppenheim, Nat. Commu. (2013); Gour *et al*., Phys. Rep. (2015)

Resource theory of **quantum coherence**

Free state: incoherent (diagonal) state; **Free operation:** incoherent operation

Baumgratz, Cramer & Plenio, PRL (2014); Winter & Yang, PRL (2016)

Resource theory of **asymmetry**

Free state: invariant state under symmetry G; **Free operation:** symmetric operation

Bartlett, Rudolph, & Spekkens, RMP (2007)

…and more.

Second law from the monotonicity

$$S_1(\rho||\sigma) \geq S_1(\boldsymbol{E}(\rho)||\boldsymbol{E}(\sigma))$$

$\boldsymbol{E}$: any CPTP map

Lieb & Ruskai (1973); Petz (1986)

The KL divergence is a *monotone*.

Gibbs-preserving map (GPM): $\boldsymbol{E}(\rho^{\mathrm{G}}) = \rho^{\mathrm{G}}$

$$\Rightarrow \quad S_1(\rho||\rho^{\mathrm{G}}) \geq S_1(\boldsymbol{E}(\rho)||\rho^{\mathrm{G}})$$

$$\Leftrightarrow \quad \Delta S_1 \geq \beta Q$$

Clausius inequality (or "Landauer principle")

$\Delta S_1 \coloneqq S_1(\boldsymbol{E}(\rho)) - S_1(\rho)$ $\quad$ $Q := \mathrm{tr}[H\boldsymbol{E}(\rho)] - \mathrm{tr}[H\rho]$ (heat)

GPM at $\beta = 0 \Leftrightarrow \boldsymbol{E}(I) = I$ (unital) $\Rightarrow$

$$S_1(\rho) \leq S_1(\boldsymbol{E}(\rho))$$

Converse?

There exists a CPTP E s.t.

$$\rho' = \boldsymbol{E}(\rho), \sigma' = \boldsymbol{E}(\sigma) \quad \overset{\Rightarrow}{\not\Leftarrow} \quad S_1(\rho||\sigma) \geq S_1(\rho'||\sigma')$$

The “second law” does not provide a *sufficient* condition for state conversion.

The KL divergence is not a *complete* monotone.

Example: $\rho = \mathrm{diag}\left(\frac{2}{3}, \frac{1}{6}, \frac{1}{6}\right) \qquad \rho' = \mathrm{diag}\left(\frac{1}{2}, \frac{1}{2}, 0\right)$

$S_1(\rho) < S_1(\rho')$ but there is *no* unital CPTP s.t. $\rho' = E(\rho)$

Asymptotic state convertibility

Definition of asymptotic state conversion

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.

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

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

We can take the asymptotic limit straightforwardly:

Thm.

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

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

Faist & Renner PRX (2018); Sagawa *et al.* arXiv (2019);
Unital case: Gour et al., Phys. Rep. (2015); i.i.d. case: Matsumoto, arXiv (2010)

A bit history of Stein’s lemma

- **Classical case**: Stein’s lemma, or asymptotic equipartition property (AEP)
  - i.i.d. case: quite 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. (Proved the “strong converse”)

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

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

Beyond ergodic states

$\hat{P}^{(k)}$: 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.

Theorem II

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.**