

Role of Quantum Coherence in Thermodynamics

Gilad Gour

University of Calgary
Department of Mathematics and Statistics
Institute of Quantum Science and Technology

Quantum Resources:
From mathematical foundations to operational characterization
Singapore, 7 December 2022

Based on PRX Quantum 3, 040323 (2022); arXiv: 2205.13612

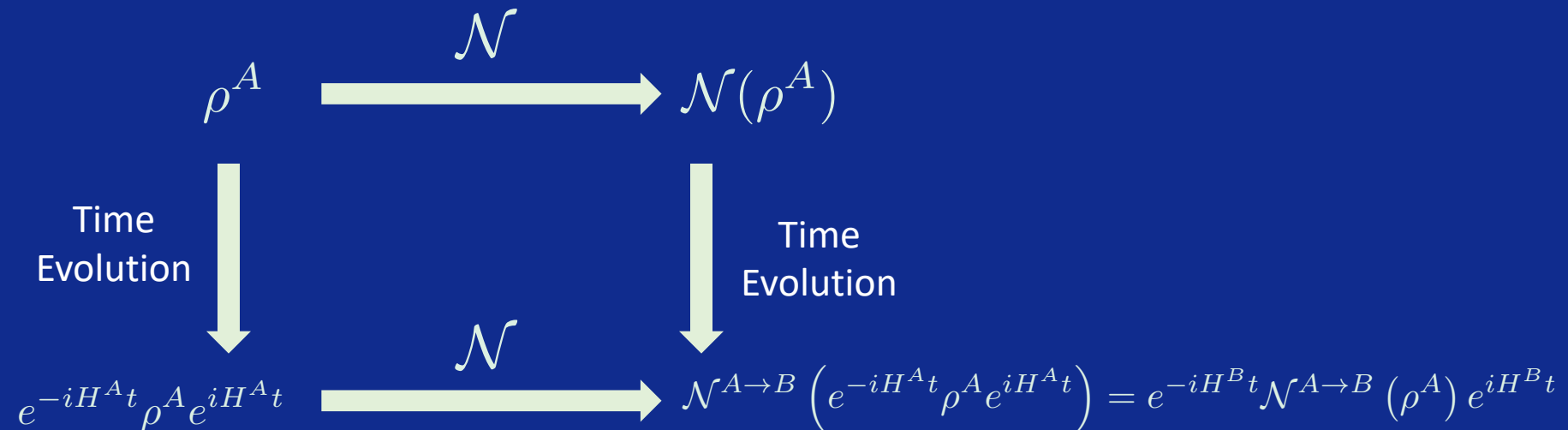
Time-Translation Symmetry

A quantum state $\rho \in \mathfrak{D}(A)$ is time-translation invariant if

$$e^{-iH^A t} \rho^A e^{iH^A t} = \rho^A \quad \forall t \in \mathbb{R}$$

A quantum channel $\mathcal{N} \in \text{CPTP}(A \rightarrow B)$ is said to be time-translation covariant if

$$\mathcal{N}^{A \rightarrow B} \left(e^{-iH^A t} \rho^A e^{iH^A t} \right) = e^{-iH^B t} \mathcal{N}^{A \rightarrow B} (\rho^A) e^{iH^B t} \quad \forall t \in \mathbb{R} \quad \forall \rho \in \mathfrak{D}(A)$$



Time-Translation Symmetry

The Pinching Channel

The pinching channel is defined with respect to an Hamiltonian $H^A = \sum_{x=1}^m a_x \Pi_x^A$

$$\mathcal{P}^{A \rightarrow A}(\rho^A) := \sum_{x=1}^m \Pi_x^A \rho^A \Pi_x^A$$

Properties:

1. The pinching channel is itself time-translation covariant.
2. The pinching channel is idempotent; i.e. $\mathcal{P} = \mathcal{P} \circ \mathcal{P}$.
3. A density matrix $\rho \in \mathfrak{D}(A)$ is time-translation invariant iff $\mathcal{P}(\rho) = \rho$.
4. If $\mathcal{N} \in \text{CPTP}(A \rightarrow B)$ is time-translation covariant then

$$\mathcal{P}^{B \rightarrow B} \circ \mathcal{N}^{A \rightarrow B} = \mathcal{N}^{A \rightarrow B} \circ \mathcal{P}^{A \rightarrow A}$$

5. The pinching channel can be expressed as a random unitary channel.

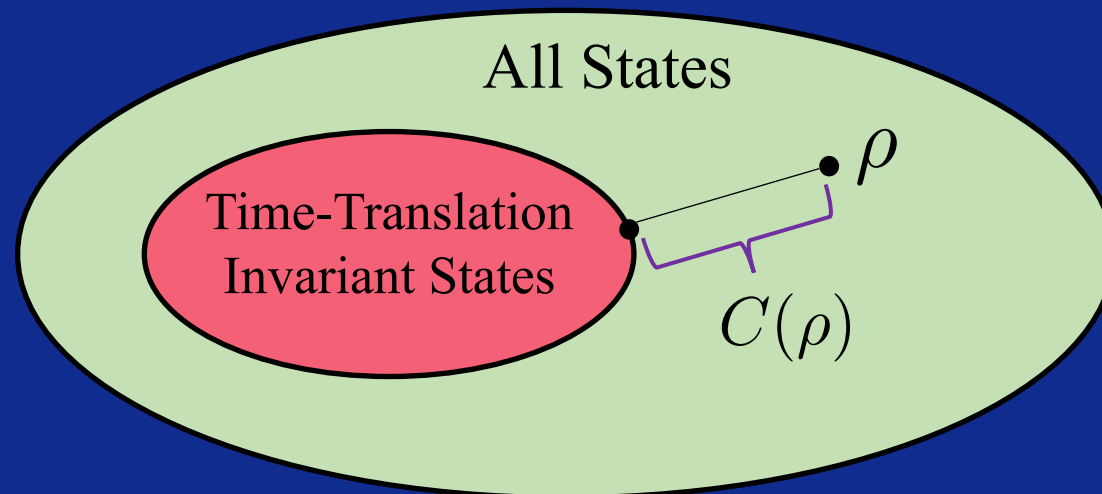
Quantification of Time-Translation Asymmetry

Let $D(\rho||\sigma) := \text{Tr}[\rho \log \rho] - \text{Tr}[\rho \log \sigma]$ and $H(\rho) := -\text{Tr}[\rho \log \rho]$. Then,

$$C(\rho) := \min_{\sigma \in \text{INV}(A)} D(\rho||\sigma) = H(\mathcal{P}(\rho)) - H(\rho)$$

For any $\rho \in \mathfrak{D}(A)$ the coherence of n copies of ρ satisfies

$$C(\rho^{\otimes n}) \leq |A| \log(n+1) \quad \xrightarrow{\text{Regularization}} \quad \lim_{n \rightarrow \infty} \frac{1}{n} C(\rho^{\otimes n}) = 0$$



Manipulation of Time-Translation Asymmetry

Consider two Hamiltonians:

$$H^A = \sum_{x=1}^m a_x |x\rangle \langle x|^A \quad H^B = \sum_{y=1}^n b_x |y\rangle \langle y|^B$$

Relatively non-degenerate Hamiltonians:

$$a_x - a_{x'} = b_y - b_{y'} \quad \Rightarrow \quad x = x' \quad \text{and} \quad y = y'$$

Theorem: For relatively non-degenerate Hamiltonians

$$\mathcal{N} \in \text{COV}(A \rightarrow B) \quad \Leftrightarrow \quad \mathcal{N} \text{ is classical; i.e. } \mathcal{N}^{A \rightarrow B} = \mathcal{P}^{B \rightarrow B} \circ \mathcal{N}^{A \rightarrow B} \circ \mathcal{P}^{A \rightarrow A}$$

Manipulation of Time-Translation Asymmetry

Consider the Hamiltonian $H^A = \sum_{x=1}^m a_x |x\rangle\langle x|^A$

Non-degenerate Bohr Spectrum: $a_x - a_y = a_{x'} - a_{y'} \iff x = x' \text{ and } y = y'$
or $x = y \text{ and } x' = y'$

Theorem:

Let A be a physical system with Bohr energy spectrum, and let $\rho, \sigma \in \mathfrak{D}(A)$. Then, the following are equivalent:

1. There exists a $\mathcal{N} \in \text{COV}(A \rightarrow A)$ such that $\sigma = \mathcal{N}(\rho)$.
2. The matrix $Q = (q_{xy})$, whose components are given by

$$q_{xy} := \begin{cases} \min \left\{ 1, \frac{s_{xx}}{r_{xx}} \right\} & \text{if } x = y \\ \frac{s_{xy}}{r_{xy}} & \text{otherwise.} \end{cases}$$

is positive semidefinite.

$$r_{xy} := \langle x | \rho | y \rangle \neq 0$$

$$s_{xy} := \langle x | \sigma | y \rangle$$

Manipulation of Time-Translation Asymmetry

Corollary:

Let $\sigma \in \mathfrak{D}(A)$ be an arbitrary state, and denote by $p_x := \langle x | \sigma | x \rangle$. Then,

$$|\psi\rangle := \sum_{x=1}^m \sqrt{p_x} |x\rangle$$

can be converted to σ by a time-translation covariant channel.

Quantum Thermodynamics



Free States: The Gibbs States

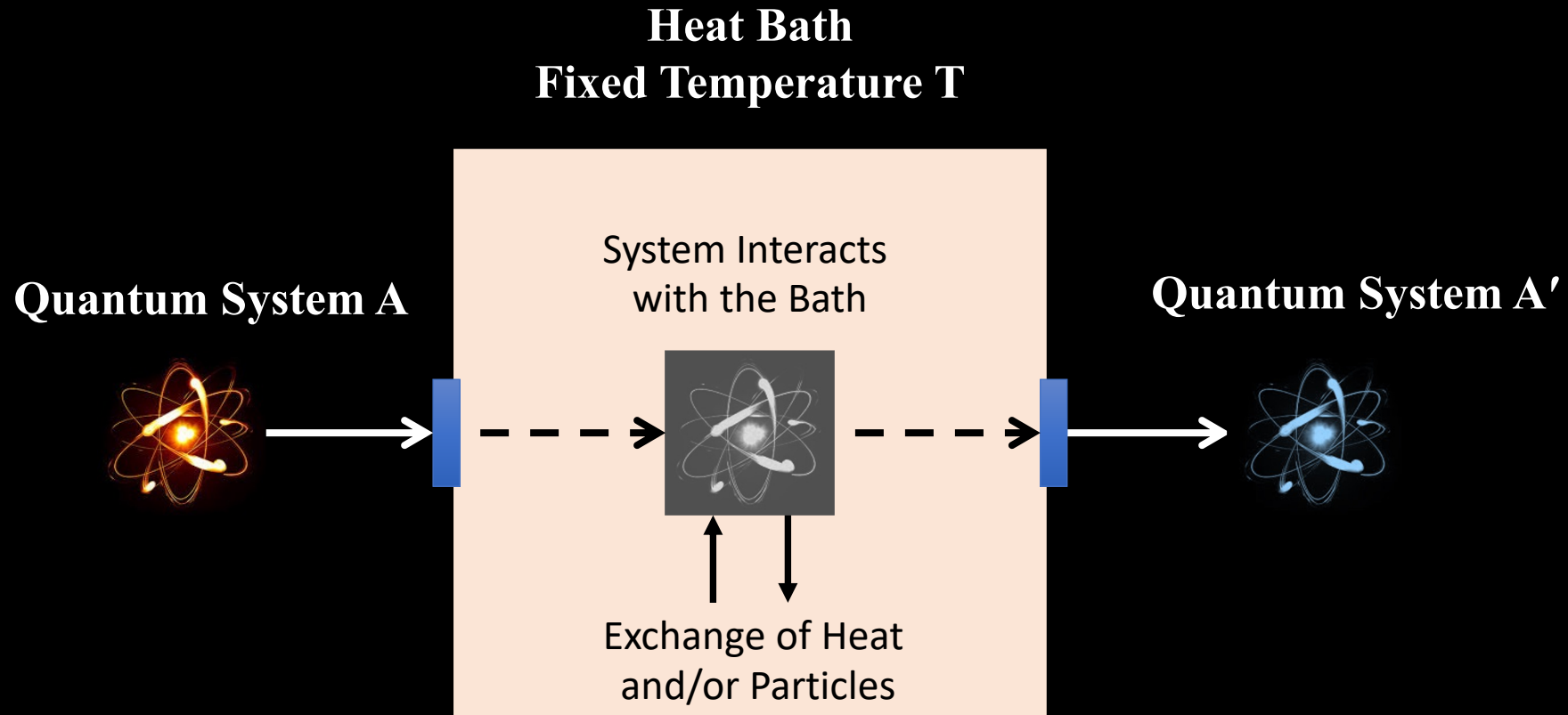
$$\gamma^A = \frac{e^{-\beta H^A}}{\text{Tr} [e^{-\beta H^A}]}$$

$$\gamma^B = \frac{e^{-\beta H^B}}{\text{Tr} [e^{-\beta H^B}]}$$

Properties:

1. Gibbs states cannot be used to extract work.
2. Gibbs states have minimal energy for a given entropy.
3. Gibbs states are the only completely passive states.

Thermal Operations



Thermal Operations

Three Basic Steps:

1. Thermal equilibrium. Any subsystem B , with Hamiltonian H^B , can be prepared in its thermal Gibbs state γ^B .

Thermal Operations

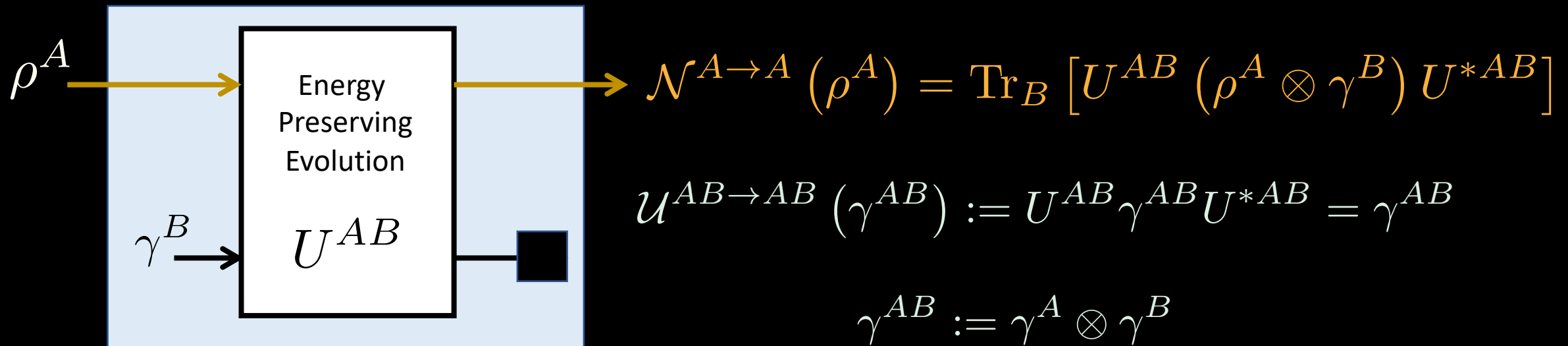
Three Basic Steps:

1. Thermal equilibrium. Any subsystem B , with Hamiltonian H^B , can be prepared in its thermal Gibbs state γ^B .
2. Conservation of energy. Unitary operation on a composite physical system that commutes with the total Hamiltonian can be implemented.

Thermal Operations

Three Basic Steps:

1. Thermal equilibrium. Any subsystem B , with Hamiltonian H^B , can be prepared in its thermal Gibbs state γ^B .
2. Conservation of energy. Unitary operation on a composite physical system that commutes with the total Hamiltonian can be implemented.
3. Discarding subsystems. It is possible to trace over any subsystem (with a well defined Hamiltonian) of a composite system.

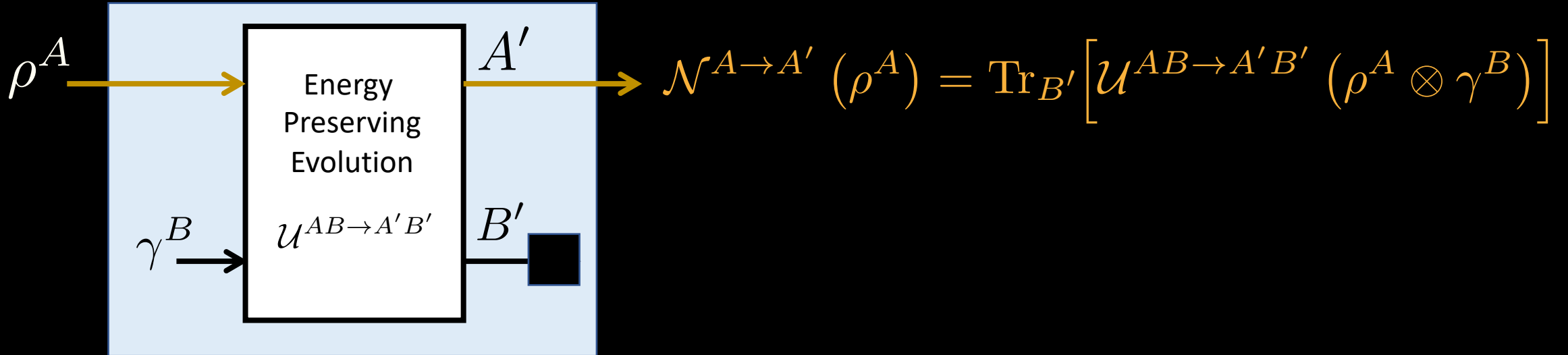


Thermal Operations

Consider a Gibbs preserving unitary channel $\mathcal{U} \in \text{CPTP}(AB \rightarrow A'B')$

$$\mathcal{U}^{AB \rightarrow A'B'} (\gamma^A \otimes \gamma^B) = \gamma^{A'} \otimes \gamma^{B'} \quad (\text{with } |A'B'| = |AB|)$$

Lemma: The quantum channel below is a thermal operation.



Closed Thermal Operations

$\text{TO}(A \rightarrow A')$ denotes the set of all thermal operations in $\text{CPTP}(A \rightarrow A')$.

Lemma: The pinching channel $\mathcal{P} \in \text{TO}(A \rightarrow A)$.

Two undesirable properties:

1. The set $\text{TO}(A \rightarrow A')$ is not closed in $\text{CPTP}(A \rightarrow A')$.
2. The set $\text{TO}(A \rightarrow A')$ is not convex.

The closure of the set $\text{TO}(A \rightarrow A')$:

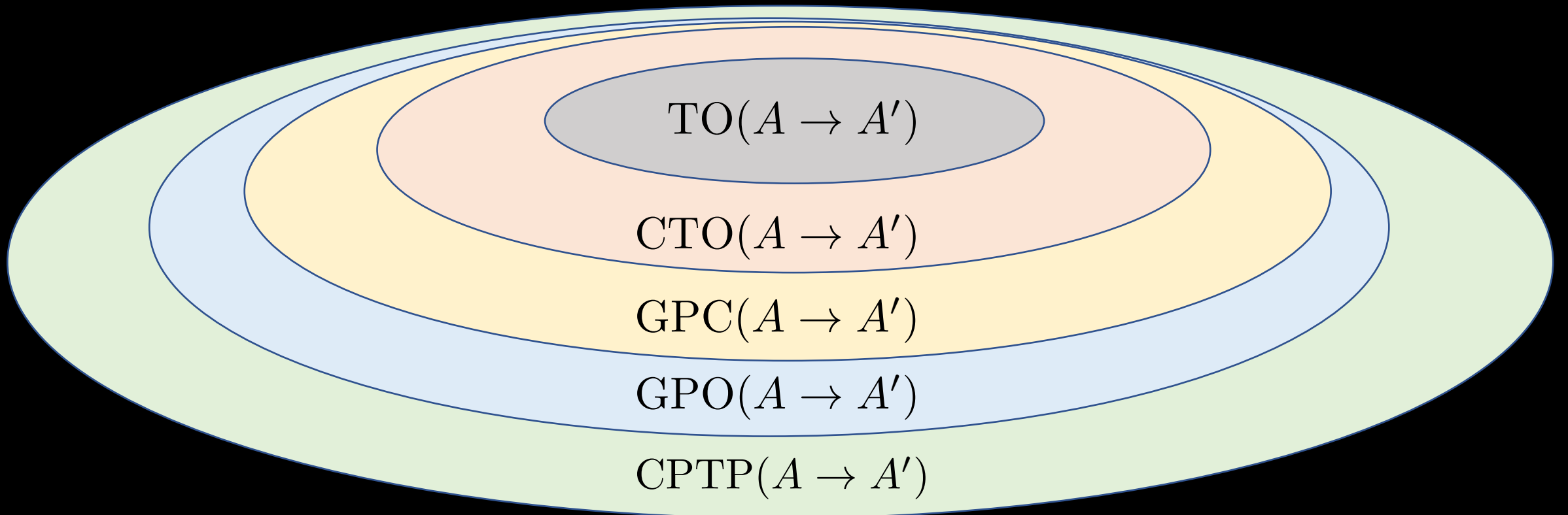
$$\text{CTO}(A \rightarrow A') := \left\{ \mathcal{N} \in \text{CPTP}(A \rightarrow A') : \mathcal{N} = \lim_{k \rightarrow \infty} \mathcal{N}_k, \mathcal{N}_k \in \text{TO}(A \rightarrow A') \right\}$$

Theorem: The set $\text{CTO}(A \rightarrow A')$ is closed and convex.

Gibbs Preserving Covariant Operations

Every thermal operation $\mathcal{N} \in \text{CPTP}(A \rightarrow A')$ has two key properties:

1. $\mathcal{N}^{A \rightarrow A'}$ is *Gibbs preserving operation* (GPO); that is, $\mathcal{N}^{A \rightarrow A'}(\gamma^A) = \gamma^{A'}$.
2. $\mathcal{N}^{A \rightarrow A'}$ is time-translation covariant; i.e. $\mathcal{N} \in \text{COV}(A \rightarrow A')$.



Quantification of Quantum Athermality

The Relative Entropy of a Resource:

$$D(\rho||\gamma) = -H(\rho) - \text{Tr}[\rho \log \gamma]$$

Quantification of Quantum Athermality

The Relative Entropy of a Resource:

$$\begin{aligned} D(\rho||\gamma) &= -H(\rho) - \text{Tr}[\rho \log \gamma] \\ &= -H(\rho) - \text{Tr}[\mathcal{P}(\rho) \log \gamma] \end{aligned}$$

Quantification of Quantum Athermality

The Relative Entropy of a Resource:

$$\begin{aligned} D(\rho||\gamma) &= -H(\rho) - \text{Tr}[\rho \log \gamma] \\ &= -H(\rho) - \text{Tr}[\mathcal{P}(\rho) \log \gamma] \\ &= D(\mathcal{P}(\rho)||\gamma) + H(\mathcal{P}(\rho)) - H(\rho) \end{aligned}$$

Quantification of Quantum Athermality

The Relative Entropy of a Resource:

$$\begin{aligned} D(\rho||\gamma) &= -H(\rho) - \text{Tr} [\rho \log \gamma] \\ &= -H(\rho) - \text{Tr} [\mathcal{P}(\rho) \log \gamma] \\ &= D(\mathcal{P}(\rho)||\gamma) + H(\mathcal{P}(\rho)) - H(\rho) \\ &= D(\mathcal{P}(\rho)||\gamma) + C(\rho) \end{aligned}$$

Quantification of Quantum Athermality

The Relative Entropy of a Resource:

$$\begin{aligned} D(\rho||\gamma) &= -H(\rho) - \text{Tr}[\rho \log \gamma] \\ &= -H(\rho) - \text{Tr}[\mathcal{P}(\rho) \log \gamma] \\ &= D(\mathcal{P}(\rho)||\gamma) + H(\mathcal{P}(\rho)) - H(\rho) \\ &= D(\mathcal{P}(\rho)||\gamma) + C(\rho) \end{aligned}$$

Nonuniformity

Quantum
Coherence

Deterministic Manipulation of Quantum Athermality

Suppose $\mathcal{P}(\rho) = \mathcal{P}(\sigma)$

$$(\rho, \gamma) \xrightarrow{\text{GPC}} (\sigma, \gamma)$$



Time-Translation
Covariant Operations

$$\rho \xrightarrow{\hspace{10em}} \sigma$$



$$Q^A := I^A + \sum_{x \neq y \in [m]} \frac{s_{xy}}{r_{xy}} |x\rangle\langle y|^A \geq 0$$

The Quasi-Classical Case

$$[\rho^A, \gamma^A] = 0 \quad \Rightarrow \quad \rho^A \sim \mathbf{p}^A \quad , \quad \gamma^A \sim \mathbf{g}^A$$

Theorem:

$$(\mathbf{p}^A, \mathbf{g}^A) \xrightarrow{\text{CTO}} (\mathbf{q}^B, \mathbf{g}^B) \quad \Leftrightarrow \quad (\mathbf{p}^A, \mathbf{g}^A) \xrightarrow{\text{GPO}} (\mathbf{q}^B, \mathbf{g}^B)$$

D. Janzing, P. Wocjan, R. Zeier, R. Geiss, and T. Beth, International Journal of Theoretical Physics 39, 2717 (2000)

Relative Majorization:

$$\begin{aligned} (\mathbf{p}^A, \mathbf{g}^A) \xrightarrow{\text{GPO}} (\mathbf{q}^B, \mathbf{g}^B) &\quad \Leftrightarrow \quad \mathbf{q}^B = E\mathbf{p}^A \quad \text{and} \quad \mathbf{g}^B = E\mathbf{g}^A \\ &\quad \Leftrightarrow \quad (\mathbf{p}^A, \mathbf{g}^A) \succ (\mathbf{q}^B, \mathbf{g}^B) \end{aligned}$$

The Church of the Trivialized Hamiltonian

For a trivial Hamiltonian $H^A = 0$ the Gibbs states is uniform:

$$\mathbf{g}^A = \mathbf{u}^{(m)} := \frac{1}{m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \quad m := |A|$$

Theorem:

If $\mathbf{g} = (\frac{k_1}{k}, \dots, \frac{k_m}{k})^T$ has rational components, then for any probability vector $\mathbf{p} = (p_1, \dots, p_m)^T$

$$(\mathbf{p}, \mathbf{g}) \xleftrightarrow{\text{CTO}} (\mathbf{r}, \mathbf{u}^{(k)}) \quad \text{where} \quad \mathbf{r} := \bigoplus_{x=1}^m p_x \mathbf{u}^{(k_x)}$$

The Golden Unit of Athermality

$$(|0\rangle\langle 0|^A, \mathbf{u}^A)$$

Pure State Maximally Mixed State.

Theorem:

$$(|0\rangle\langle 0|^A, \mathbf{u}^A) \xleftrightarrow{\text{CTO}} (|0\rangle\langle 0|^X, \mathbf{u}_m^X)$$

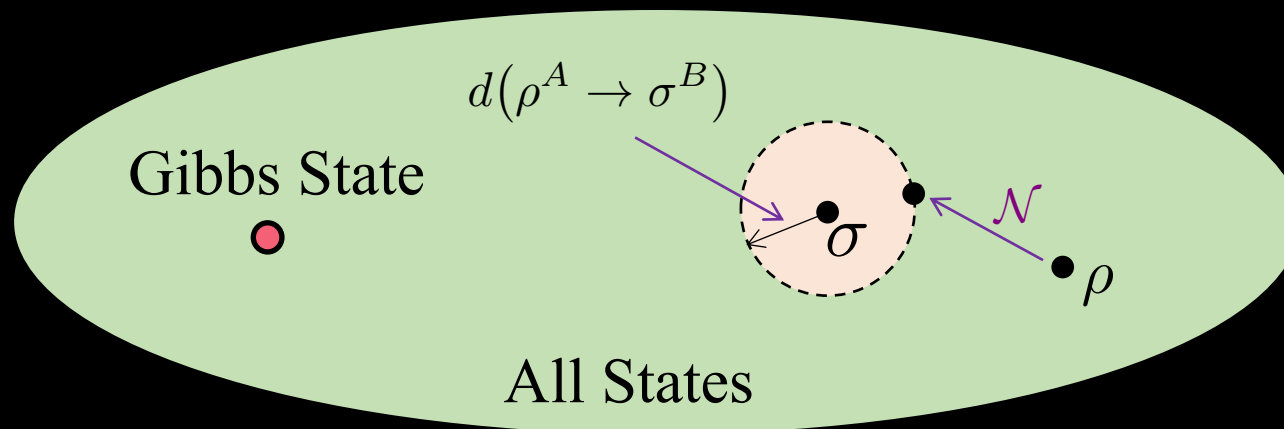
$$|A| = m$$

$$|X| = 2$$

$$\mathbf{u}_m^X := \frac{1}{m} |0\rangle\langle 0|^X + \frac{m-1}{m} |1\rangle\langle 1|^X .$$

Distillation

$$d(\rho^A \rightarrow \sigma^B) := \min_{\mathcal{N} \in \text{CTO}(A \rightarrow B)} \frac{1}{2} \|\sigma^B - \mathcal{N}(\rho^A)\|_1$$



$$\begin{aligned} \text{Distill}^\varepsilon(\rho) &= \log \sup_{0 < m \in \mathbb{R}} \left\{ m : d\left((\rho^A, \gamma^A) \rightarrow (|0\rangle\langle 0|^X, \mathbf{u}_m^X)\right) \leq \varepsilon \right\} \\ &= D_{\min}^\varepsilon(\mathcal{P}(\rho) \parallel \gamma) \end{aligned}$$

Hypothesis Testing Divergence: $D_{\min}^\varepsilon(\rho \parallel \gamma) := \min_{0 \leq \Lambda \leq I^A} \left\{ \text{Tr}[\gamma \Lambda] : \text{Tr}[\Lambda \rho] \geq 1 - \varepsilon \right\}$

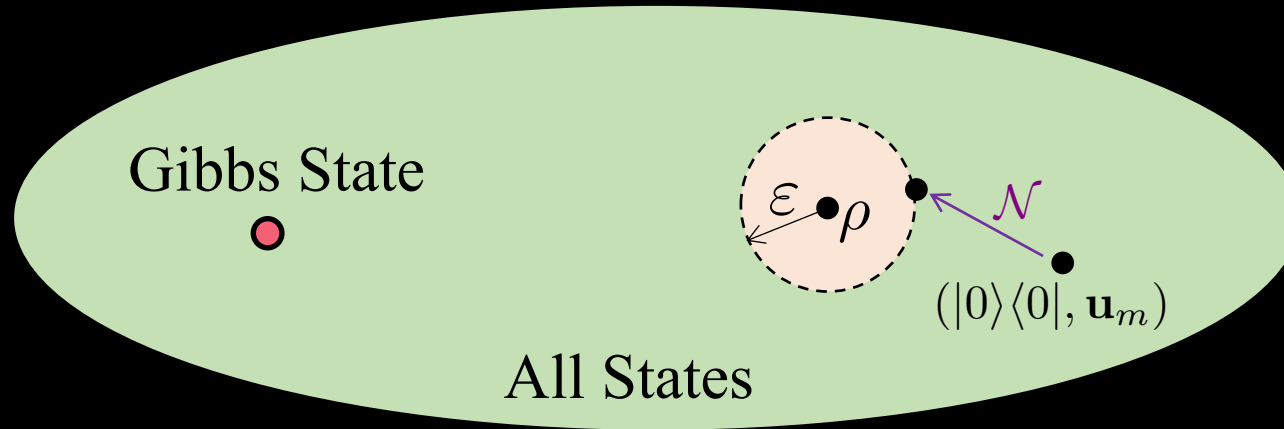
Distillation

$$\begin{aligned}\text{Distill}^\varepsilon(\rho) &= \log \sup_{0 < m \in \mathbb{R}} \left\{ m : d\left((\rho^A, \gamma^A) \rightarrow (|0\rangle\langle 0|^X, \mathbf{u}_m^X)\right) \leq \varepsilon \right\} \\ &= D_{\min}^\varepsilon(\mathcal{P}(\rho) \parallel \gamma)\end{aligned}$$

Asymptotically:

$$\begin{aligned}\text{Distill}(\rho) &= \lim_{\varepsilon \rightarrow 0^+} \limsup_{n \rightarrow \infty} \frac{1}{n} \text{Distill}^\varepsilon(\rho^{\otimes n}) \\ &= \lim_{\varepsilon \rightarrow 0^+} \limsup_{n \rightarrow \infty} \frac{1}{n} D_{\min}^\varepsilon(\mathcal{P}(\rho^{\otimes n}) \parallel \gamma) \\ &= D(\rho \parallel \gamma)\end{aligned}$$

Cost



$$\text{Cost}^\varepsilon(\rho) = \log \inf_{0 < m \in \mathbb{R}} \left\{ m : d\left((|0\rangle\langle 0|^X, \mathbf{u}_m^X) \rightarrow (\rho^A, \gamma^A) \right) \leq \varepsilon \right\}$$

$$= D_{\max}^\varepsilon(\rho \| \gamma) \quad (\text{Under Gibbs Preserving Operations})$$

$$= \infty \quad (\text{Under GPC or CTO or TO})$$

Sublinear Athermality Resources (SLAR)

Definition: A sublinear athermality resource (SLAR) is a sequence of quantum athermality systems $\{R_n\}_{n \in \mathbb{N}}$, such that:

1. $|R_n| = \text{Poly}(n)$
2. There exists $c > 0$ and $0 \leq \alpha < 1$ such that $\|H^{R_n}\|_\infty \leq cn^\alpha$ for all $n \in \mathbb{N}$.

$$(|0\rangle\langle 0|, \mathbf{u}_m) \xrightarrow{\text{CTO}+\text{SLAR}} (\rho^{\otimes n}, \gamma^{\otimes n})$$



$$(|0\rangle\langle 0|, \mathbf{u}_m) \otimes (\eta^{R_n}, \gamma^{R_n}) \xrightarrow{\text{CTO}} (\rho^{\otimes n}, \gamma^{\otimes n})$$

Asymptotic Cost

$$(|0\rangle\langle 0|, \mathbf{u}_m) \xrightarrow{\text{CTO+SLAR}} (\rho^{\otimes n}, \gamma^{\otimes n})$$



$$(|0\rangle\langle 0|, \mathbf{u}_m) \otimes (\eta^{R_n}, \gamma^{R_n}) \xrightarrow{\text{CTO}} (\rho^{\otimes n}, \gamma^{\otimes n})$$

Theorem: If ρ is a pure state then

$$\text{Cost}(\rho) := \lim_{n \rightarrow \infty} \frac{m}{n} = D(\rho \| \gamma)$$

Future Work

State with zero non-uniformity and the most coherence for a given Gibbs state:

$$|\psi_\gamma\rangle := \sum_{x=1}^m \sqrt{g_x} |x\rangle \quad \text{and} \quad \gamma = \sum_{x=1}^m g_x |x\rangle \langle x|$$

Interconversions with two types of resources:

$$\begin{array}{ccc} (\psi_\gamma, \gamma)^{\otimes k} \otimes (|0\rangle\langle 0|, \mathbf{u})^{\otimes m} & \xrightarrow{\text{GPC}} & (\rho, \gamma)^{\otimes n} \\ \begin{array}{c} \nearrow \\ \text{Coherence/Asymmetry} \end{array} & & \begin{array}{c} \nwarrow \\ \text{Nonuniformity} \end{array} \end{array}$$

Thank You!