Title: Limitations of statistical mechanics for quantum thermodynamics.

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Abstract: How should we describe the thermodynamics of extreme quantum regimes, where features such as coherence and entanglement dominate?

I will discuss possible limitations of a traditional statistical mechanics approach, and then describe work that applies modern techniques from the theory of quantum information to the foundations of thermodynamics. In particular I discuss recent progress in quantum resource theories and argue that to properly encapsulate the thermodynamic structure of quantum coherence and entanglement we must make use of concepts beyond free energies.

Limitations of statistical mechanics for quantum thermodynamics.

Imperial College London

THE ROYAL SOCIETY

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Trajectory

- Motivations + background.
- Possible limitations of traditional approaches.
- Resource theories & symmetry principles.
- Quantum coherence in thermodynamics.

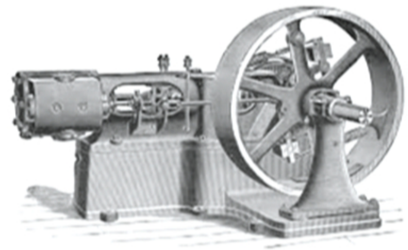
(Work with M. Lostaglio, K Korzekwa, T. Rudolph, J. Oppenheim, M. Frenzel.)

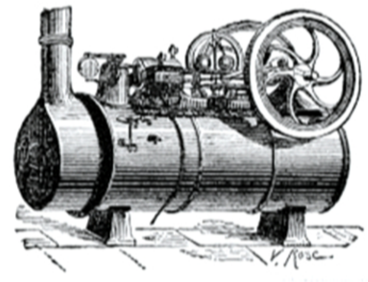
2nd Law of Thermodynamics

- "It is impossible to construct a device who's sole effect is the extraction of work from heat."
- "It is impossible to construct a device who's sole effect is the erasure of a bit."
- "It is impossible to see inside a furnace, solely by the light of the furnace."*

* Bennett (1987)

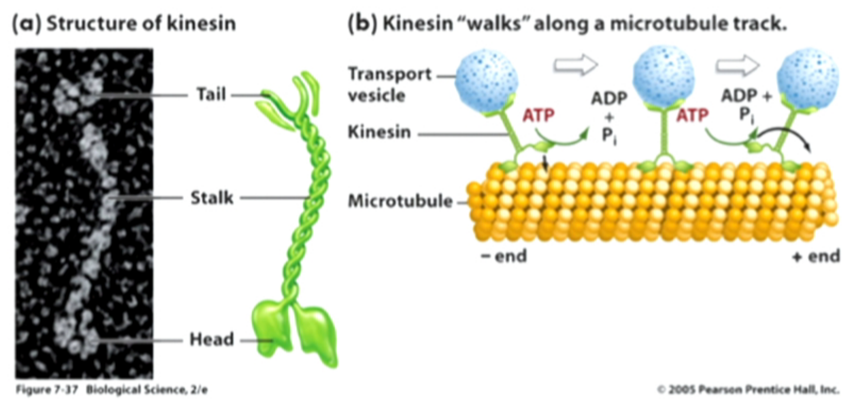
Limitations of existing thermodynamics



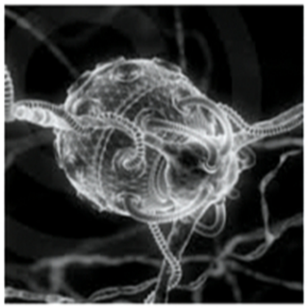


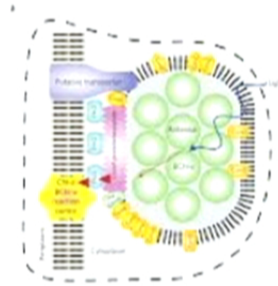
The Thermodynamic Limit

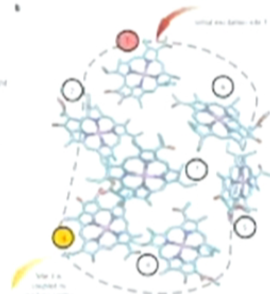
- *"Thermodynamics means the thermodynamic limit."*
- (Except it doesn't)



Non-asymptotic thermodynamics







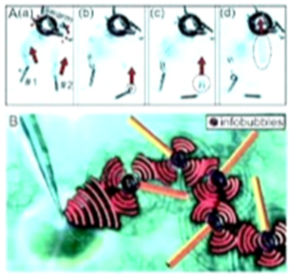
- **Q: What thermodynamic laws operate at micro/nano/pico/… scales?**
- **Q: How do coherent superpositions extend thermodynamic processes?**

Applications

- Active work to develop nanoscale thermodynamic machines.

- Nanotechnology ~$6 billion (currently)

What are the fundamental thermodynamic laws beyond the thermodynamic limit?



Applications

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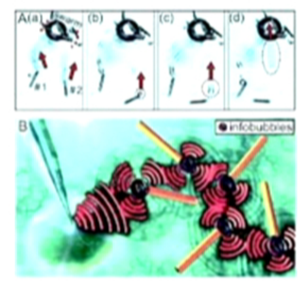
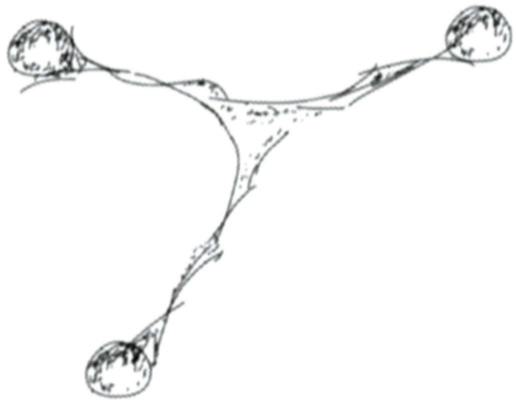
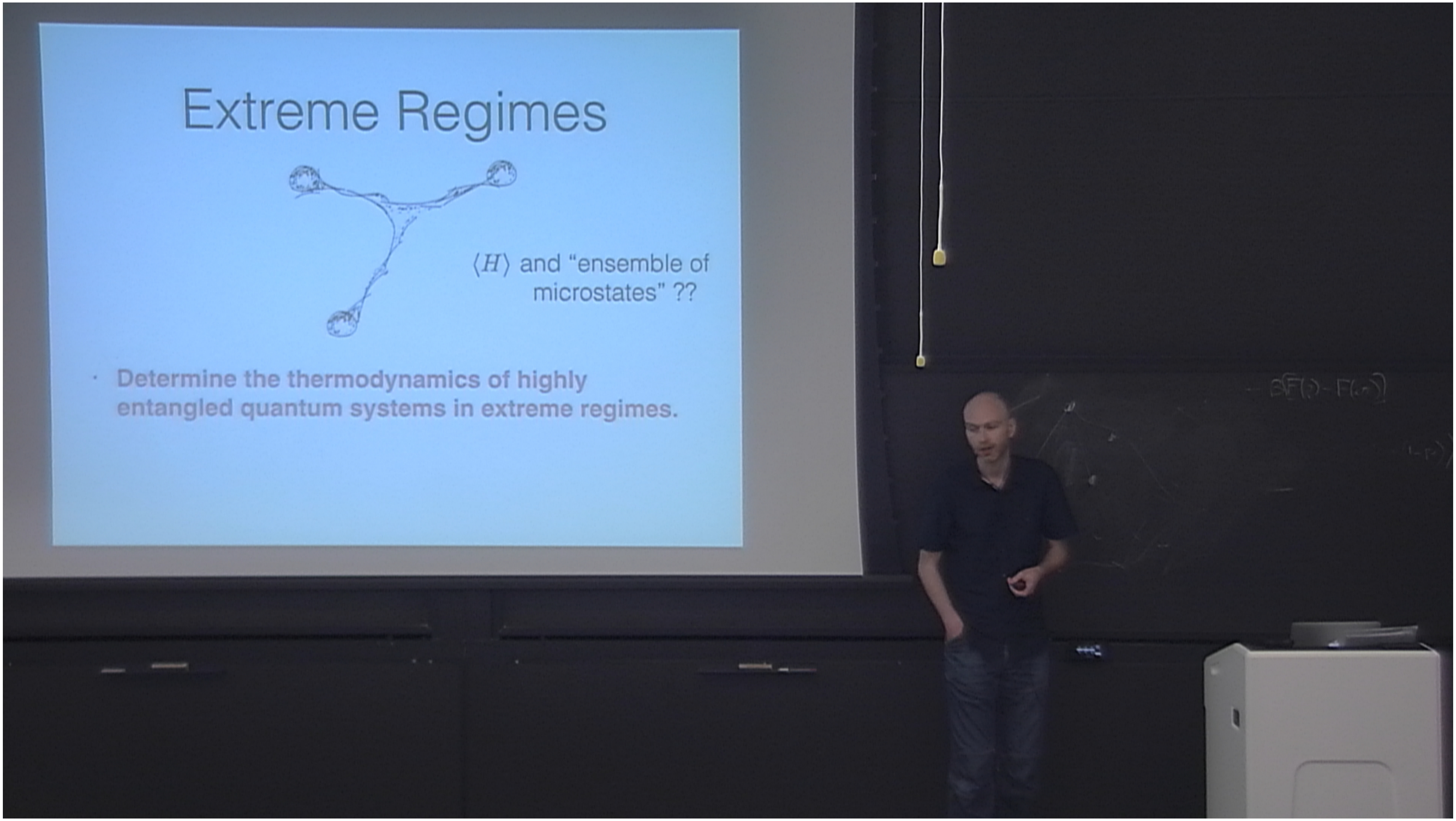


What are the fundamental thermodynamic laws beyond the thermodynamic limit?

Extreme Regimes



- **Determine the thermodynamics of highly entangled quantum systems in extreme regimes.**


Extreme Regimes
⟨H⟩ and "ensemble of microstates" ??
Determine the thermodynamics of highly entangled quantum systems in extreme regimes.

Potential limitations of more traditional analysis

Traditional 2nd Law

- **"It is impossible to construct a device who's sole effect is the extraction of work from heat."**

$$\langle W \rangle \leq -\Delta F$$

Fluctuation Theorems?

- **Arbitrarily violent dynamics** on thermal state.
- Sharpening of 2nd Law to an **equality**.

Core structure: $\mathcal{P}_{\gamma_*}(x) = e^{-\beta x}\mathcal{P}_{\gamma}(-x)$ $\qquad \beta = \frac{1}{kT}$

Distribution for backward process

Distribution for forward process

$$\downarrow$$

$$\boxed{\langle e^{-\beta(W-\Delta F)}\rangle = 1}$$

$$\downarrow$$

$$\langle W \rangle \leq -\Delta F$$

* C. Jarzynski, Phys. Rev. Lett. (1997)

Fluctuation Theorems?

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Distribution for backward process

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$$\Downarrow$$

$$\langle W \rangle \leq -\Delta F$$

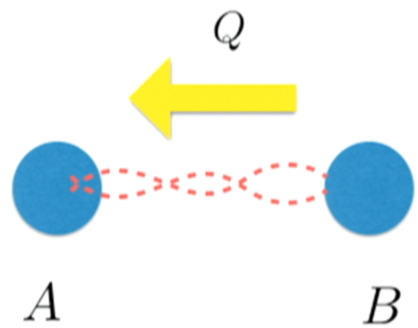
* C. Jarzynski, Phys. Rev. Lett. (1997)

Fluctuation Theorems

$$\langle e^{-\Delta\beta Q}\rangle = \gamma := \langle e^{-\Delta\mathcal{I}}\rangle$$

Energy exchange

Initial correlations



$$\langle \Delta\mathcal{I}\rangle = I_c(A:B)$$

$$\rho_{AB} \rightarrow \sum_{j,k} \Pi_{j,k}\rho_{AB}\Pi_{j,k}$$

Only **classical** correlations contribute.

Poorly suited to handling **coherence** and **entanglement**.

* DJ, et al, Phys. Rev. E (2015)

how *should* we handle intrinsically quantum-mechanical properties?

Maximum entropy principles?

Thermodynamics

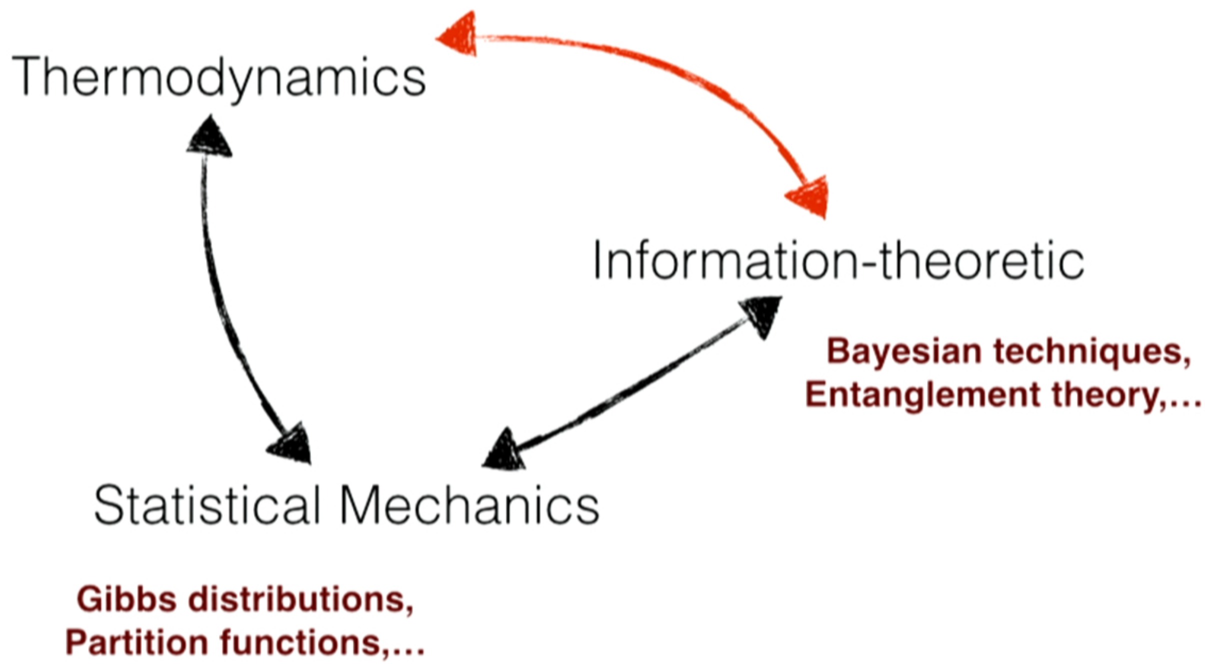
Information-theoretic

Bayesian techniques, Entanglement theory,….

Statistical Mechanics

Gibbs distributions, Partition functions,…

Maximum entropy principles?



A different kind of analysis

- "***Heat***", "***temperature***" — ambiguous/complex/ indirect…or maybe not even definable.
- **Giles (1964)**: *thermodynamics ultimately concerns the accessibility/inaccessibility of one physical state from another.*

"The mathematical foundations of thermodynamics", R. Giles (1964)

A different kind of analysis

- **Thermodynamics**: *the accessibility/ inaccessibility of one physical state from another under particular operations.*

- **Entanglement theory**: *the accessibility/ inaccessibility of one quantum state from another under Local operations and Classical Communications.*

Primitive measures

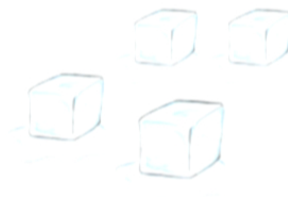
A single unit of "entropy"

1g of ice @ 0 Celsius **1g of water @ 0 Celsius**

A single unit of entanglement

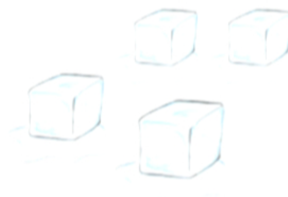
$|\psi^{-}\rangle$

An adiabatic process



Star

An adiabatic process



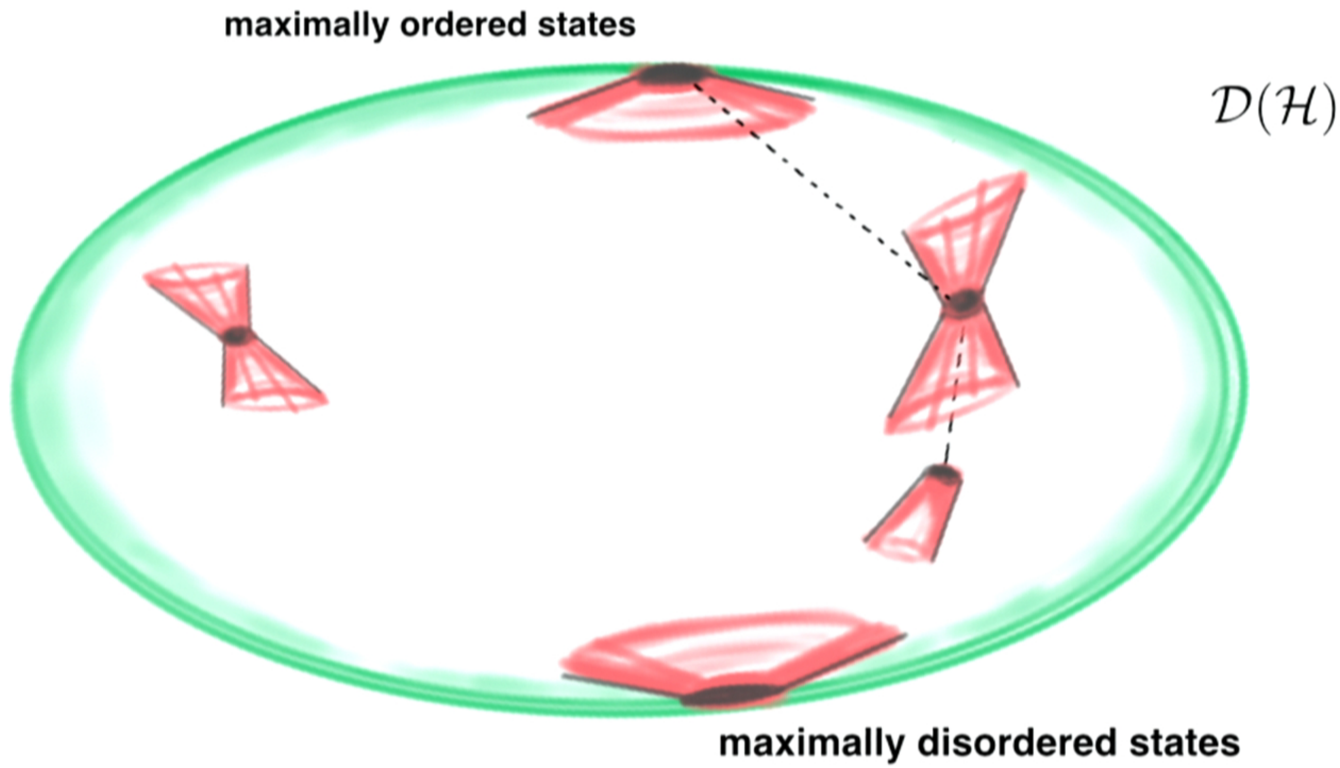
Star

Supernova

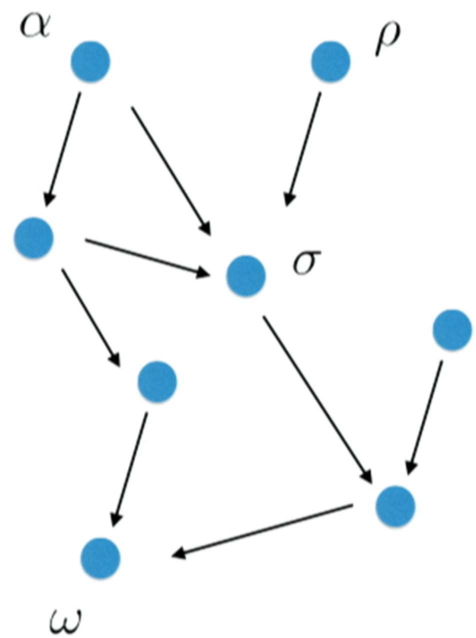
Remnant

Maximum # ice cubes that can be melted?

Thermodynamics



Thermodynamic Entropy



When does thermodynamic ordering have a unique entropic formulation?

$$\rho \to \sigma$$
$$\Leftrightarrow S(\rho) \leq S(\sigma)$$

A unique additive entropy exists if and only if the following 7 conditions hold:

Reflexivity	$\rho \to \rho$
Transitivity	$\rho \to \sigma$ and $\sigma \to \tau$ implies $\rho \to \tau$
Consistency	$\rho_1 \to \sigma_1$ and $\rho_2 \to \sigma_2$ then $(\rho_1, \rho_2) \to (\sigma_1, \sigma_2)$
Scale invariance	$\rho \to \sigma$ then $\rho^{\otimes t} \to \sigma^{\otimes t}$ for $t \geq 0$
Splitting	$\rho \leftrightarrow (\rho^{\otimes t}, \rho^{\otimes (1-t)})$
Stability	$(\rho, \epsilon_1) \to (\sigma, \epsilon_2)$ then $\rho \to \sigma$
Comparability	if $\alpha \to \rho$ and $\beta \to \rho$ then $\alpha \to \beta$ or $\beta \to \alpha$

** E. Lieb & J. Ingvason The physics and mathematics of the second law (1999)*

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Consistency $\rho_1 \to \sigma_1$ and $\rho_2 \to \sigma_2$ then $(\rho_1, \rho_2) \to (\sigma_1, \sigma_2)$

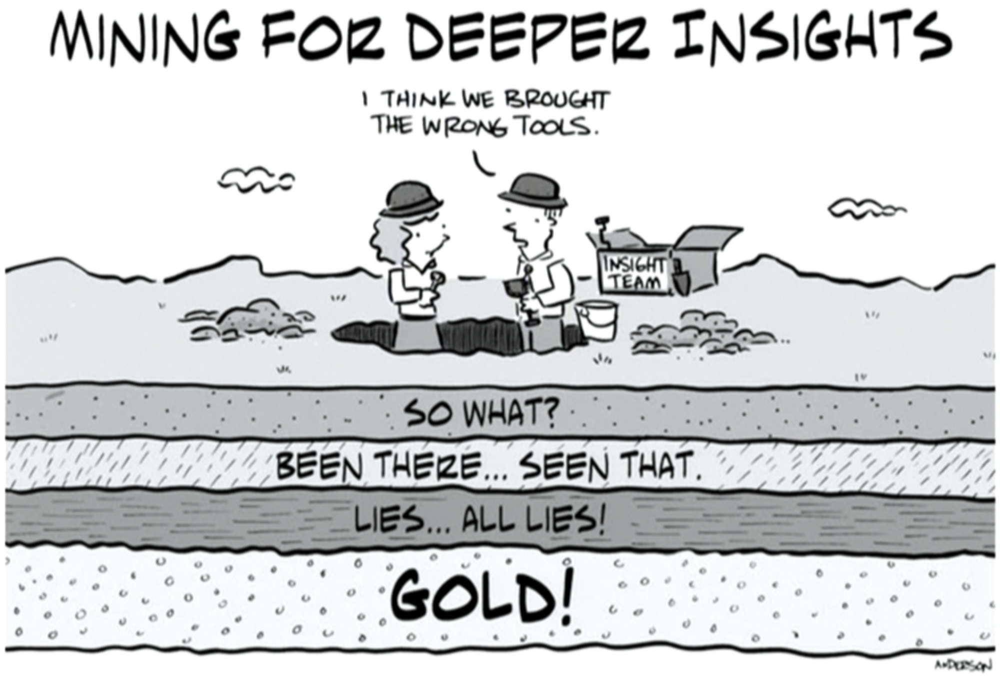
Scale invariance $\rho \to \sigma$ then $\rho^{\otimes t} \to \sigma^{\otimes t}$ for $t \geq 0$

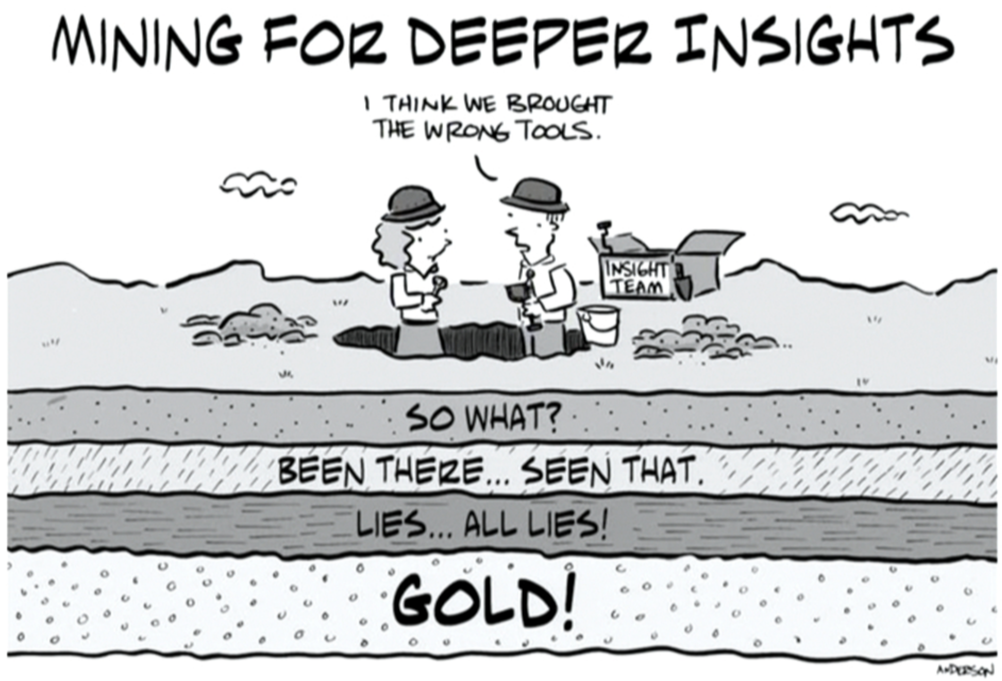
Splitting $\rho \leftrightarrow (\rho^{\otimes t}, \rho^{\otimes(1-t)})$

Stability $(\rho, \epsilon_1) \to (\sigma, \epsilon_2)$ then $\rho \to \sigma$

Comparability if $\alpha \to \rho$ and $\beta \to \rho$ then $\alpha \to \beta$ or $\beta \to \alpha$

** E. Lieb & J. Ingvason The physics and mathematics of the second law (1999)*


MINING FOR DEEPER INSIGHTS
I THINK WE BROUGHT THE WRONG TOOLS.
INSIGHT TEAM
SO WHAT?
BEEN THERE... SEEN THAT.
LIES... ALL LIES!
GOLD!
ANDERSON



Learn from Entanglement Theory

The Quantum Resource Theory Recipe:

Step 1: Define "free states"

Step 2: Define "free operations"

1. **Ordering** of accessible/inaccessible states
2. **Resource states**.
3. Resource **measures**.

Entanglement

1. **Free states:** **separable states** $\sum_k p_k \rho_k \otimes \sigma_k$
2. **Free quantum operations:**

Local Operations & Classical Communications

—Entanglement is non-increasing—

Some very recent resource directions

- Weilenmann, Kramer, Faist, Renner (2015)
- Fritz (2015)
- Brandao, Gour (2015)
- Coecke, Fritz, Spekkens (2014)
- and others…..

Resource Theory of Thermodynamics

1. **Free states: thermal states** $\gamma = e^{-\beta H}/Z$

2. **Free quantum operations:**

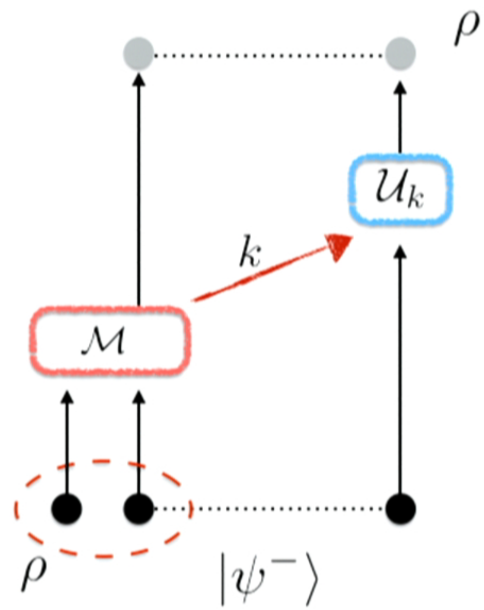
$$\mathcal{E}(\rho) = \mathrm{tr_b}[\mathrm{U}(\rho \otimes \gamma_\mathrm{b})\mathrm{U}^\dagger]$$

$$[U, H_\mathrm{tot}] = 0$$

—athermality is non-increasing—

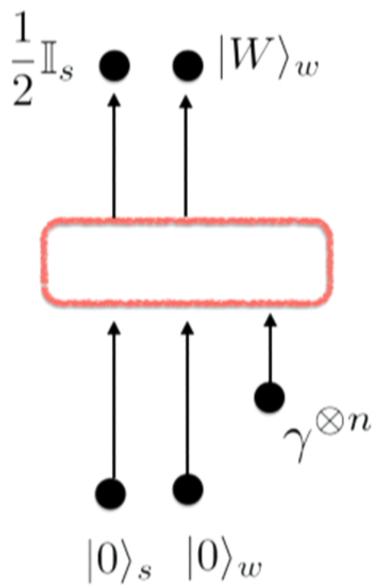
** Brandao et al, Phys. Rev. Lett. (2013)*

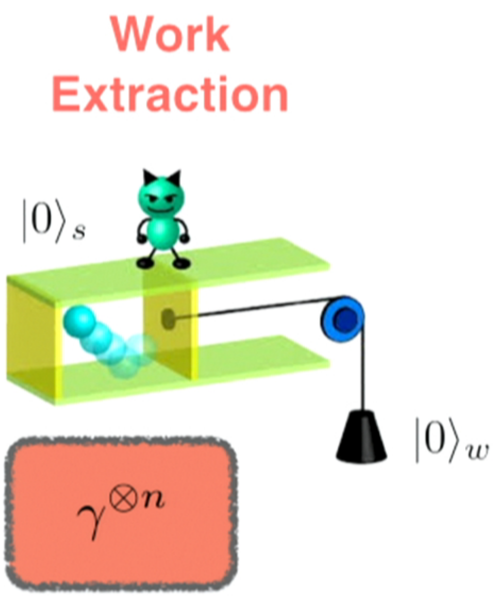
Use of resources: Entanglement



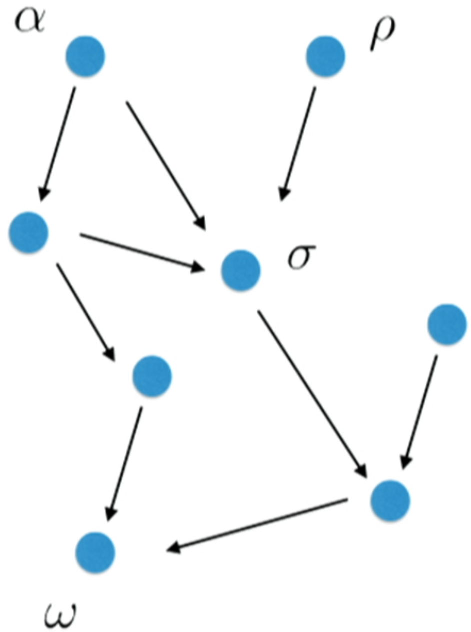
Quantum Teleportation

Use of resources: Thermodynamics

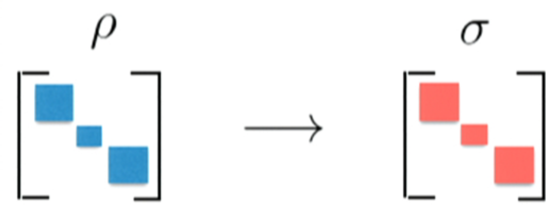




Mapping the general thermal structure



Zero-coherence states:



Q: Does the ordering of states admit an entropic formulation?

"A Set of Second Laws" (Jonathan's talk!)

Theorem: For zero coherence states, the transformation $\rho \to \sigma$ is possible

if and only if $F_\alpha(\rho) \geq F_\alpha(\sigma) \quad \forall\alpha$

A **set** of entropy conditions

Renyi-divergences: $D_\alpha(\rho||\sigma) = \frac{1}{\alpha - 1} \log\left[\mathrm{tr}(\sigma^\kappa \rho \sigma^\kappa)^\alpha)\right]$

$$F_\alpha(\rho) := D_\alpha(\rho||\gamma)$$

$$\kappa = \frac{1-\alpha}{2\alpha}$$

* Brandao et al, PNAS (2014)

But what about
Quantum Coherence
& Thermodynamics?

But what about
Quantum Coherence
& Thermodynamics?

Symmetry & the 1st Law of Thermodynamics

- Traditional form: $dE = dQ + dW$
- Microscopic energy conservation (system+bath).

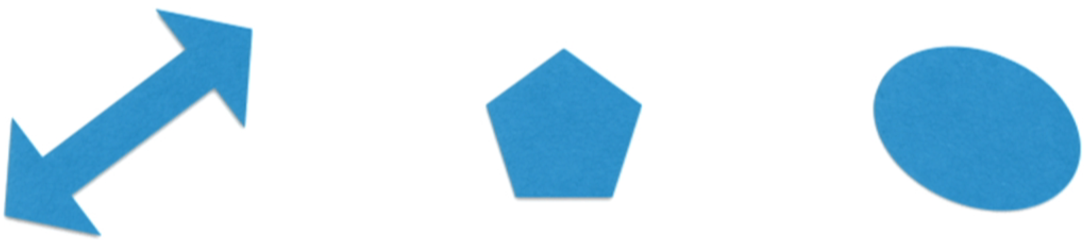
Quantum Mechanical <u>Symmetry</u>:

$$[U, H_{\mathrm{tot}}] = 0$$

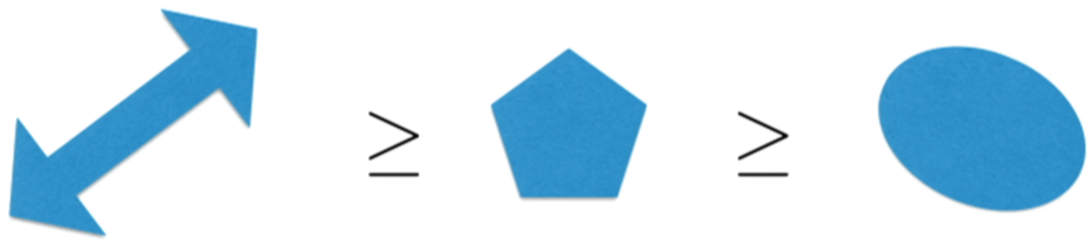
$$t \mapsto e^{-itH_{\mathrm{tot}}}$$

Constrains **non-conservation** of **two** quantities:

(a) System energy
(b) System "coherence"



When is A is more asymmetric than B?



A theory of asymmetry

Related papers:

- *I. Marvian,R. Spekkens Phys. Rev. A 90, (2014)*
- *I. Marvian, R. Spekkens, New J. Phys. 15, (2013)*
- *G. Gour, I Marvian, R. Spekkens Phys. Rev. A 80, 012307 (2009)*
- *M. Ahmadi, DJ, T. Rudolph, New. J. Phys. 15 (2013)*

A theory of asymmetry

- "Group-theoretic Anna Karenina Principle":

"all symmetric objects are alike; each asymmetric object can be asymmetric in its own way."

A theory of asymmetry

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"all symmetric objects are alike; each asymmetric object can be asymmetric in its own way."

Resource Theory of Asymmetry

$U : G \to U(g)$

1. **Free states:** **symmetric states** $U\rho U^\dagger = \rho$

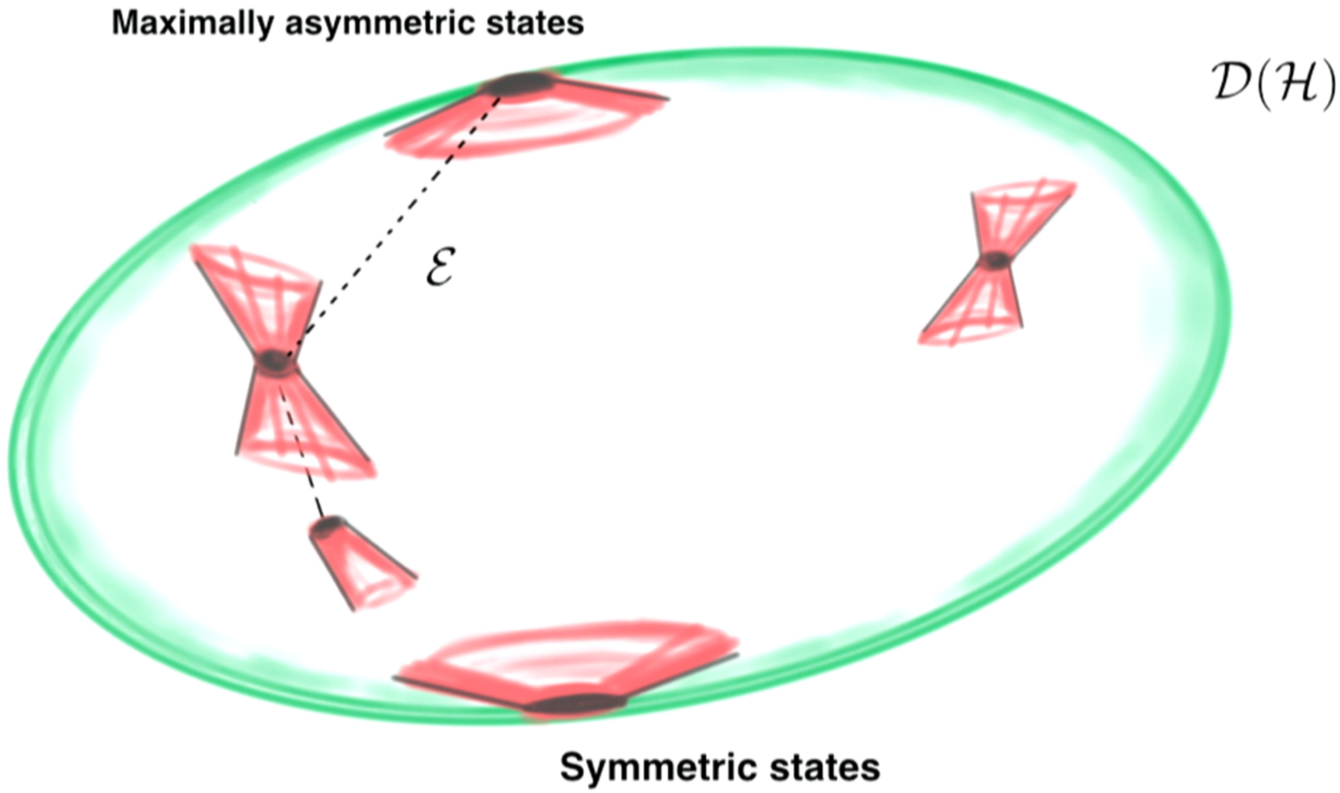
2. **Free quantum operations:**

symmetric/covariant operations

$$U\mathcal{E}(\rho)U^\dagger = \mathcal{E}(U\rho U^\dagger)$$

—asymmetry is non-increasing—

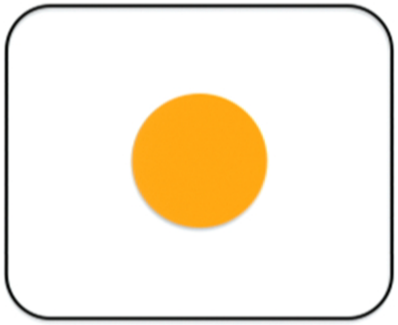
A theory of asymmetry



Example, $G = SU(2)$

Rotationally invariant states

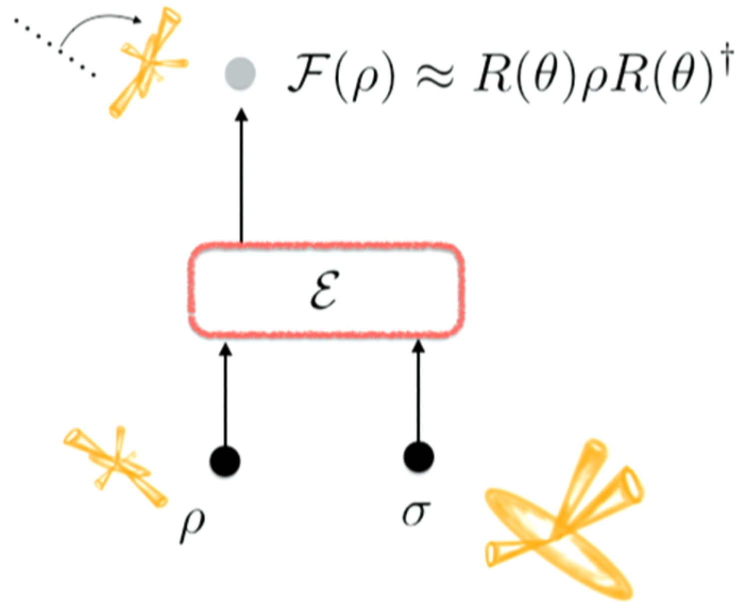
$|\psi^-\rangle, \; \rho_s = \frac{1}{2}\mathbb{I}$



Pointy/Asymmetric states

$\rho_s = |\uparrow\uparrow\rangle, \quad \frac{1}{3}|l,l\rangle\langle l,l| + \frac{2}{3}|l,0\rangle\langle l,0|$

Use of resources: asymmetry



Spatial Rotation

Asymmetry structure

Resource state

symmetry restoration

G-orbit

$\downarrow$

metric

$\downarrow$

resource measures

*C. Cirstoiu, DJ, (2015)

The 1st Law of Thermodynamics

- Traditional form: $dE = dQ + dW$
- Microscopic energy conservation. $[U, H_{\rm tot}] = 0$

$$t \mapsto e^{-itH_{\rm tot}}$$

$$\sqrt{p}|E_0\rangle + \sqrt{1-p}|E_1\rangle \to e^{-itE_0}\sqrt{p}|E_0\rangle + e^{-itE_1}\sqrt{1-p}|E_1\rangle$$

Core connection

$[U, H_{\text{tot}}] = 0$

Global energy conservation
+
Thermal states

$\gamma = \frac{e^{-\beta H}}{Z}$

Thermodynamics is a **particular** asymmetry theory

Coherence $\Longleftrightarrow$ U(1)-asymmetry

THERMAL $\subset U(1)$ COVARIANT

Thermal operations: $\mathcal{E}(\rho) = \mathrm{tr_b}[\mathrm{U}(\rho \otimes \gamma)\mathrm{U}^\dagger]$

Covariant operations: $\mathcal{F}(U_1(g)\rho U_1(g)^\dagger) = U_2(g)\mathcal{F}(\rho)U_2(g)^\dagger$

$\forall g \in G$

* M. Lostaglio, DJ, T. Rudolph, Nature Comm. (2015)

$\text{THERMAL} \subset U(1)\ \text{COVARIANT}$

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$\forall g \in G$

Covariant Stinespring dilation: $\mathcal{F}(\rho) = \mathrm{tr}_2[\mathrm{V}(\rho \otimes \sigma)\mathrm{V}^\dagger]$

symmetric auxiliary state

* *M. Keyl, R. Werner J.Math.Phys. (1998)*

$\text{THERMAL} \subset U(1) \text{ COVARIANT}$

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symmetric auxiliary state

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Applications of Framework:

1. The insufficiency of free energy relations.
2. Coherence “work-locking”.
3. General thermodynamic bounds on coherence.
4. Intrinsically-quantum 2nd law constraints.

Based on:

- *Lostaglio, Korzekwa, Oppenheim, DJ, arxiv:05.xx (2015)*
- *Lostaglio, DJ, Rudolph, Nature Comm. (2015)*
- *Lostaglio, Korzekwa, DJ, Rudolph, Phys. Rev. X (2015)*

(1). Insufficiency of free energies in thermodynamics.

Consider <u>any</u> set of functions $\{D_\alpha(\cdot)\}_\alpha$ that **"behave like free energies"**:

If $\rho \to \sigma$ then we have $\{D_\alpha(\rho) \geq D_\alpha(\sigma)\}_\alpha$

and $D_\alpha(\rho) \geq c||\rho - \gamma||$

then

$\{D_\alpha(\cdot)\}_\alpha$ cannot provide a complete set of thermodynamic constraints.

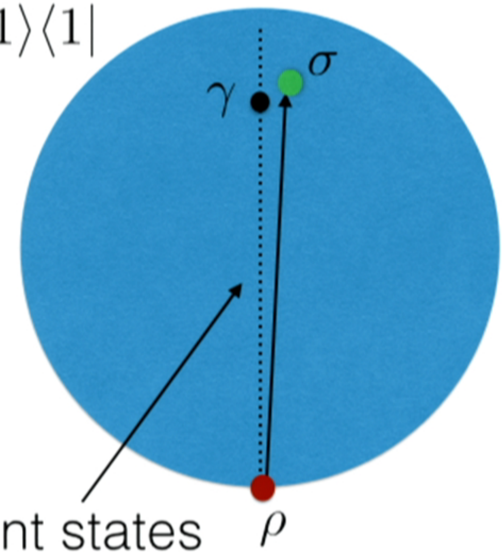
(1). Insufficiency of free energies in thermodynamics.

$H = |1\rangle\langle 1|$

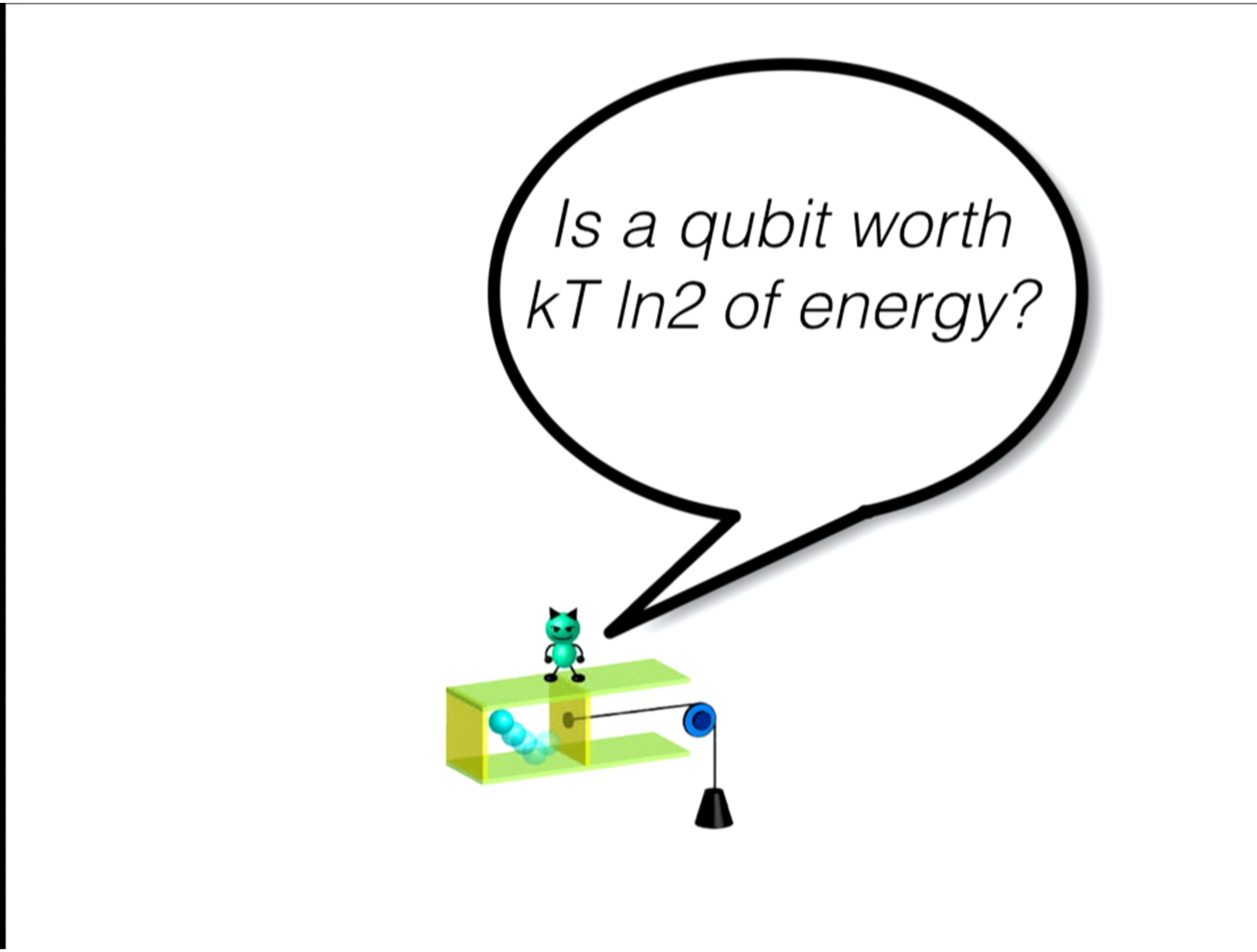
Proof:

D_α say "get closer to γ."

Symmetry says:
"asymmetry non-increasing." $\blacksquare$



$$\sigma = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$

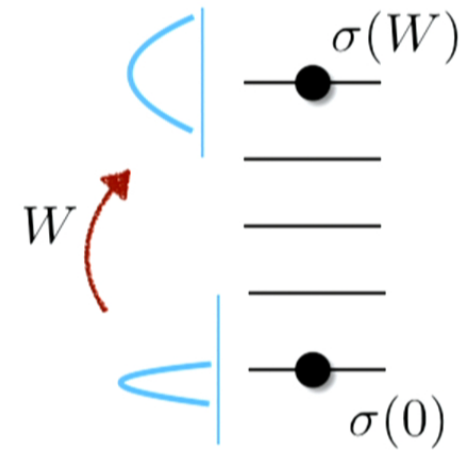

Is a qubit worth
kT ln2 of energy?

Work / Ordered Energy

Allow a broad work definition:
"raising a weight up a ladder by height W"

$$\sigma(0) \to \sigma(W)$$

$$W = f(\langle H \rangle, \langle H^2 \rangle, \langle H^3 \rangle, \dots)$$



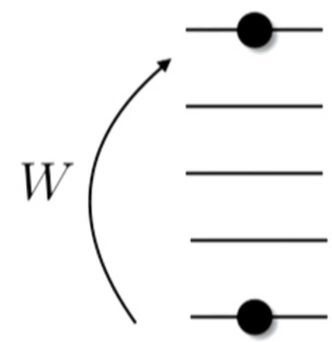
(2).Work-locked in coherence

Theorem:

$$[\rho \to W] \Leftrightarrow [\mathcal{D}(\rho) \to W]$$

where

$$\mathcal{D}(\rho) = \mathcal{G}_H(\rho) = \int dt e^{-itH} \rho e^{itH}$$

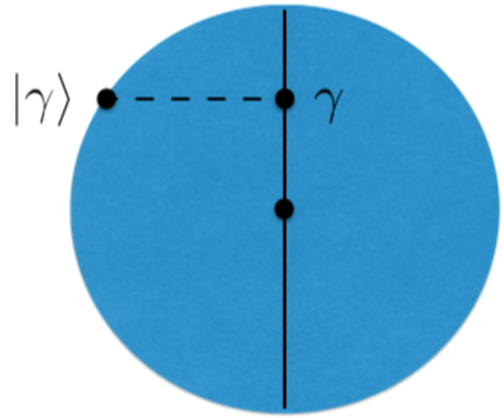


Szilard and coherence

Pure state $|\gamma\rangle$

$\mathcal{D}(|\gamma\rangle\langle\gamma|) = \gamma$

$\Rightarrow$ **No work** can be extracted from $|\gamma\rangle$ **on its own.**



Value of a qubit ? Non-trivial.

Requires careful "resource counting".

Unlocking coherence for work.

- Use a second coherent source:

(*relational* coherence protected)

$$\mathcal{D}(|\gamma\rangle\langle\gamma|) = \gamma$$

$$\mathcal{D}(|\gamma\rangle\langle\gamma| \otimes \sigma_R) \neq \mathcal{D}(|\gamma\rangle\langle\gamma|) \otimes \mathcal{D}(\sigma_R)$$

σ_R acts as quantum reference frame for $|\gamma\rangle$

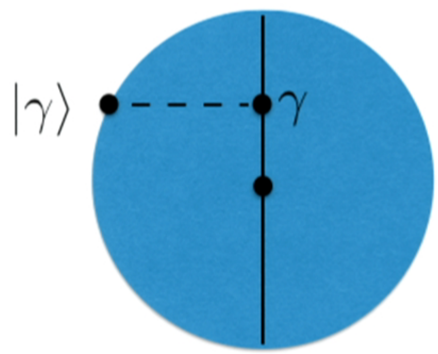
E.g.

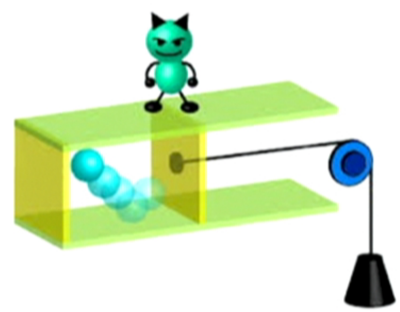
$$\boxed{\begin{aligned} |\gamma\rangle \otimes |\gamma\rangle \rightarrow W &\leq Z^{-1} e^{-\frac{E}{kT}} (E - 2kT \ln Z) \\ &= kT \ln 2 \ (\text{for } E = 0) \end{aligned}}$$

Quantum Szilard engine

- It is only for a particular "classical" regime that we can associate the free energy to every qubit state.

$$|\Psi\rangle \longrightarrow W = -\Delta F$$





M. Lostaglio, K. Korzekwa, J. Oppenheim, DJ, "Extracting work from quantum coherence" arXiv 05.xx (2015)

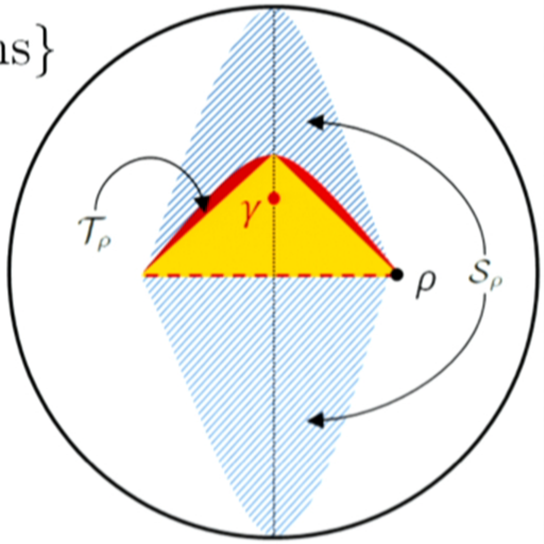
Is free energy all there is to thermo?

$$\mathcal{T}_\rho := \{\sigma : \rho \to \sigma \text{ under thermal operations}\}$$

Now allow **arbitrarily** many $|w\rangle^{\otimes n}$

Extends $\mathcal{T}_\rho$ only to:

$$\mathcal{S}_\rho := \{\sigma : \rho \to \sigma \text{ under covariant maps}\}$$



From Covariant-Stinespring:

$$\mathcal{E}(\rho) = \mathrm{tr}_\mathrm{b}[\mathrm{U}(\rho \otimes \gamma_\mathrm{b})\mathrm{U}^\dagger]$$

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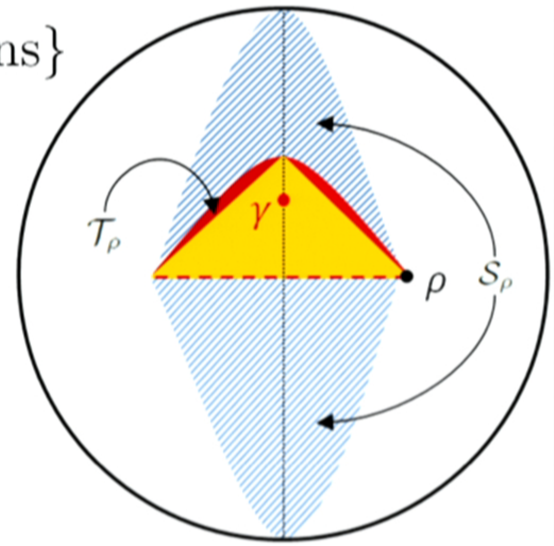

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$$\mathcal{E}(\rho) = \mathrm{tr_b}[\mathrm{U}(\rho \otimes \gamma_\mathrm{b})\mathrm{U}^\dagger]$$

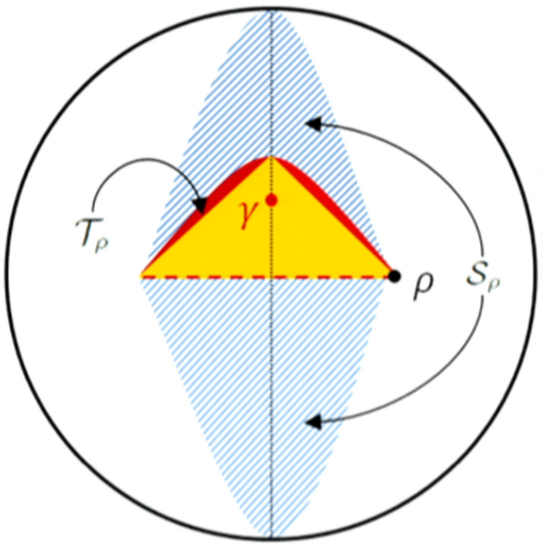
Non-trivial Coherence

Yellow region:

$$\{\sigma = p\rho + (1-p)\mathcal{E}(\mathcal{D}(\rho))\}$$

(thermal map on dephased state)

Suggests at least two resources at play: (purity, asymmetry)



Mode operators

- Apply harmonic analysis to operators: irreps of group action.

$$\mathcal{B}(\mathcal{H}) = \bigoplus_{\nu} V_\nu$$

$$U(t)\rho^{(\nu)}U(t)^\dagger = e^{-i\nu t}\rho^{(\nu)}$$

$$\rho = \sum_{\nu=-d}^{d} \rho^{(\nu)}$$

Thermal operations

$$[\mathcal{E}(\rho)]^{(\nu)} = \mathcal{E}(\rho^{(\nu)})$$

$$||\mathcal{E}(\rho)^{(\nu)}||_1 \leq ||\rho^{(\nu)}||_1$$

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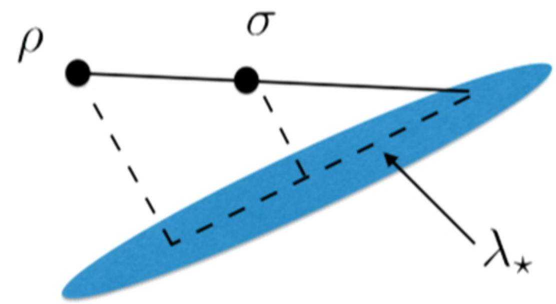
(3). General Bounds on Coherence

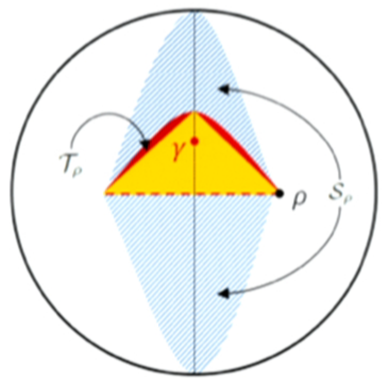
Lower bound:

$$\sigma^{(\nu)} = \lambda_\star \rho^{(\nu)}$$



Upper bound:

$$|\sigma_k^{(\nu)}| \leq \sum_{c:\omega_c \leq \omega_k} |\rho_c^{(\nu)}| e^{-\beta\hbar(\omega_k - \omega_c)} + \sum_{c:\omega_c > \omega_k} |\rho_c^{(\nu)}|$$



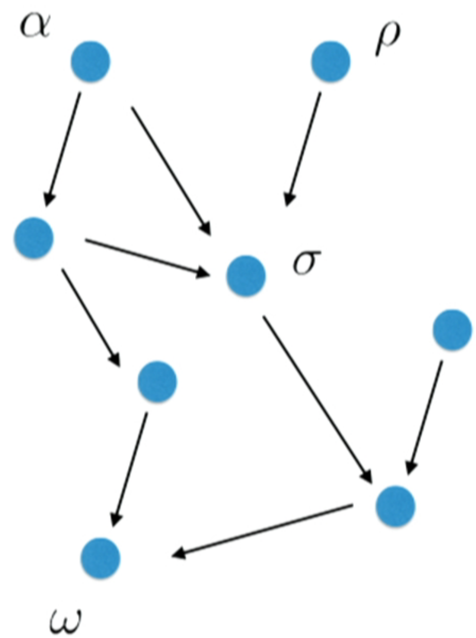
Previous bound:

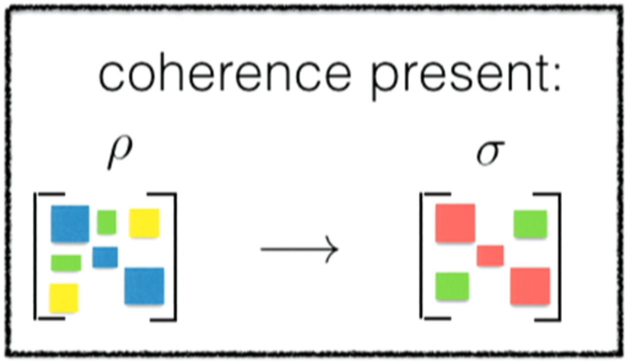
$$|\sigma_{nm}| \leq |\rho_{nm}| \sqrt{p_{n|n} p_{m|m}}$$

* Cwiklinski, Studzinski, Horodecki, Oppenheim, arxiv (2014)

*M. Lostaglio, K. Korzekwa, DJ, T. Rudolph, Phys. Rev. X (2015)

(4). The full thermodynamic ordering of states?





Q: Does the ordering of states admit an entropic formulation?

Thermodynamic structure

- Entanglement theory ~ non-locality monotones.
- Asymmetry theory ~ asymmetry monotones.
- Thermodynamics ~ **ordered energy + asymmetry**

Work

Quantum coherence

Distillation/Formation

Work:

$|w\rangle = |1\rangle^{\otimes w}$

$$W_{\text{form}} \to \rho \to W_{\text{distill}}$$

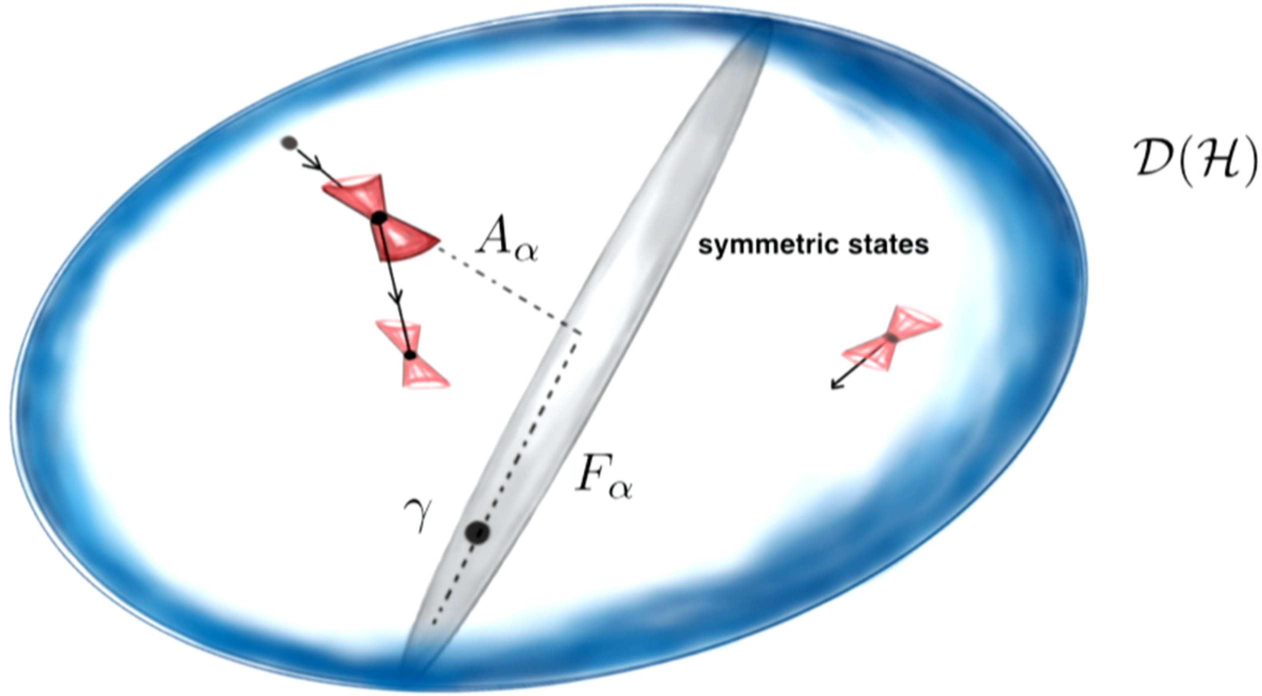
$D_\infty(\rho||\gamma)$ $D_0(\rho||\gamma)$

Coherence:

$|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$

ρ

$A_\infty(\rho)$ $A_0(\rho)$


$\mathcal{D}(\mathcal{H})$
A_α
symmetric states
F_α
γ

(4). Necessary entropic constraints

Theorem: For arbitrary quantum states, the thermodynamic transformation $\rho \to \sigma$ is possible provided

$$F_\alpha(\rho) \geq F_\alpha(\sigma)$$

$$A_\alpha(\rho) \geq A_\alpha(\sigma) \qquad \forall \alpha \geq 0$$

Asymmetry monotones:

$$A_\alpha(\rho) := D_\alpha(\rho||\mathcal{G}(\rho))$$

$$\mathcal{G}(\rho) = \int_G dg \; U(g)\rho U(g)^\dagger$$

$$F = U - TS$$

$$F(\rho) = F(\mathcal{G}(\rho)) + A_1(\rho)$$

incoherent component

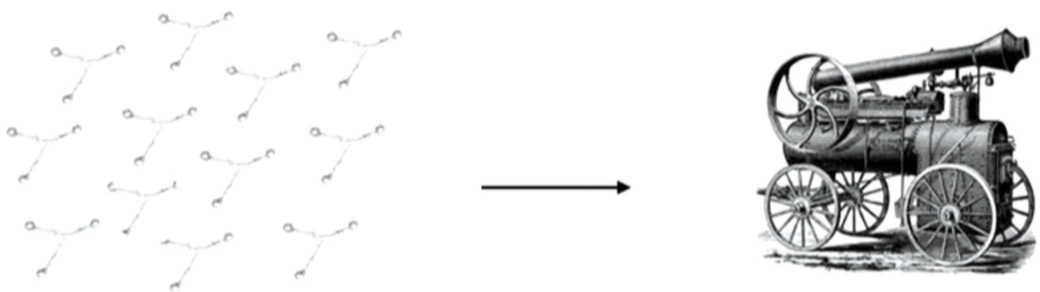
coherent component

Macroscopic regime

- **Theorem:** for any $\rho \in \mathcal{B}(\mathcal{H})$ we have

$$\lim_{n\to\infty} \frac{1}{n} \begin{bmatrix} F_\alpha(\rho^{\otimes n}) \\ A_\alpha(\rho^{\otimes n}) \end{bmatrix} = \begin{bmatrix} F(\rho) - F(\gamma) \\ 0 \end{bmatrix}$$

$$F = \langle H \rangle - TS$$



Review

Essentially unique entropy.

$$\rho \to \sigma \;\Leftrightarrow\; S(\rho) \leq S(\sigma)$$

$$\langle e^{-\beta(W-\Delta F)} \rangle = 1$$ (provably incomplete)

$$\rho \to \sigma \;\Leftrightarrow\; D_\alpha(\rho||\gamma) \leq D_\alpha(\sigma||\gamma)$$

$$\begin{bmatrix} F_\alpha(\rho) \\ A_\alpha(\rho) \end{bmatrix} \leq \begin{bmatrix} F_\alpha(\sigma) \\ A_\alpha(\sigma) \end{bmatrix} +$$

Outlook

- Applications: coherent transport systems (conductivity, energy transport scenarios) ?
- Non-equilibrium state states? Feedback control?
- New entropic conditions — are they both necessary and sufficient?