Quantum thermodynamics of correlated-catalytic state conversion at small-scale

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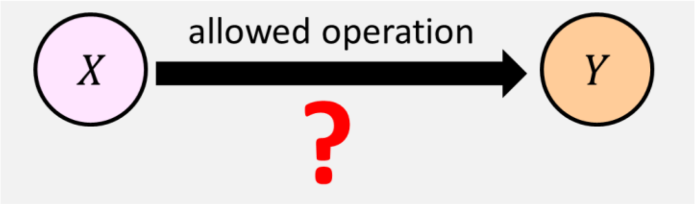
(collaborator: Takahiro Sagawa)

N. Shiraishi and T. Sagawa, Phys. Rev. Lett. 126, 150502 (2021)

One slide summary



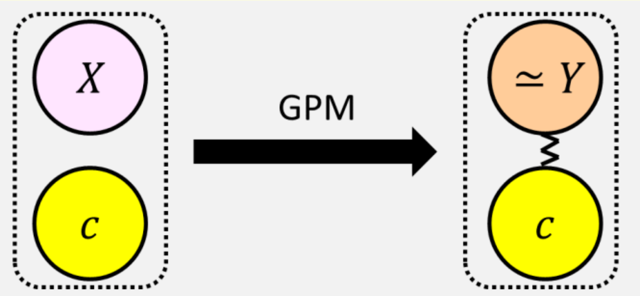
State convertibility (thermo)

macro: second law

micro: (usually) infinite ineq.

Main result

In small quantum systems, ρ is convertible to ρ' via a thermodynamic process with **correlated catalyst** if and only if $\boldsymbol{F(\rho) \geq F(\rho')}$.



Outline

Motivation and background

Main result and its proof

Remarks and future prospects

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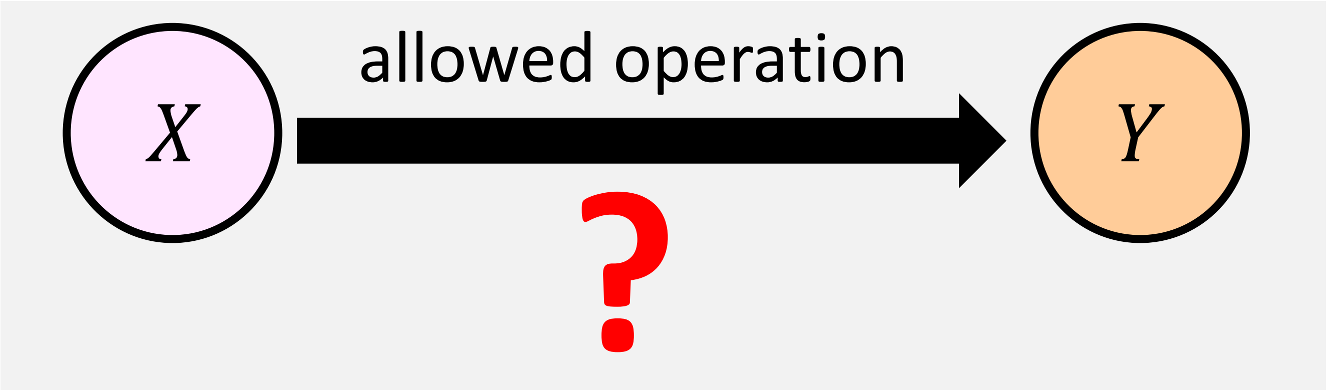
Remarks and future prospects

Motivation from macroscopic thermodynamics

X, Y: equilibrium states



In conventional thermodynamics,

$$\text{(adiabatic operation)}: S(X) \leq S(Y)$$

$$\text{(isothermal operation)}: F(X) \geq F(Y)$$

is the **necessary and sufficient condition**.

(E. H.Lieb and J. Yngvason, Phys. Rep. 310, 1 (1999).)

Situation is completely different in microscopic case

In contrast, in microscopic cases various **new constraints** other than the second law emerge.

Ex) majorization, infinite inequalities…

Questions in quantum thermodynamics

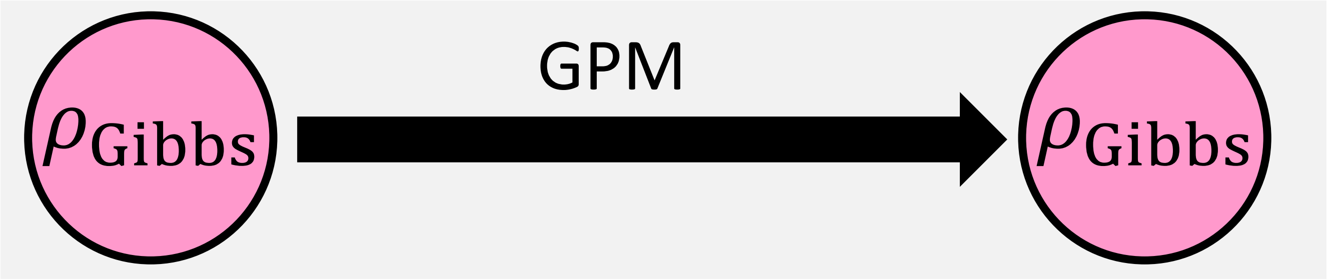
- What is the **necessary and sufficient condition** (nec.&suff.) for state conversions?
- Does **the second law** become a unique criterion? (i.e., a single monotone)

Gibbs-preserving map

We restrict the class of allowed operations to a set of **Gibbs-preserving maps** (with a fixed temperature).

Gibbs-preserving map (GPM)

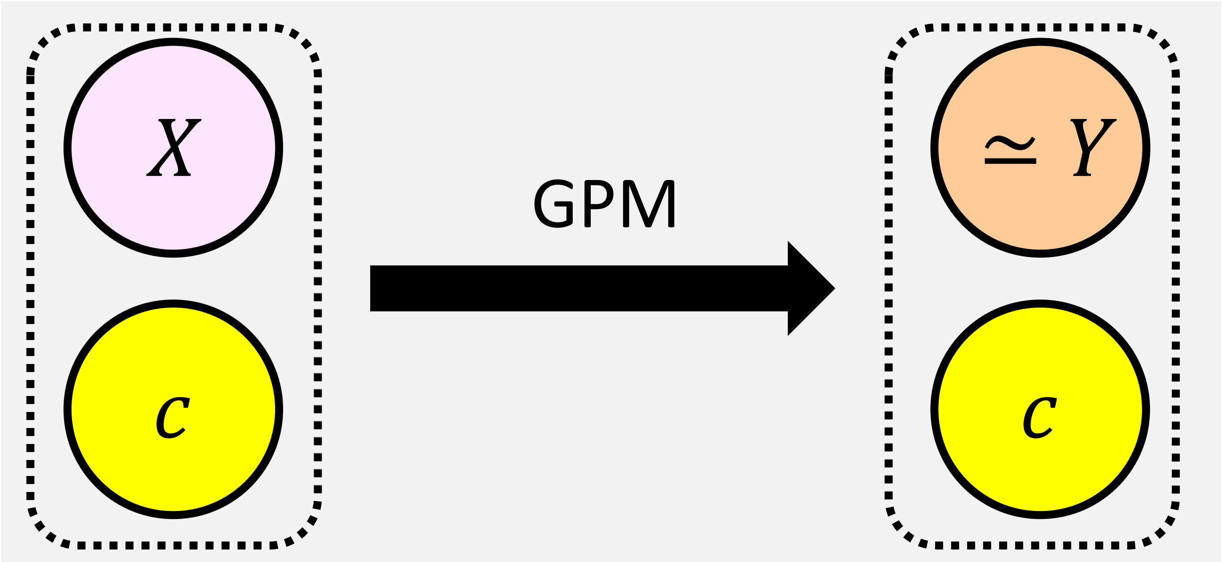
CPTP map satisfying $\boldsymbol{\Lambda(\rho_{\mathrm{Gibbs}}) = \rho_{Gibbs}}$



GPM is a standard class of thermodynamic operations

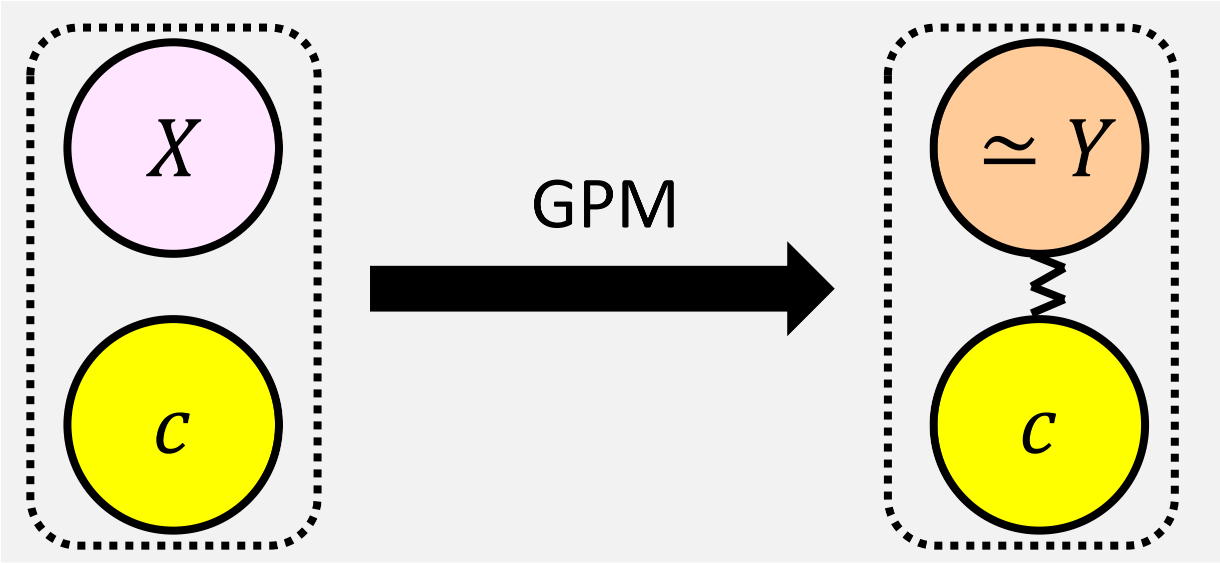
State conversion with catalyst

We introduce a **catalyst** system, which does not change through the map but helps conversion.



We say that $X \to Y$ is **convertible with a catalyst** if for any $\varepsilon > 0$ there exist proper Λ and c s.t. $\Lambda(X \otimes c) = Y' \otimes c$ with $d(Y, Y') < \varepsilon$

State conversion with **correlated** catalyst



$X \to Y$ is **convertible with a correlated catalyst** if for any $\varepsilon > 0$ there exist proper Λ and c s.t. $\Lambda(X \otimes c) = \tau$ with $\mathbf{Tr}_S[\boldsymbol{\tau}] = \boldsymbol{c}$, $\boldsymbol{d}(\boldsymbol{Y}, \mathbf{Tr}_C[\boldsymbol{\tau}]) < \boldsymbol{\varepsilon}$, and the correlation is arbitrarily small.

Summarizing known results

	Classical	**Quantum**
GPM	d-majorization	**No simple criterion**
GPM with catalyst	Infinite inequalities $F_\alpha(\rho) \geq F_\alpha(\rho\,')$	**No simple criterion**
GPM with correlated catalyst	The second law $F(\rho) \geq F(\rho')$	**???**

GPM: D. Blackwell, Proc. Math. Statist. and Prob. 93 (1951)

GPM with catalyst: F. Brandao, *et al.*, PNAS 112, 3275 (2015)

GPM with correlated catalyst: M. P. Muller, Phys. Rev. X 8, 041051 (2018)

There is a conjecture

In the quantum case, it is conjectured that…

Conjecture

In the quantum case, the nec.&suff. condition to convert $\rho \to \rho'$ by GPM with a correlated catalyst is the second law with quantum KL divergence ($F(\rho) = S(\rho||\rho_{\mathrm{Gibbs}})$):

$$F(\rho) \geq F(\rho')$$

(H. Wilming, R. Gallego, and J. Eisert, Entropy 19, 241 (2017).
M. Lostaglio and M. P. Muller, Phys. Rev. Lett. 123, 020403 (2019))

Single thermodynamic potential!

We need new approach!

	Classical	Quantum
GPM	d-majorization	**No simple criterion**
GPM with catalyst	Infinite inequalities $F_\alpha(\rho) \geq F_\alpha(\rho')$	**No simple criterion**
GPM with correlated catalyst	The second law $F(\rho) \geq F(\rho')$	???

used in proof

used in proof

We cannot follow the approach in classical cases.

Completely new approach is needed!

Outline

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Main result and its proof

Remarks and future prospects

Main result

Main result

In the quantum case, nec.&suff. condition to convert $\rho \to \rho'$ by GPM with a correlated catalyst is the second law with quantum KL divergence ($F(\rho) = S(\rho||\rho_{\mathrm{Gibbs}})$):

$$F(\rho) \geq F(\rho')$$

(N. Shiraishi and T. Sagawa, Phys. Rev. Lett. 126, 150502 (2021))

The conjecture is solved in positive.
The second law is recovered in quantum microscopic systems.

Necessary part (easy part)

Let $\Lambda(\rho \otimes c) = \tau$ with $\mathrm{Tr}_S[\tau] = c$.
Using the additivity, superadditivity, and monotonicity of KL divergence, we have

$$
\begin{aligned}
& S(\rho||\rho_{\mathrm{Gibbs}}) + S(c||c_{\mathrm{Gibbs}}) \\
= & S(\rho \otimes c||\rho_{\mathrm{Gibbs}} \otimes c_{\mathrm{Gibbs}}) \\
\geq & S(\tau||\rho_{\mathrm{Gibbs}} \otimes c_{\mathrm{Gibbs}}) \\
\geq & S(\underline{\mathrm{Tr}_C[\tau]}||\rho_{\mathrm{Gibbs}}) + S(c||c_{\mathrm{Gibbs}})
\end{aligned}
$$

arbitrarily close to ρ'

Proof strategy of the sufficient part

Our proof consists of three parts.

1: Sufficient condition for state conversions
(measurement-preparation method)

2: Condition for asymptotic conversions

3: Reduction from asymptotic conversions to
(correlated-)catalytic conversions

(Note: This proof technique is not only for q-thermo but for other resource theories)

Before step 1: Renyi-divergence

Renyi-0 divergence: $S_0(\rho||\sigma) := -\ln[\mathrm{Tr}[P_\rho \sigma]]$

(P_ρ: projection onto the support of ρ)

Renyi-∞ divergence: $S_\infty(\rho||\sigma) := \ln[\min\{\lambda | \rho \leq \lambda\sigma\}]$

$S_\infty(\rho||\sigma)$ (highest distinguishability)

$\rotatebox{90}{$\leq$}$

$S_1(\rho||\sigma)$ (KL divergence)

$\rotatebox{90}{$\leq$}$

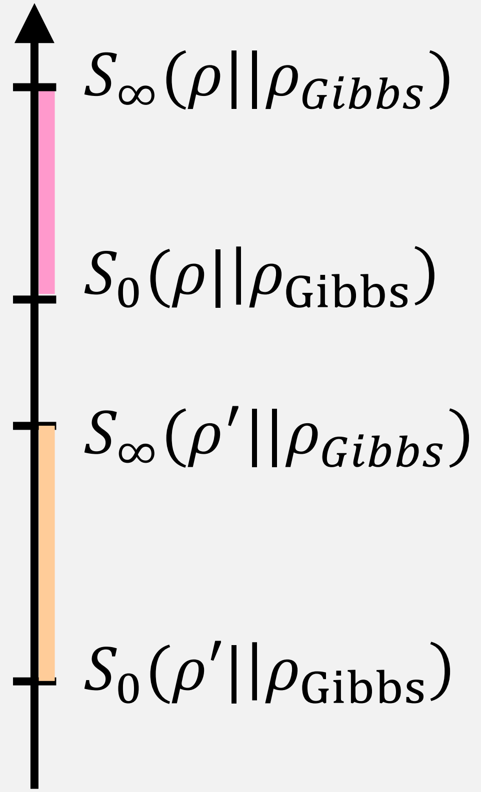
$S_0(\rho||\sigma)$ (lowest distinguishability)

Step 1: sufficient condition for state conversion

Theorem 1: There exists a GPM with $\Lambda(\rho) = \rho'$ if

$$\boldsymbol{S_0(\rho||\rho_{\mathrm{Gibbs}}) \geq S_\infty(\rho'||\rho_{Gibbs})}$$

(P. Faist and R. Renner, Phys. Rev. X 8, 021011 (2018).)



Intuitive picture

ρ is more distinguishable than ρ' from ρ_{Gibbs} in any sense.

→ ρ is convertible to ρ' via GPM

Proof of Theorem 1: Measurement-preparation method

i. Perform a measurement with $\{P_\rho, 1 - P_\rho\}$.

$$\rho \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \rho_{\mathrm{Gibbs}} \to \begin{pmatrix} k \\ 1 - k \end{pmatrix} \text{ with } k = e^{-S_0(\rho || \rho_{\mathrm{Gibbs}})}$$

ii. Prepare a state as $\begin{pmatrix} p \\ q \end{pmatrix} \to p\rho' + q\eta$ with

$$\eta = \frac{\rho_{\mathrm{Gibbs}} - k\rho'}{1 - k}$$

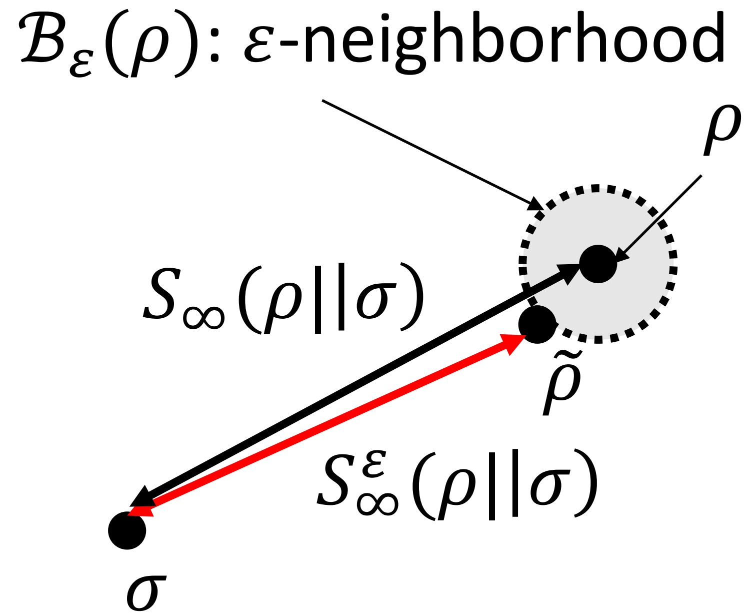
($S_0(\rho || \rho_{\mathrm{Gibbs}}) \geq S_\infty(\rho' || \rho_{Gibbs})$ confirms that η is positive-semidefinite)

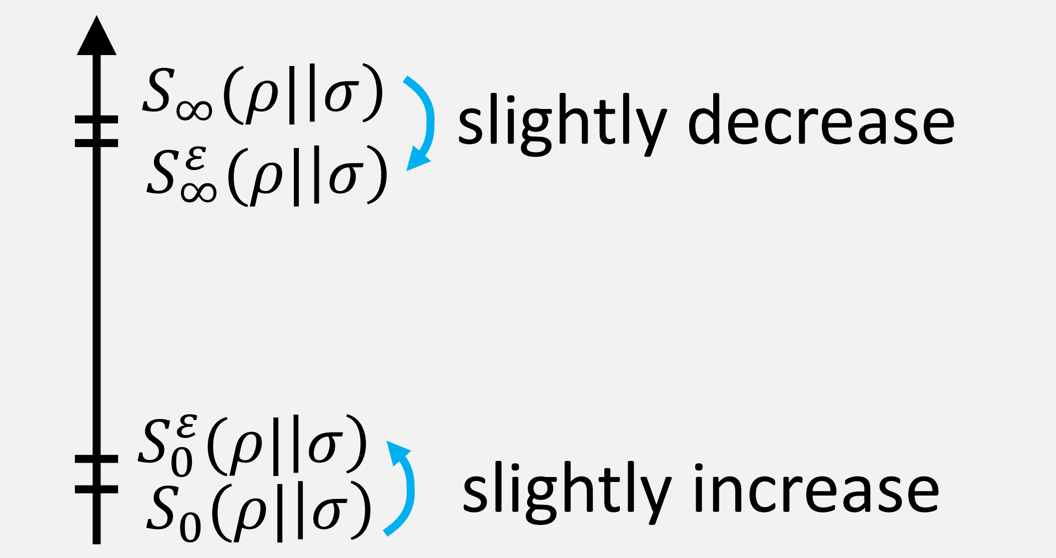
Before step 2: ε-smoothing

<u>Def: smoothed divergence</u>

$$S_\infty^\varepsilon(\rho||\sigma) = \min_{\tilde{\rho}\in\mathcal{B}_\varepsilon(\rho)} S_\infty(\tilde{\rho}||\sigma)$$

$$S_0^\varepsilon(\rho||\sigma) = \max_{\tilde{\rho}\in\mathcal{B}_\varepsilon(\rho)} S_0(\tilde{\rho}||\sigma)$$





(Note: previous sufficient condition is still valid for ε-smoothed version)

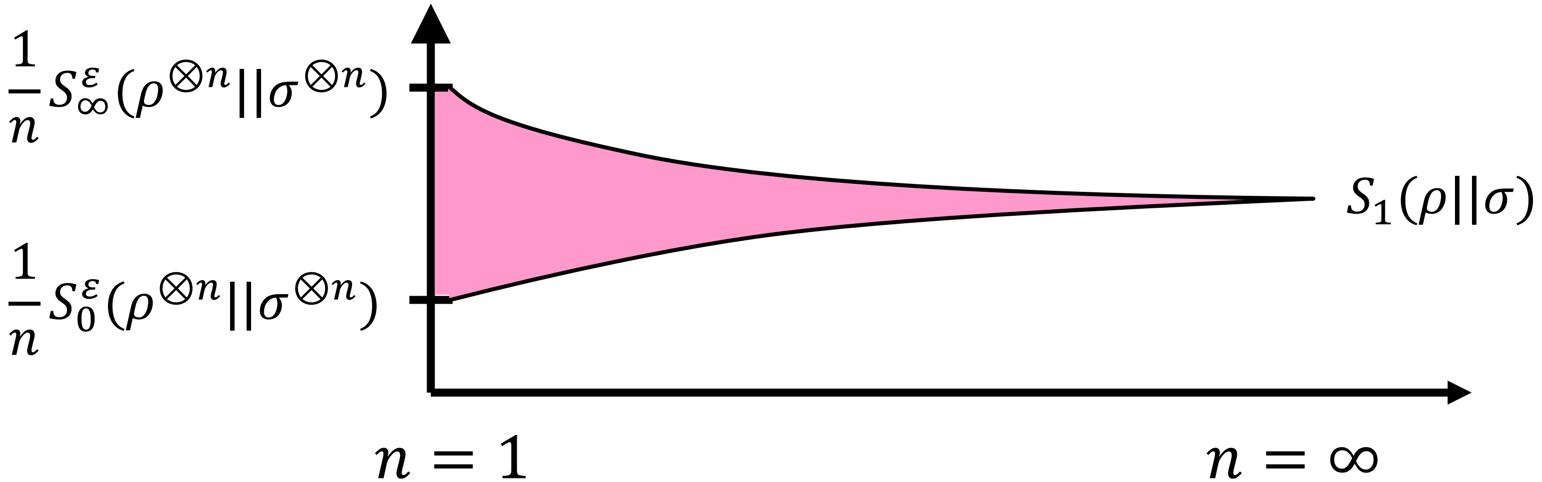
Step 2: Convergence of α-Renyi divergence

Using the quantum Stain's lemma, we have

Theorem 2: For any $0 < \varepsilon < 1/2$ and $0 \leq \alpha \leq \infty$,

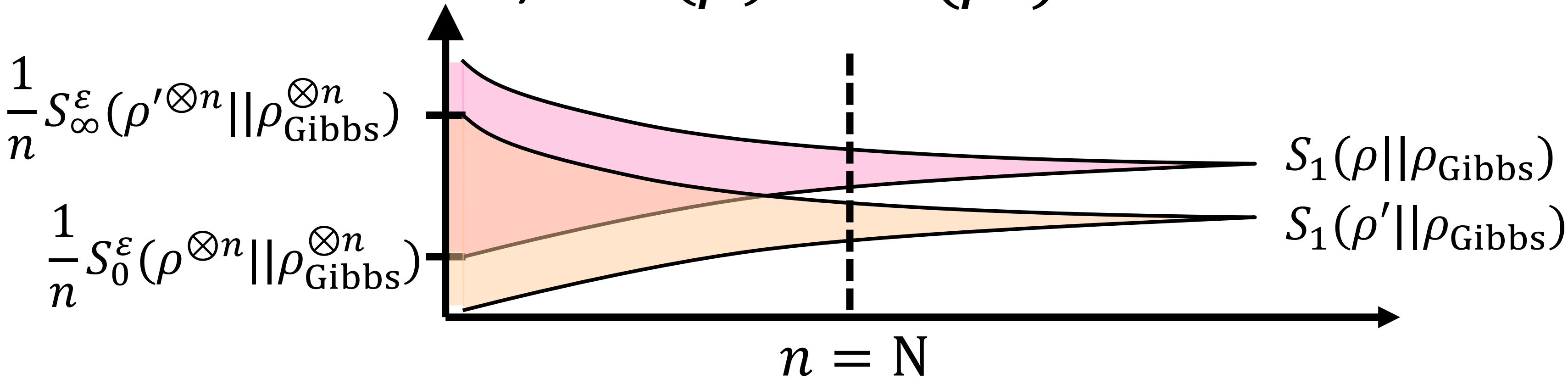
$$\lim_{n\to\infty} \frac{1}{n} S_\alpha^\varepsilon(\rho^{\otimes n}||\sigma^{\otimes n}) = S_1(\rho||\sigma)$$

(N. Datta, IEEE Trans. 55, 2816 (2009))

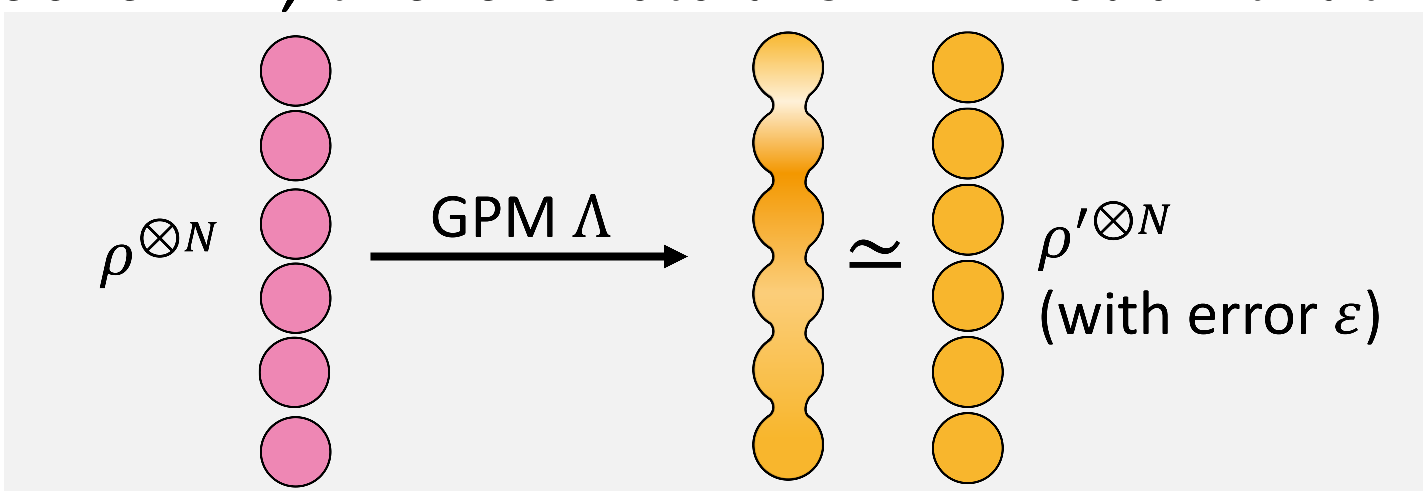


Combining Theorem 1 and 2

From Theorem 2, if $F(\rho) \geq F(\rho')$



From Theorem 1, there exists a GPM Λ such that

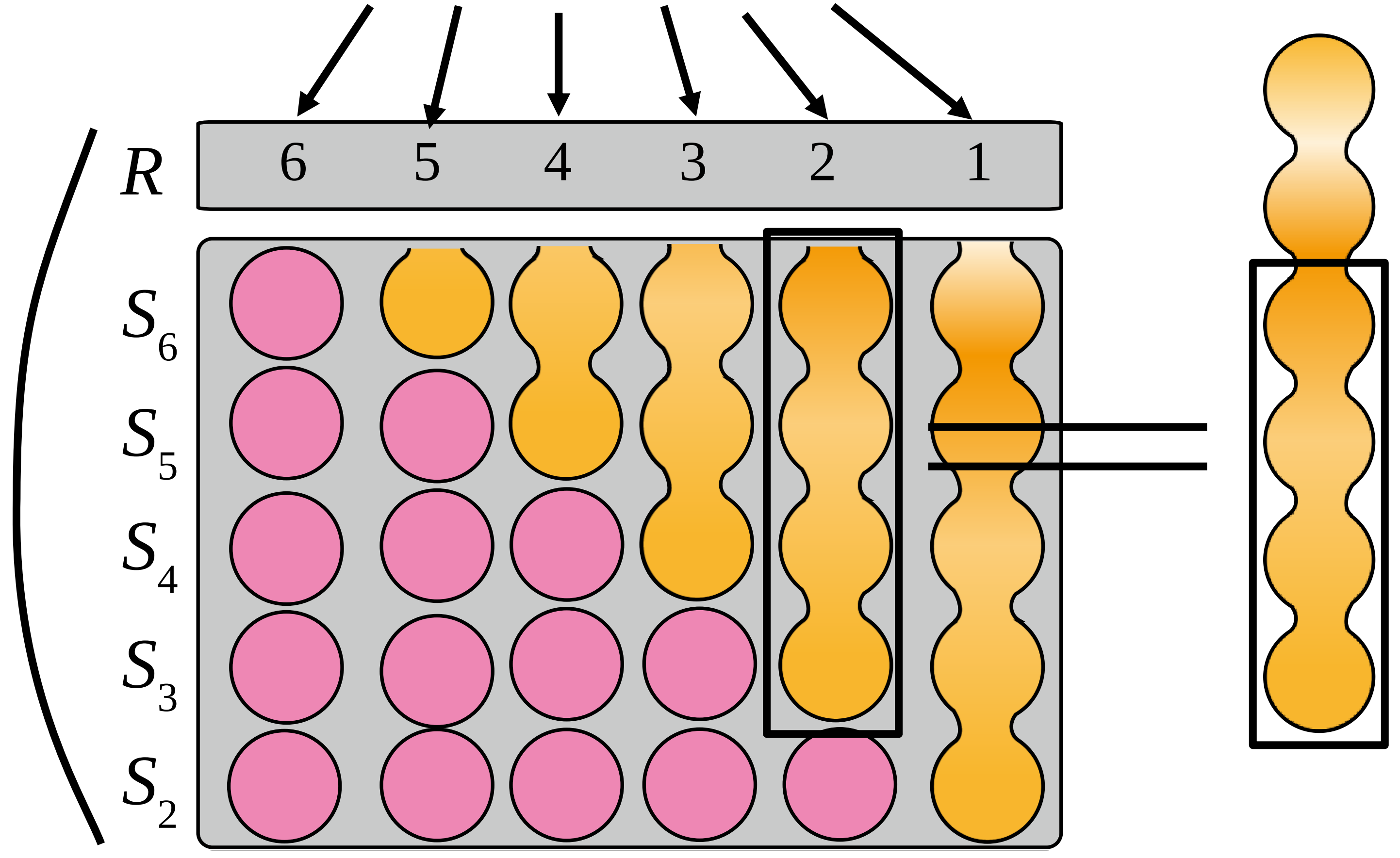


Step 3: From asymptotic to catalytic

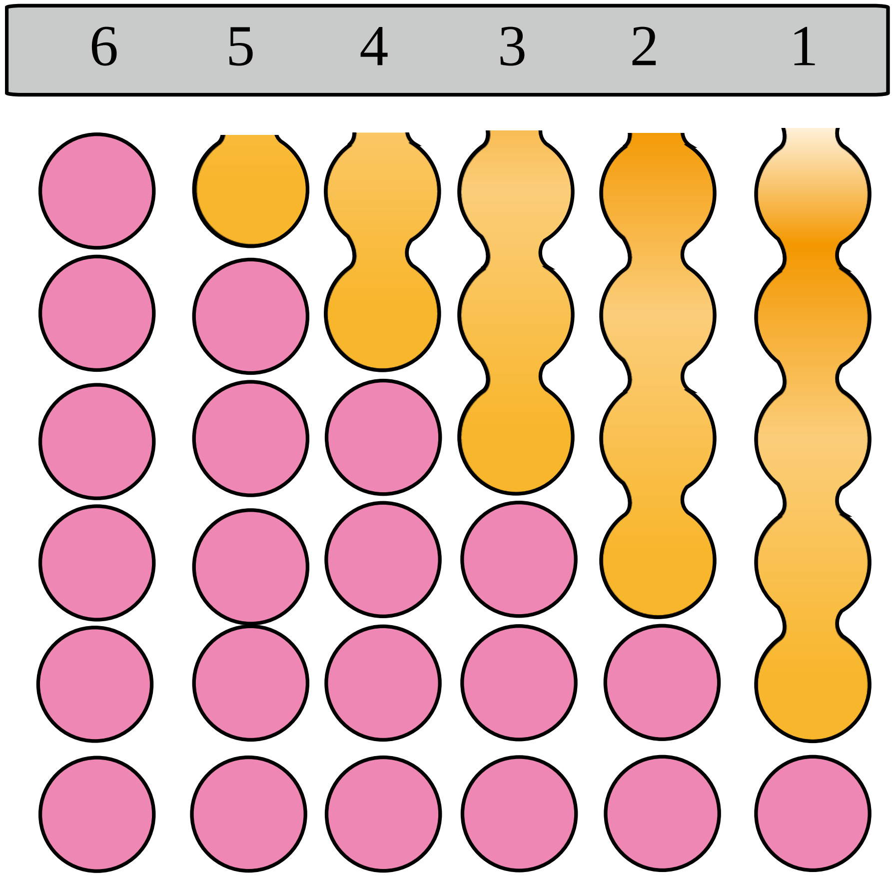
classical mixture of 6 states with equal weights

Ex) $N = 6$

catalyst



Step 3: From multi-copy to catalytic



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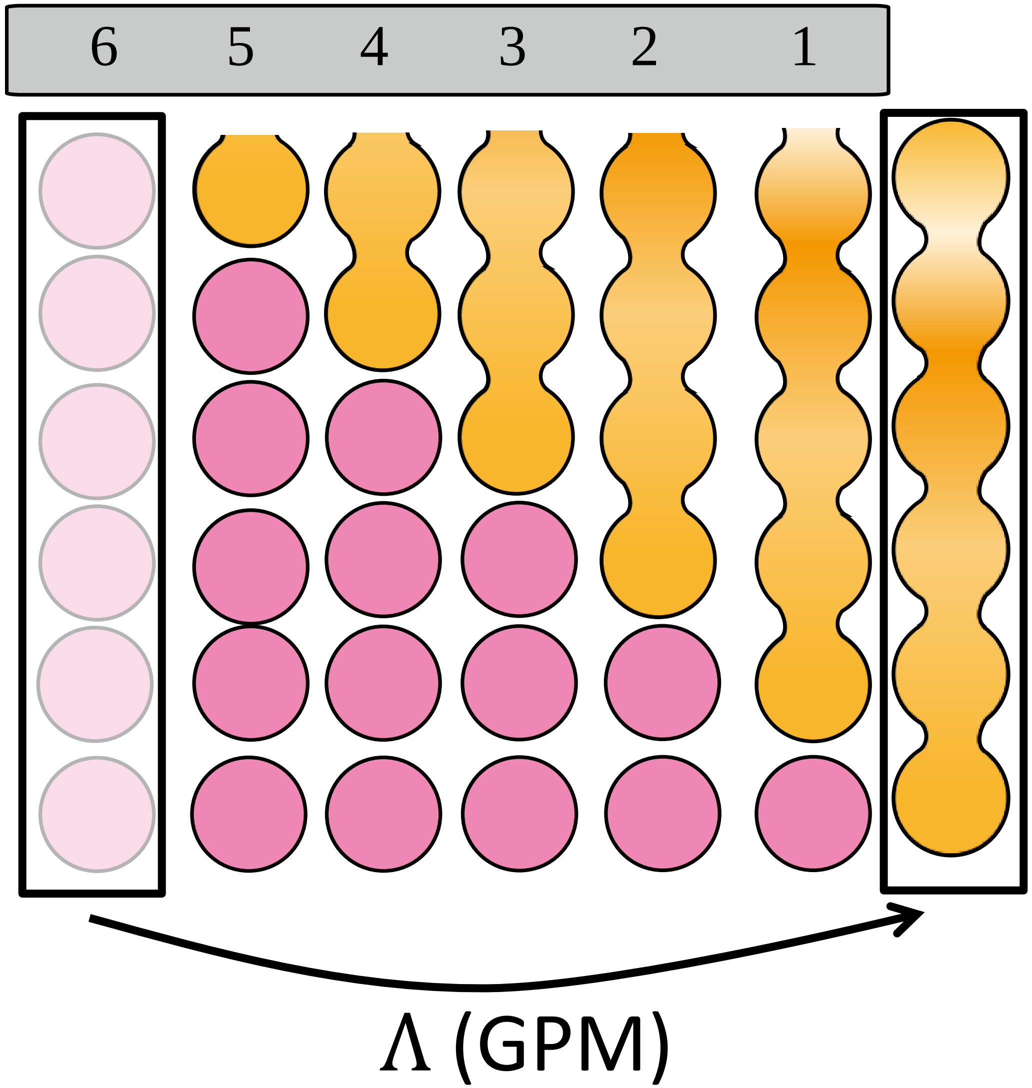

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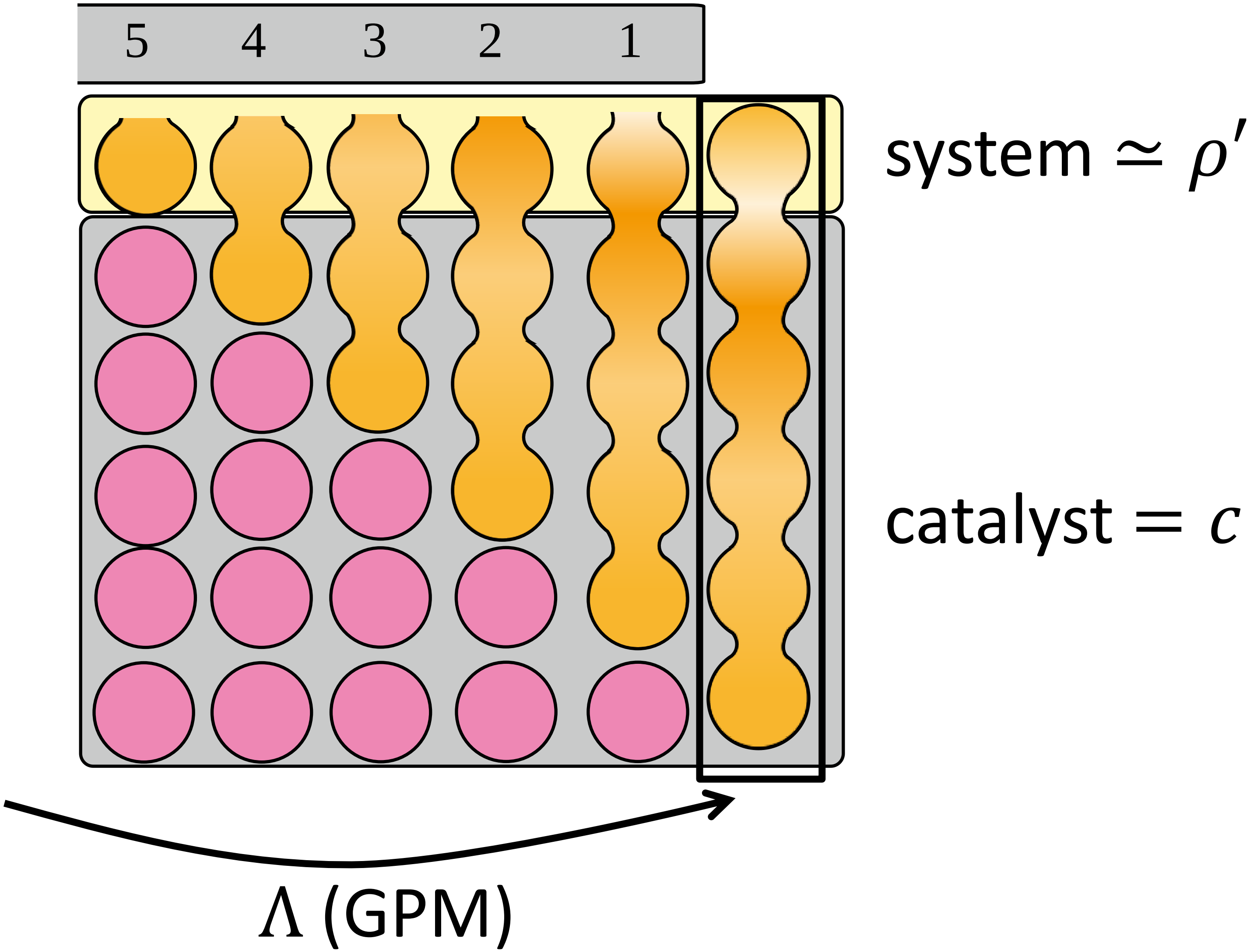

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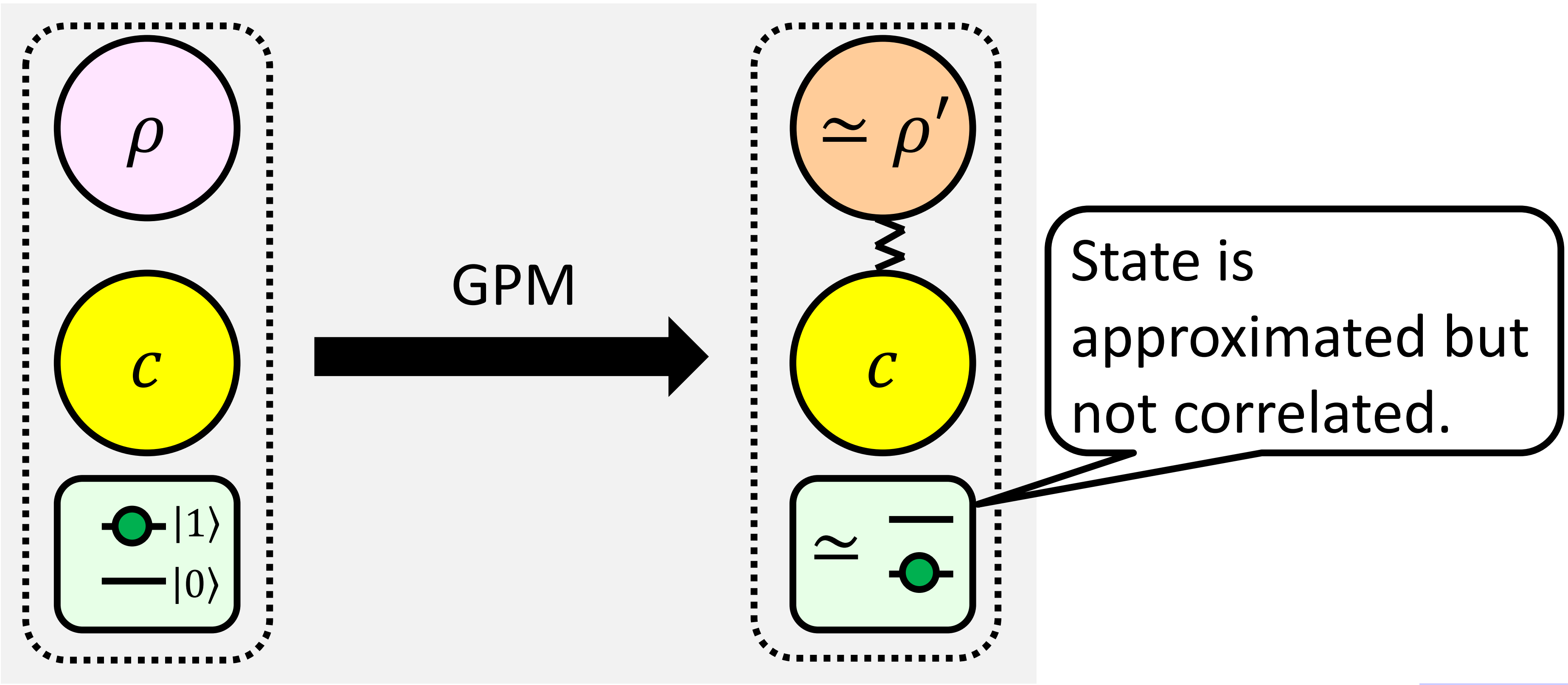
Remark 1: case with work storage

We introduce a two-level system called **work storage**, which compensate the energy change.



Conversion against free energy difference with the aid of work storage

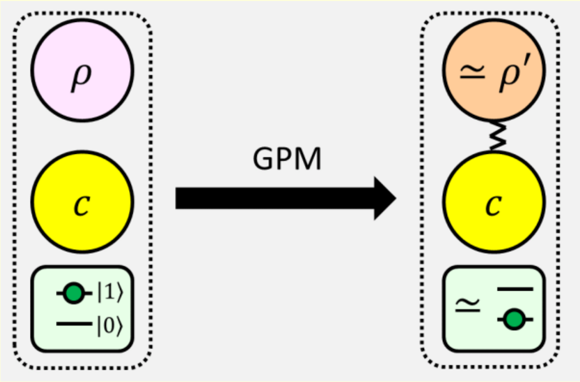
Theorem

If $F(\rho) < F(\rho')$, for any $\varepsilon > 0$, there exist a catalyst, a work storage with $\boldsymbol{\Delta E = F(\rho') - F(\rho)}$, and a GPM Λ such that

$$\boldsymbol{\Lambda(\rho \otimes c \otimes |1\rangle\langle 1|) = \tau \otimes \omega}$$

with

$$d(\mathrm{Tr}_C[\tau], \rho') < \varepsilon$$
$$\mathrm{Tr}_S[\tau] = c$$
$$d(\omega, |0\rangle\langle 0|) < \varepsilon$$



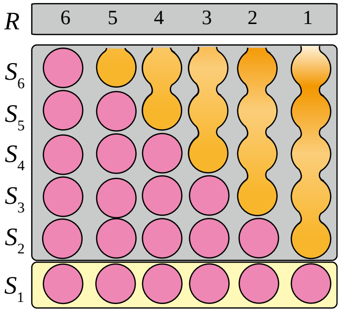
(N. Shiraishi and T. Sagawa, Phys. Rev. Lett. 126, 150502 (2021))

(Remark: the case of work extraction is not shown at present)

Remark 2: Other applications

This proof method applies other resource theories.

Sufficient condition for **asymptotic conversion** is also that for **catalytic conversion** (see Step 3).



<u>Various applications of our proof method</u>:

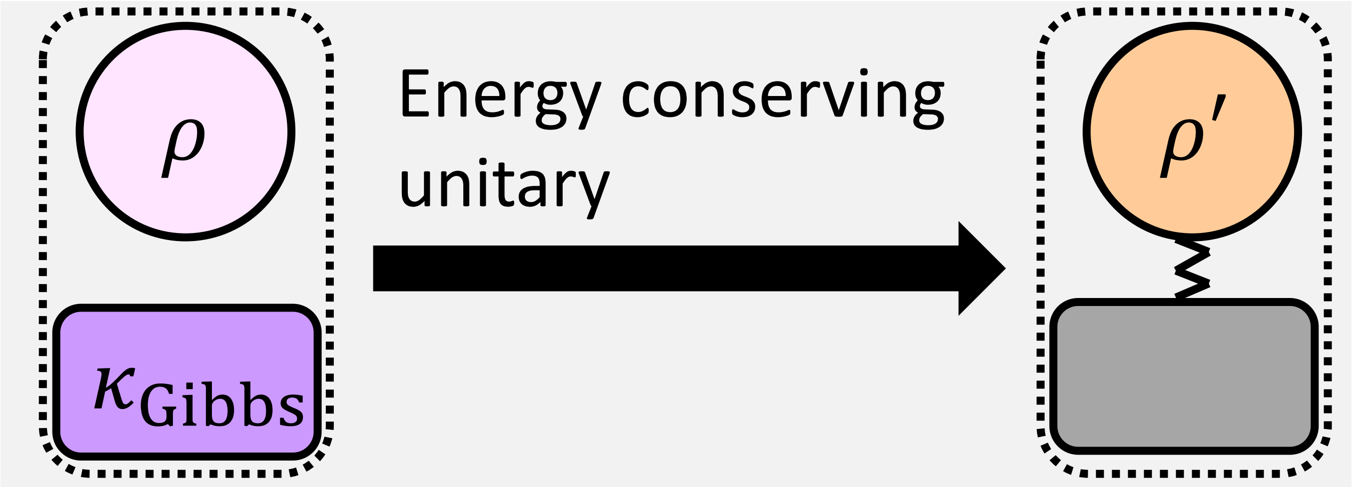
Entropy conjecture: (H. Wilming, arXiv:2012.05573)
Entanglement: (T. V. Kondra, C. Datta, and A. Streltsov, arXiv:2102.11136)
Teleportation: (P. Lipka-Bartosik and P. Skrzypczyk, PRL 127, 080502 (2021))

See N. Shiraishi and T. Sagawa, Phys. Rev. Lett. 126, 150502 (2021) and R. Takagi and N. Shiraishi, arXiv:2106.12592 for further discussion.

Remark 3: Thermal operation

<u>Def</u>: $\rho \to \rho'$ is convertible via **Thermal operation (TO)** if there exist an energy conserving unitary and an auxiliary system A with a state κ_{Gibbs} such that

$$\mathrm{Tr}_{\mathrm{A}}\left[U(\rho \otimes \kappa_{\mathrm{Gibbs}})U^{\dagger}\right] = \rho'$$



If κ_{Gibbs} is a general incoherent state, this map is called a **symmetric map** (with respect to energy).

Status of thermal operation

Classical case: GPM=TO

(M. Horodecki and J. Oppenheim, Nat. Comm. 4, 2059 (2013), N. Shiraishi, J. Phys. A Math. Theor. 53 425301 (2020))

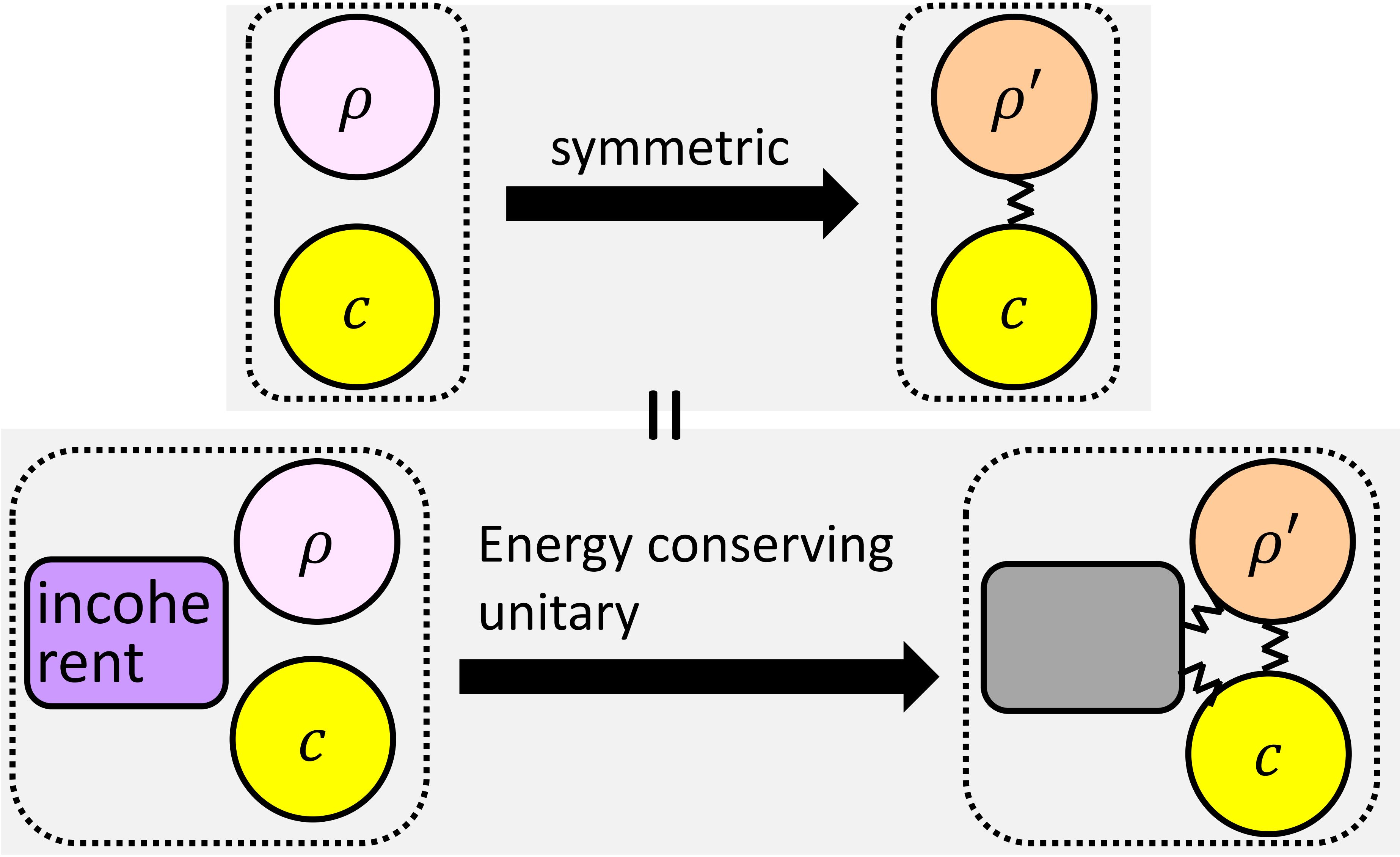
Quantum case: GPM⊃TO and GPM≠TO

(P. Faist, J. Oppenheim, and R. Renner, New J. Phys. 17, 043003 (2015))

Symmetric map (TO) cannot create energy coherence.

$$|E_1\rangle \not\longrightarrow \frac{1}{\sqrt{2}}(|E_1\rangle + |E_2\rangle)$$

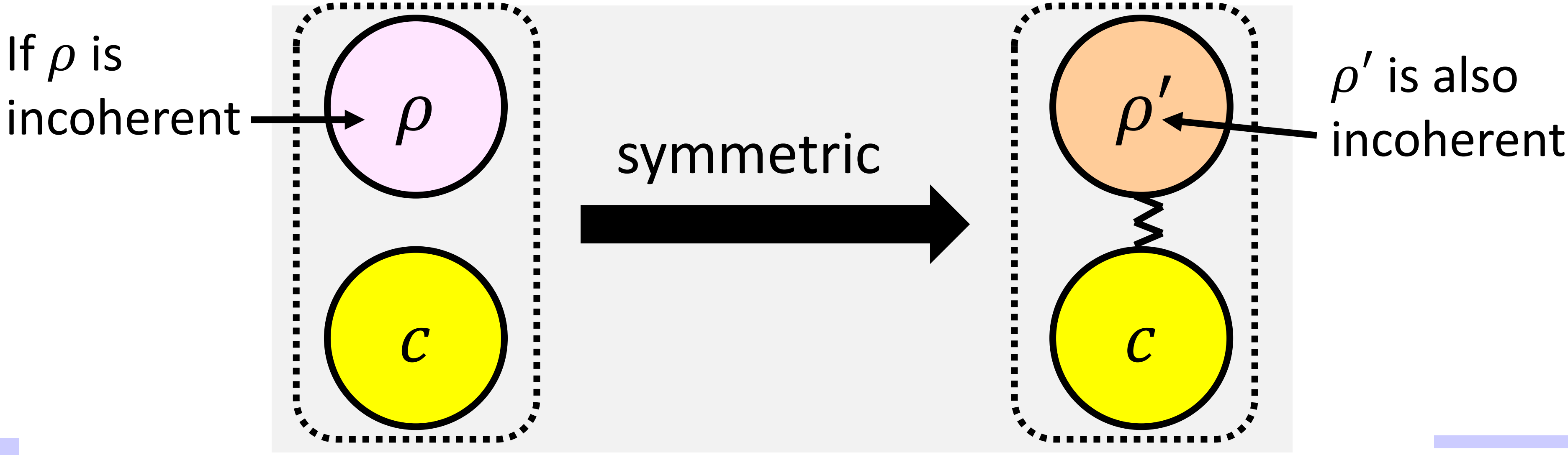
Symmetric map with correlated catalyst



No broadcasting theorem

Theorem: Let ρ be an incoherent state, and Λ be a symmetric map. If $\mathrm{Tr}_S[\Lambda(\rho \otimes c)] = c$, then $\rho' = \mathrm{Tr}_C[\Lambda(\rho \otimes c)]$ is an incoherent state.

(M. Lostaglio and M. P. Muller, Phys. Rev. Lett. 123, 020403 (2019),
I. Marvian and R. W. Spekkens, Phys. Rev. Lett. 123, 020404 (2019).)



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(M. Lostaglio and M. P. Muller, Phys. Rev. Lett. 123, 020403 (2019),
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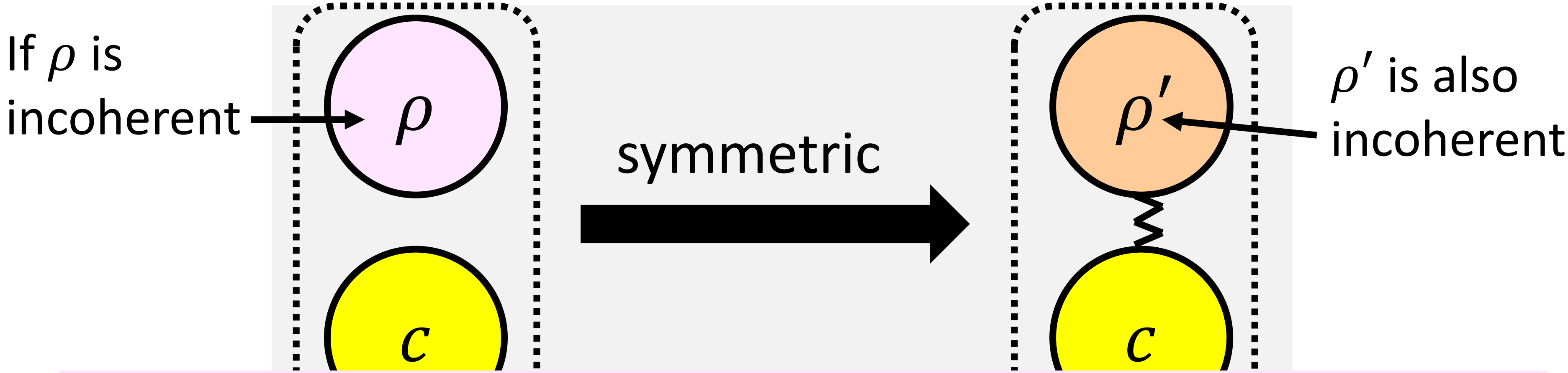
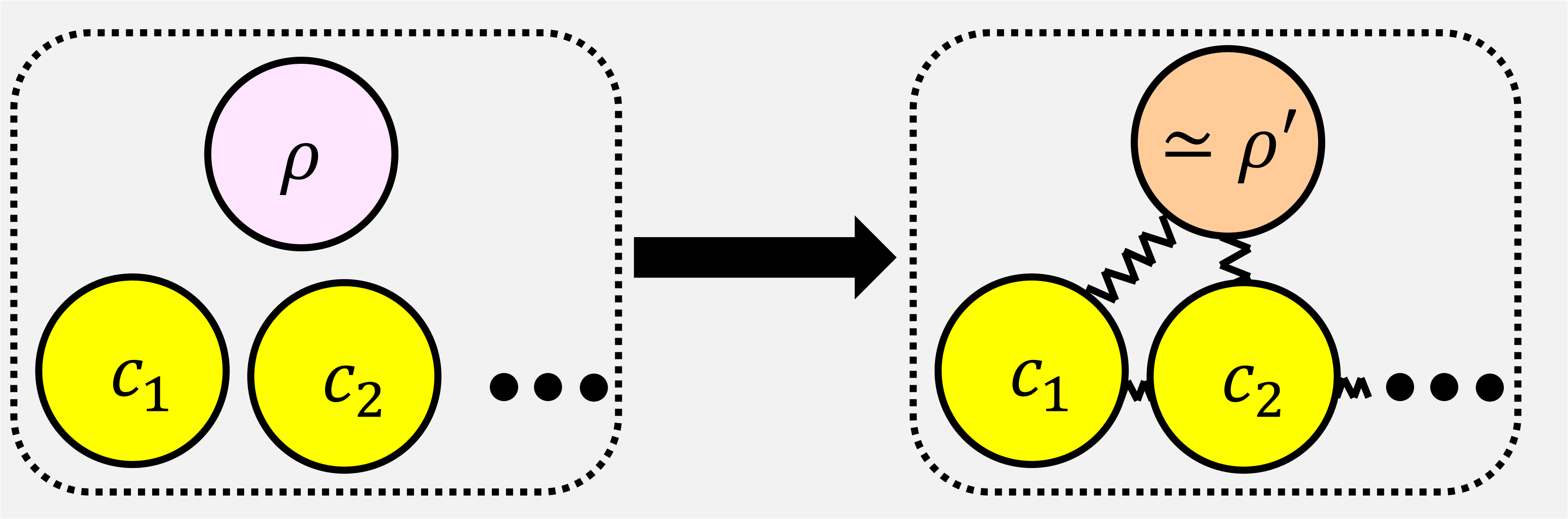


TO is NOT characterized solely by the second law.

…but coherence might be almost no barrier

Suppose that catalysts can correlate with each other (marginal catalytic operation).



We consider the power of symmetric maps with marginal catalysts.

…but coherence might be almost no barrier

<u>Theorem</u>: Any ρ can be converted to any ρ' via a symmetric map with marginal catalysts.

Coherence gives no restriction!

(i.e, resource theory of asymmetry (unspeakable coherence) with marginal catalyst is trivial.)

<u>Conjecture (intuitive)</u>: If ρ has nonzero coherence, ρ can be converted to any ρ' via a symmetric map with correlated catalyst.

Please see the lightning talk “Correlation in catalysts enables arbitrary manipulation of quantum coherence” by Ryuji Takagi

(R. Takagi and N. Shiraishi, arXiv:2106.12592)

Summary

- In small quantum systems, the nec.&suff. condition for conversion $\rho \to \rho'$ via GPM with correlated catalyst is given by the second law:

$$\boldsymbol{F(\rho) \geq F(\rho')}$$

- The proof technique can be extended to other problems in resource theories.

- Case of work cost is also treated well.

N. Shiraishi and T. Sagawa, Phys. Rev. Lett. 126, 150502 (2021)

END

Formulation of the problem

State: <u>classical case</u>: probability distribution $\boldsymbol{p}$

<u>quantum case</u>: density matrix ρ

operation: <u>classical case</u>: stochastic matrix T

$$\boldsymbol{p}' = T\boldsymbol{p}$$

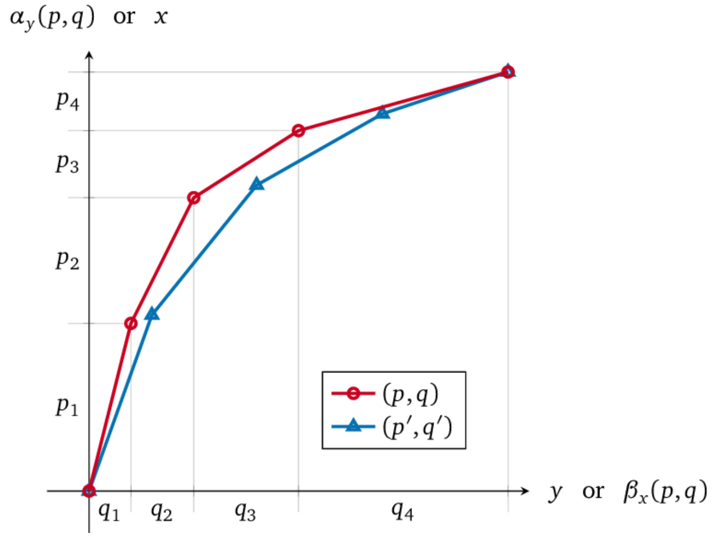
<u>quantum case</u>: CPTP map Λ

$$\rho' = \Lambda(\rho)$$

(Note: q-states in energy diagonal = c-states)

State conversion via GPM (classical)

In classical case, the nec.&suff. condition for GPM is given by **d-majorization**.



(J. M. Renes, J. Math. Phys. 57, 122202 (2016))

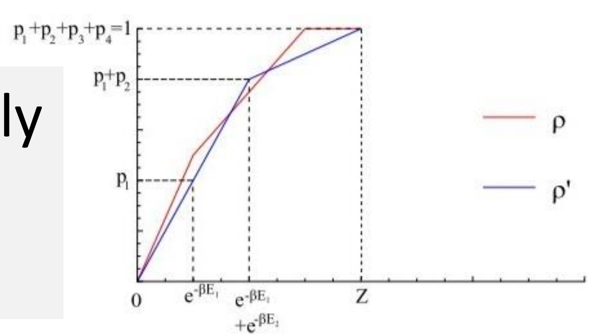
(<u>Various proofs</u>: D. Blackwell, Proc. Math. Statist. and Prob. 93 (1951), F. Veinott. Jr., Man. Sci. 19, 547 (1971), E. Ruch, R. Schranner, and T. H. Seligman, J. Chem. Phys. 69, 1 (1978). N. Shiraishi, J. Phys. A Math. Theor. 53 425301 (2020))

State conversion via GPM with catalyst (classical)

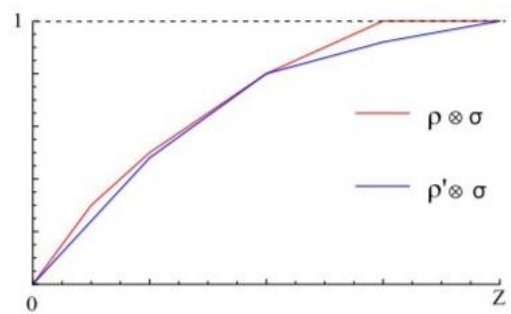
In classical case, the nec.&suff. condition for GPM with catalyst is given by **infinite inequalities** with α-Renyi divergence.

$$\boldsymbol{F_\alpha(p)} \geq \boldsymbol{F_\alpha(p')} \text{ where } F_\alpha(p) := S_\alpha(p||p_{\mathrm{Gibbs}})$$

<u>proof idea</u>: construct highly elaborated catalyst and reduce to majorization



without catalyst



with catalyst

(F. Brandao, *et al.*, PNAS 112, 3275 (2015). [Its essential idea] M. Klimesh, arXiv:0709.3680 (2007), S. Turgut, J. Phys. A Math. Theor. 40, 12185 (2007)).

State conversion via GPM with catalyst (classical)

In classical case, the nec.&suff. condition for GPM with correlated catalyst is given by **the single free energy with KL divergence (the second law!)**.

$$\boldsymbol{F}(\boldsymbol{p}) \geq \boldsymbol{F}(\boldsymbol{p}') \text{ where } F(p) \coloneqq S(p||p_{\text{Gibbs}})$$

$$p'_{XY_1} = \begin{pmatrix} \underbrace{\begin{matrix} \delta/n^2 & \cdots & \delta/n^2 \\ \delta/n^2 & \cdots & \delta/n^2 \\ \vdots & & \vdots \\ \delta/n^2 & \cdots & \delta/n^2 \end{matrix}}_{n^2} & \underbrace{\begin{matrix} (p'_1 - 2\delta)/n & \cdots & (p'_1 - 2\delta)/n \\ (p'_2 - 2\delta)/n & \cdots & (p'_2 - 2\delta)/n \\ \vdots & & \vdots \\ (p'_m - 2\delta)/n & \cdots & (p'_m - 2\delta)/n \end{matrix}}_{n} & \begin{matrix} \delta \\ \delta \\ \vdots \\ \delta \end{matrix} \end{pmatrix}$$

<u>proof idea</u>: construct highly elaborated catalyst and reduce to the case of (uncorrelated) catalyst

(M. P. Muller, Phys. Rev. X 8, 041051 (2018).)

Classical α-Renyi divergence

For two probability distributions p, q, the α-Renyi divergence except $\alpha = 0,1,\infty$ is defined as

$$S_\alpha(p||q) := \frac{1}{\alpha - 1} \ln\left(\sum_i \frac{p_i^\alpha}{q_i^{\alpha-1}}\right)$$

For $\alpha = 0,1,\infty$, we define

$$S_0(p||q) := -\ln\left(\sum_{i;p_i>0} q_i\right)$$
$$S_1(p||q) := \sum_i p_i \ln\frac{p_i}{q_i}$$
$$S_\infty(p||q) := \ln\left(\max_i \frac{p_i}{q_i}\right)$$

Quantum α-Renyi divergence

Unlike classical cases, quantum α-Renyi divergence is not uniquely defined.

Def 1: $\tilde{S}_\alpha(\rho||\sigma) := \frac{1}{\alpha-1}\ln(\mathrm{Tr}[\rho^\alpha\sigma^{1-\alpha}])$

Def 2: $S_\alpha(\rho||\sigma) := \frac{1}{1-\alpha}\ln\left(\mathrm{Tr}\left[\left(\sigma^{\frac{1-\alpha}{2\alpha}}\rho\sigma^{\frac{1-\alpha}{2\alpha}}\right)^\alpha\right]\right)$

Roughly speaking, Def 1 is good (monotonic) in $0 \leq \alpha \leq 2$, while Def 2 is good in $\frac{1}{2} \leq \alpha \leq \infty$.

Case of equality

In case of $F(\rho) = F(\rho')$, we consider another state ρ'' which is close to ρ' as satisfying $F(\rho) > F(\rho'')$ and $d(\rho', \rho'') < \frac{\varepsilon}{2}$.

Then, we consider transition $\rho \to \rho''$ with error margin $\frac{\varepsilon}{2}$ instead of ε.

Validity of Theorem 1 under ε-smoothing

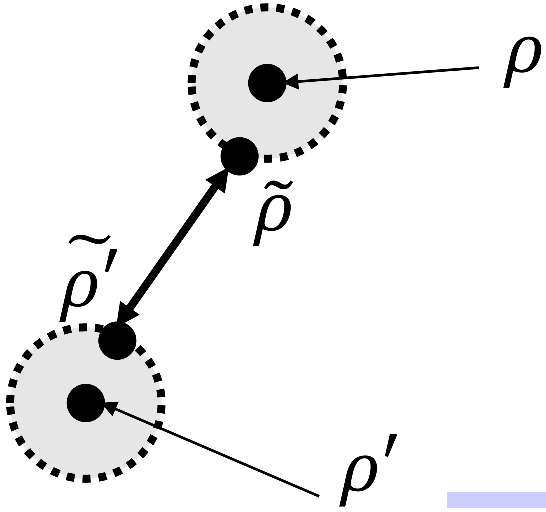
Suppose $S_0^{\varepsilon/2}(\rho||\rho_{\mathrm{Gibbs}}) \geq S_\infty^{\varepsilon/2}(\rho'||\rho_{Gibbs})$.

Then, there exist $\tilde{\rho} \in \mathcal{B}_{\varepsilon/2}(\rho)$ and $\widetilde{\rho'} \in \mathcal{B}_{\varepsilon/2}(\rho')$ s.t.

$$S_0(\tilde{\rho}||\rho_{\mathrm{Gibbs}}) \geq S_\infty(\widetilde{\rho'}||\rho_{Gibbs})$$

The map Λ guaranteed by Theorem 1 satisfies

$$d(\Lambda(\rho), \rho') < \varepsilon$$



No broadcasting theorem

Even with correlated catalyst, incoherent state cannot be transformed into coherent state via TO.

Theorem: Let ρ be an incoherent state, and Λ be an energy conserving map. If $\mathrm{Tr}_S[\Lambda(\rho \otimes c)] = c$, then $\rho' = \mathrm{Tr}_\mathrm{C}[\Lambda(\rho \otimes c)]$ is an incoherent state.

(M. Lostaglio and M. P. Muller, Phys. Rev. Lett. 123, 020403 (2019),
I. Marvian and R. W. Spekkens, Phys. Rev. Lett. 123, 020404 (2019).)

TO is not characterized solely by the second law.

But, is there any clue to investigate TO?

Precise statement of conjecture

Let $I(\rho)$ be a set of pairs (i,j) where $\rho_{ij} \neq 0$.

Let $J(\rho)$ be a set of pairs (i,j) such that $E_i - E_j$ can be written as a linear combination of integer multiple of energy difference in $I(\rho)$:

$$E_i - E_j = \sum_{(k,l)\in I(\rho)} c_{kl}(E_k - E_l), \qquad c_{kl} \in \mathbb{Z}$$

<u>Conjecture</u>:
ρ is transformable to ρ' via energy conserving map with correlated catalyst if and only if $I(\rho') \subset J(\rho)$.