ÖAW AUSTRIAN ACADEMY OF SCIENCES

IQOQI – INSTITUTE FOR QUANTUM OPTICS AND QUANTUM INFORMATION VIENNA

Exact characterization of entropy and free energy without thermodynamic limit or averaging

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PERIMETER INSTITUTE

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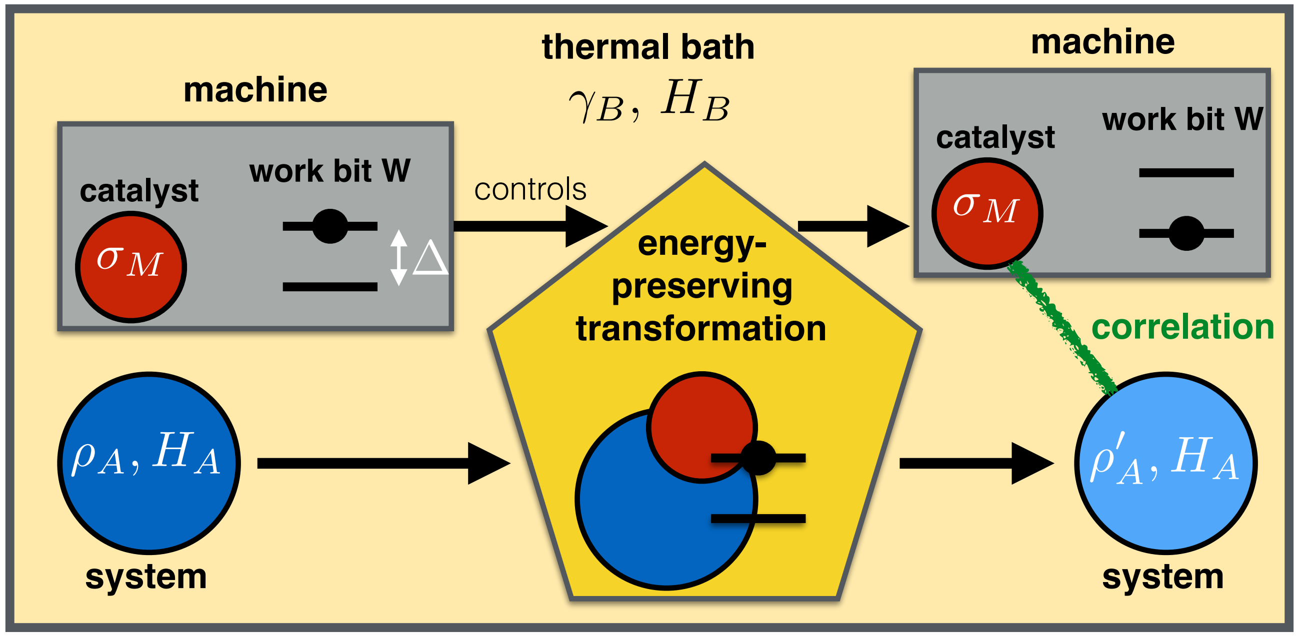
Quantum Information and Foundations of Physics @ IQOQI

May '24, *left to right:* Manuel Mekonnen (PhD student), MM, Stefan Ludescher (PhD student), Thomas Galley (postdoc), Caroline Jones (PhD student), Albert Aloy (postdoc). *Not in the picture:* Andrew J. P. Garner (postdoc).

Overview

1. Standard view: thermodynamic limit

2. Thermodynamics as a resource theory



3. Characterization of *F* and *S* without thermodynamic limit

4. How about coherence? A no-broadcasting theorem

5. Consequences for quantum information theory

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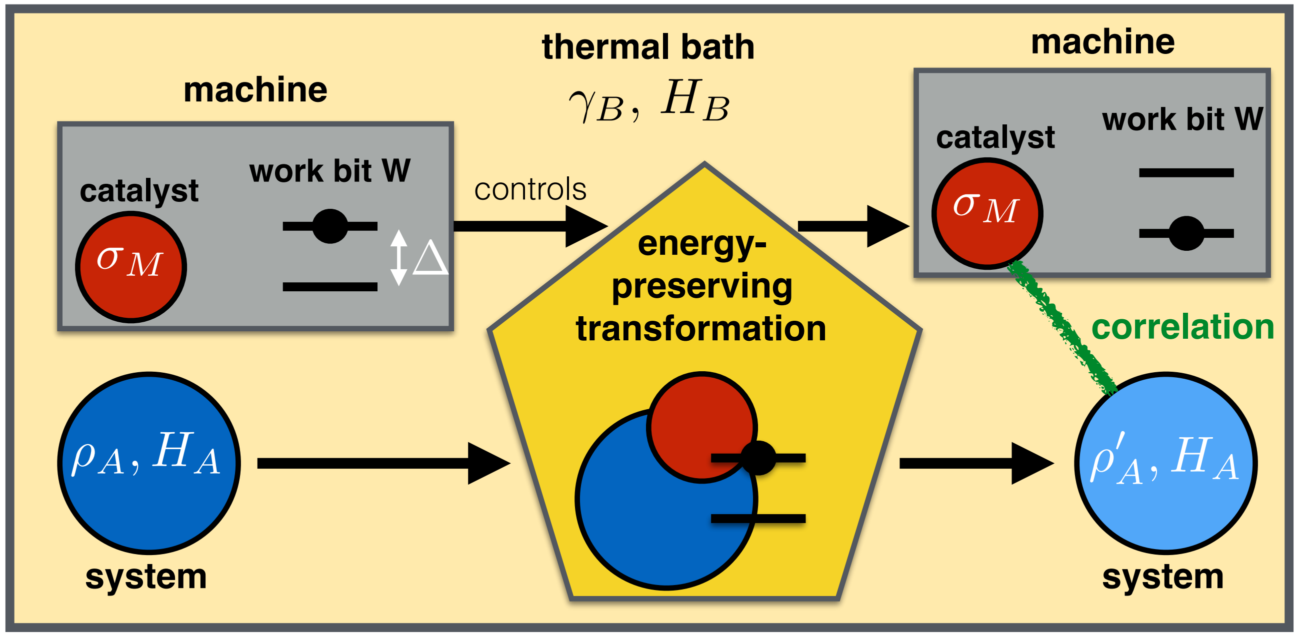

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$$\Delta F \leq 0 \qquad \text{(2nd law)},$$

where $F = U - TS$.
If this is negative, then we can extract $|\Delta F|$ of work from the system.

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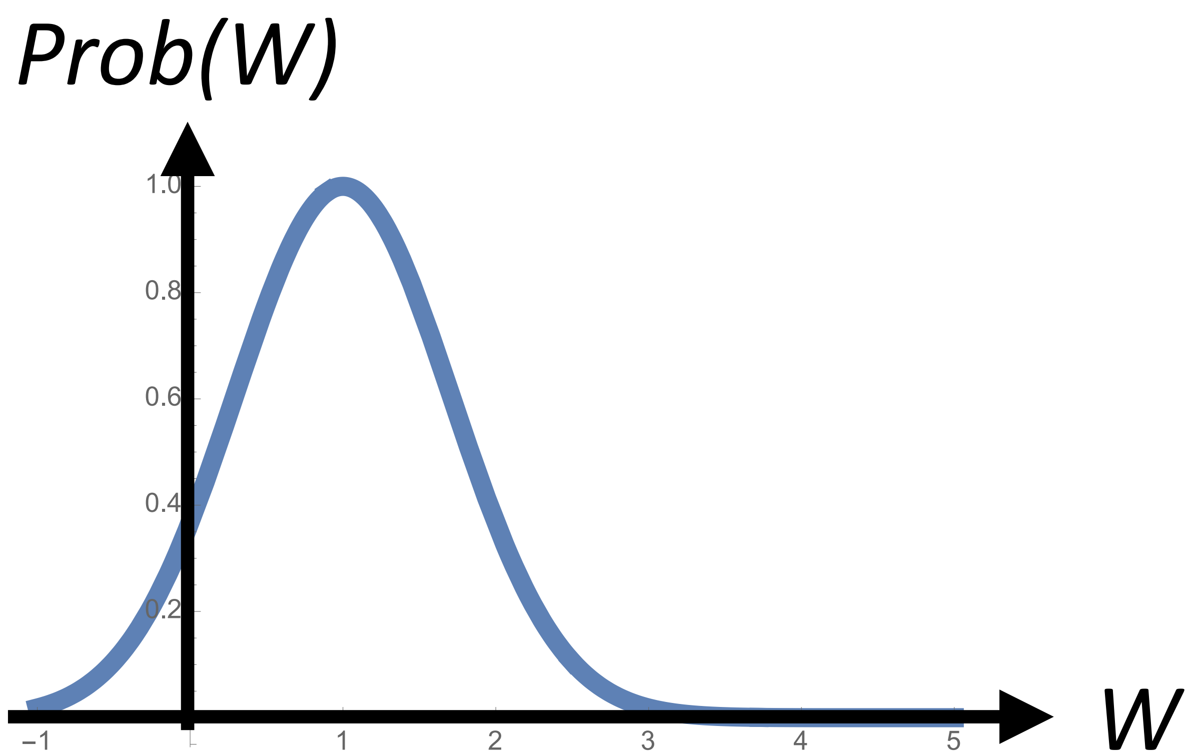
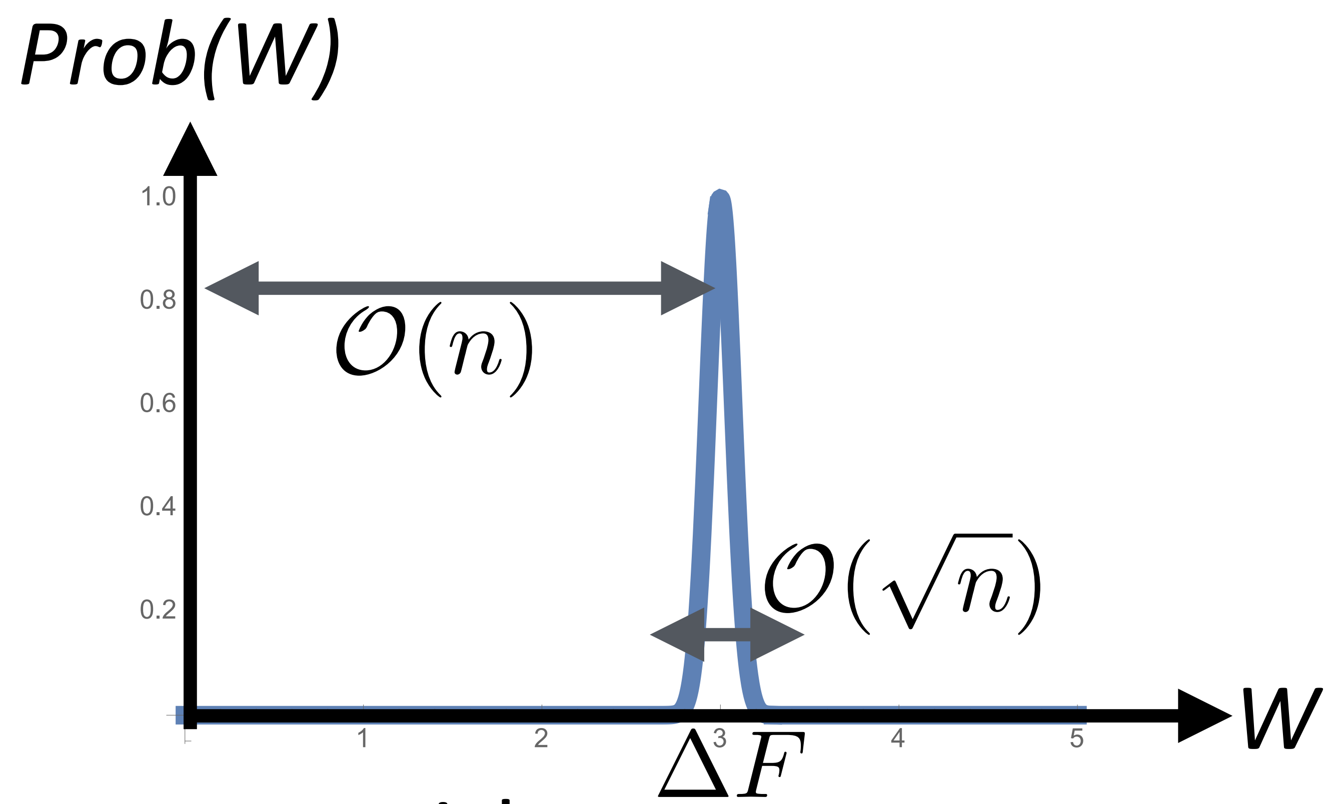
But this is a statement **on average**, since "work" is a random variable.

Standard view: thermodynamic limit

Work is a **random variable** (for any given process):



small # of particles



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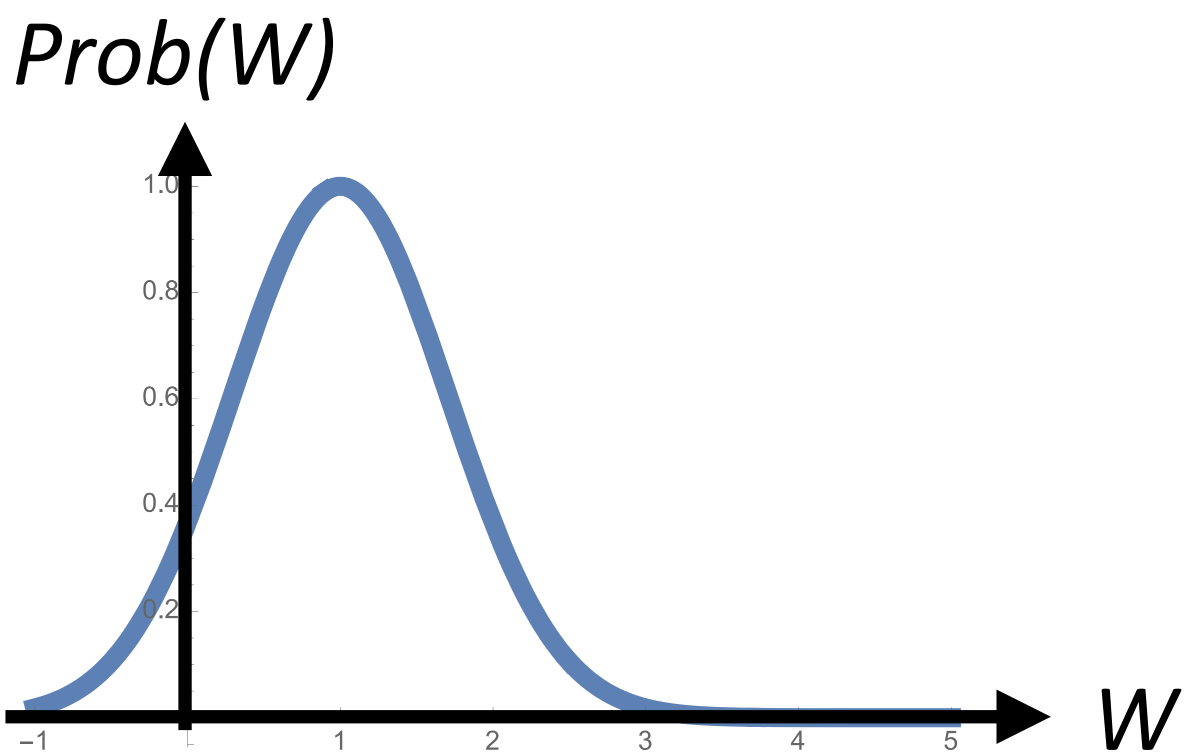

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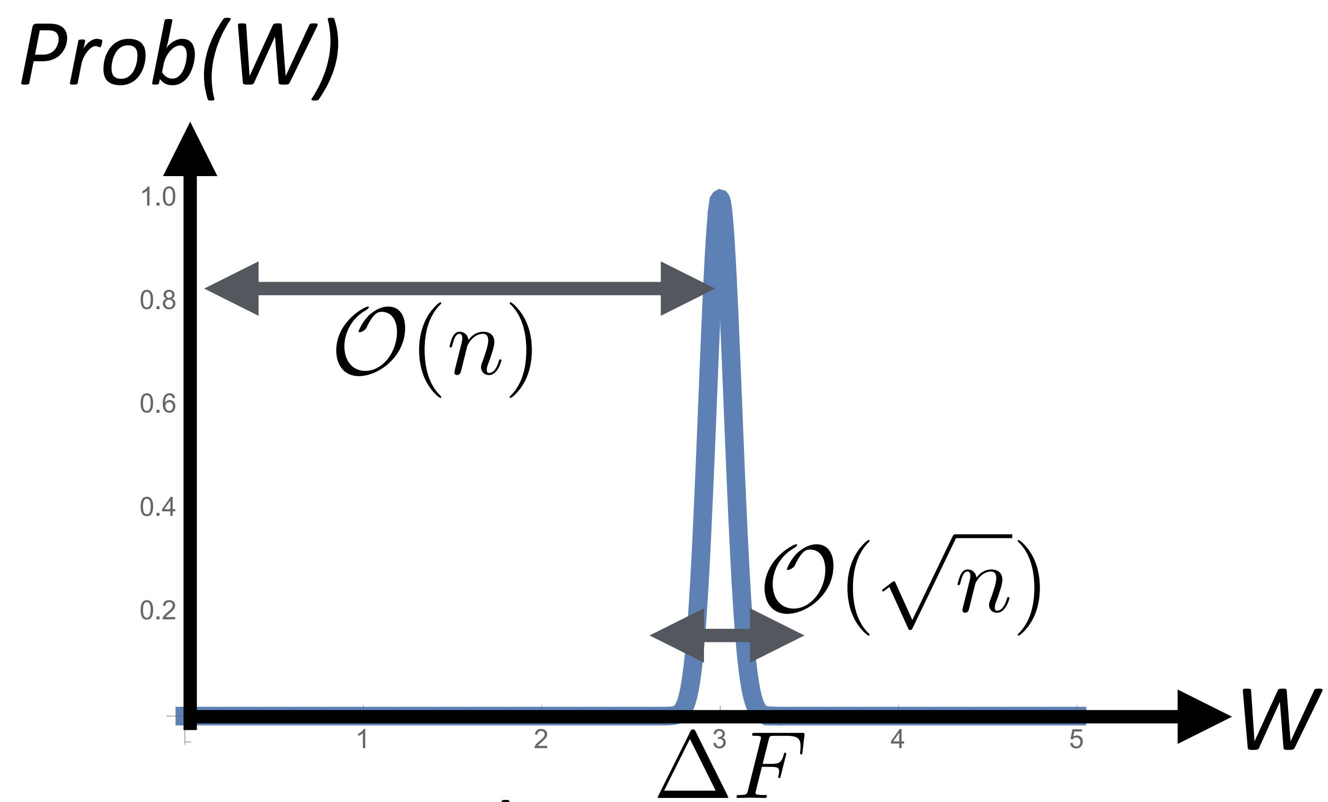

n particles

Reliably extractable work "is" ΔF :
only true in the thermodynamic limit $n \to \infty$
when fluctuations become irrelevant (law of large numbers).

Standard view: thermodynamic limit

But what can we say in the case of "small" or strongly correlated systems? Work $\approx$ its fluctuations $\longrightarrow$ reliability?

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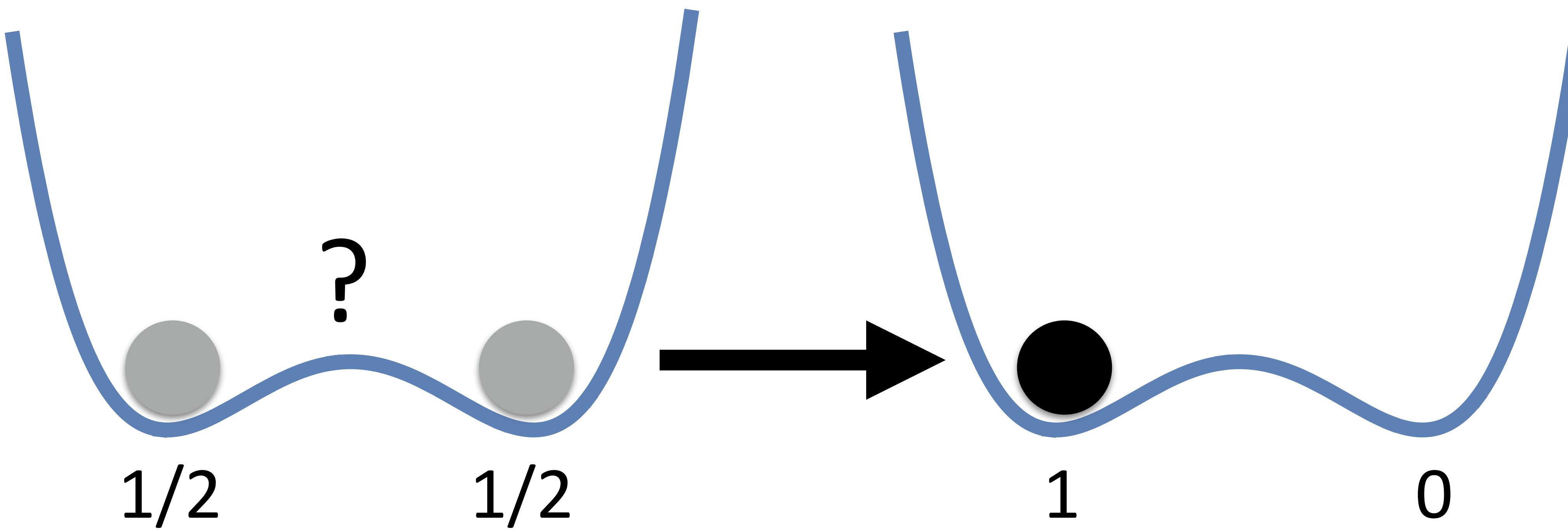
Landauer erasure:



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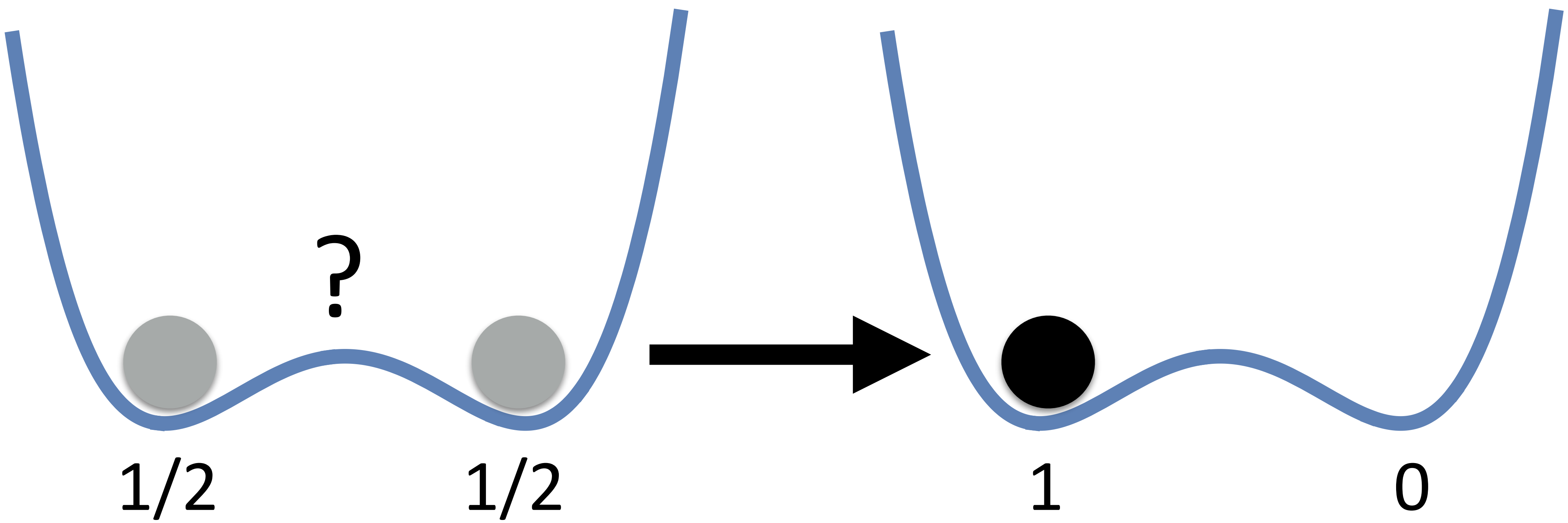

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But: Bennett's puzzle:

$$\left(\frac{1}{2}, \frac{1}{2}, 0, \ldots, 0\right) \longrightarrow \left(1-\epsilon, \frac{\epsilon}{N}, \frac{\epsilon}{N}, \ldots, \frac{\epsilon}{N}\right)$$

has $\Delta S > 0 \Rightarrow \Delta F < 0$ so this should be possible?!?

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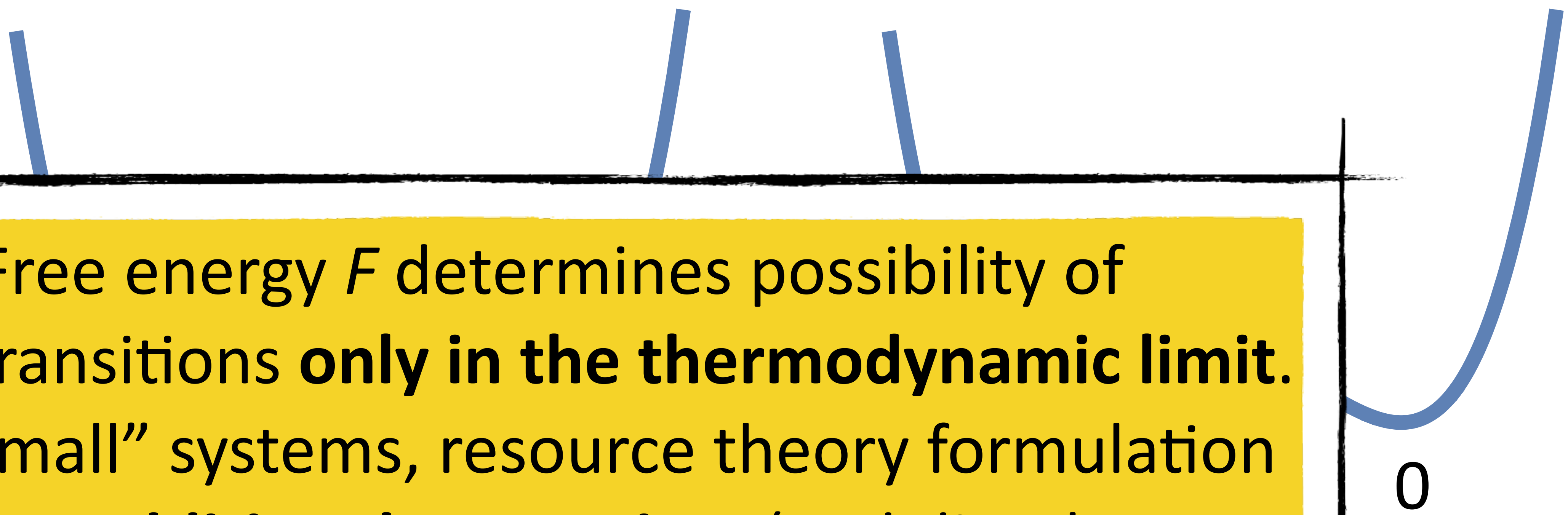

Impo

Free energy *F* determines possibility of state transitions **only in the thermodynamic limit**. For “small” systems, resource theory formulation gives **additional constraints** (and dissolves Bennett’s puzzle). More soon.

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Shannon / von Neumann entropy and data compression

Schumacher compression:

Given n copies of a quantum state $\rho,$ we would like to project into a smaller subspace (with projection $P^{(n)}$) such that

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where *S* is von Neumann entropy, $S(\rho) = -\mathrm{tr}(\rho \log \rho)$.

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Conventionally, F and S attain their operational meaning **only in the limit of very large ensembles**, due to version of the (statistical) law of large numbers.
But we would like to say more without this limit.

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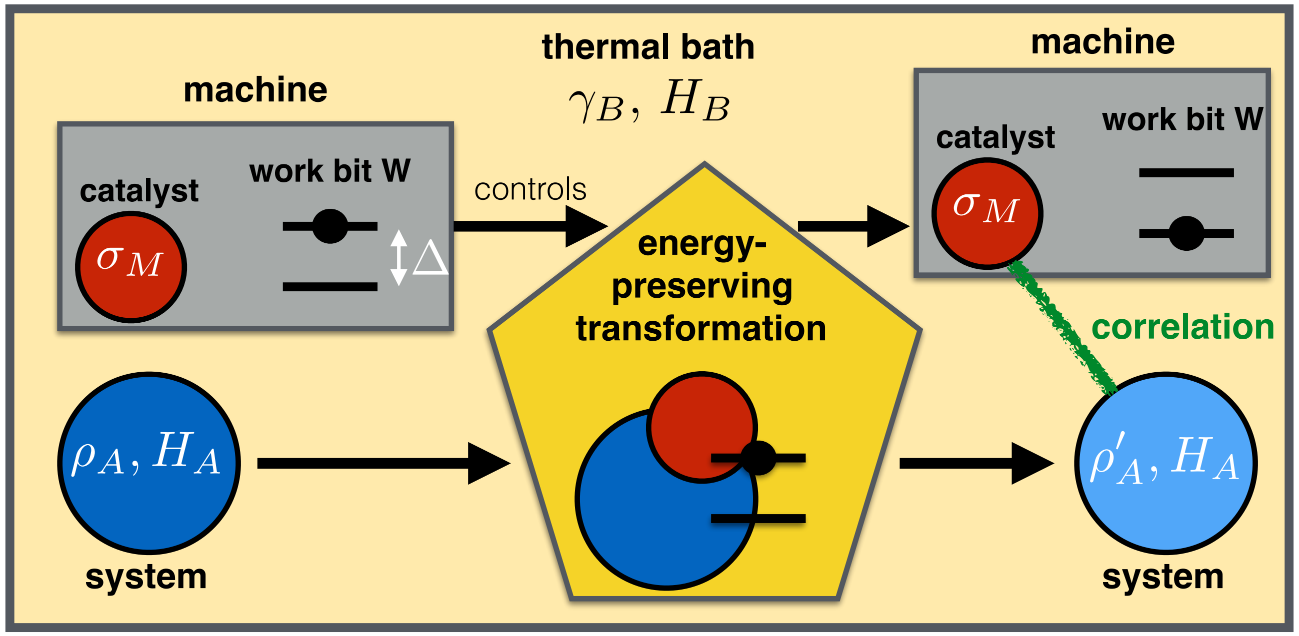

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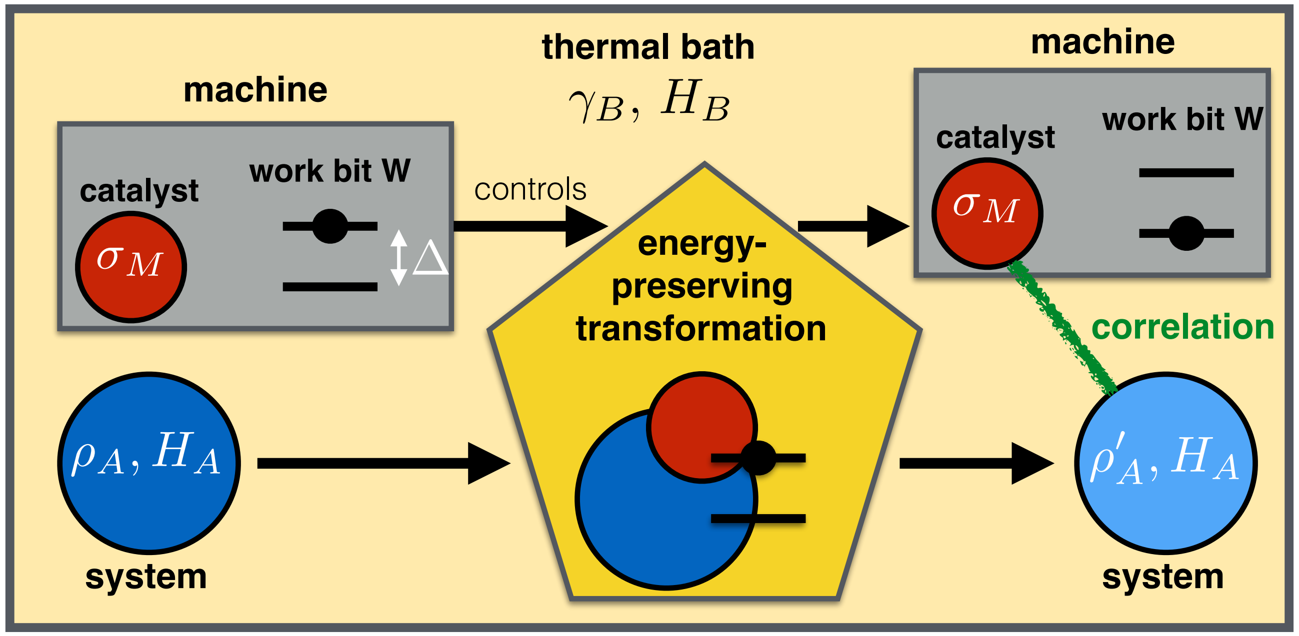

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Thermodynamics as a resource theory

The second laws of quantum thermodynamics

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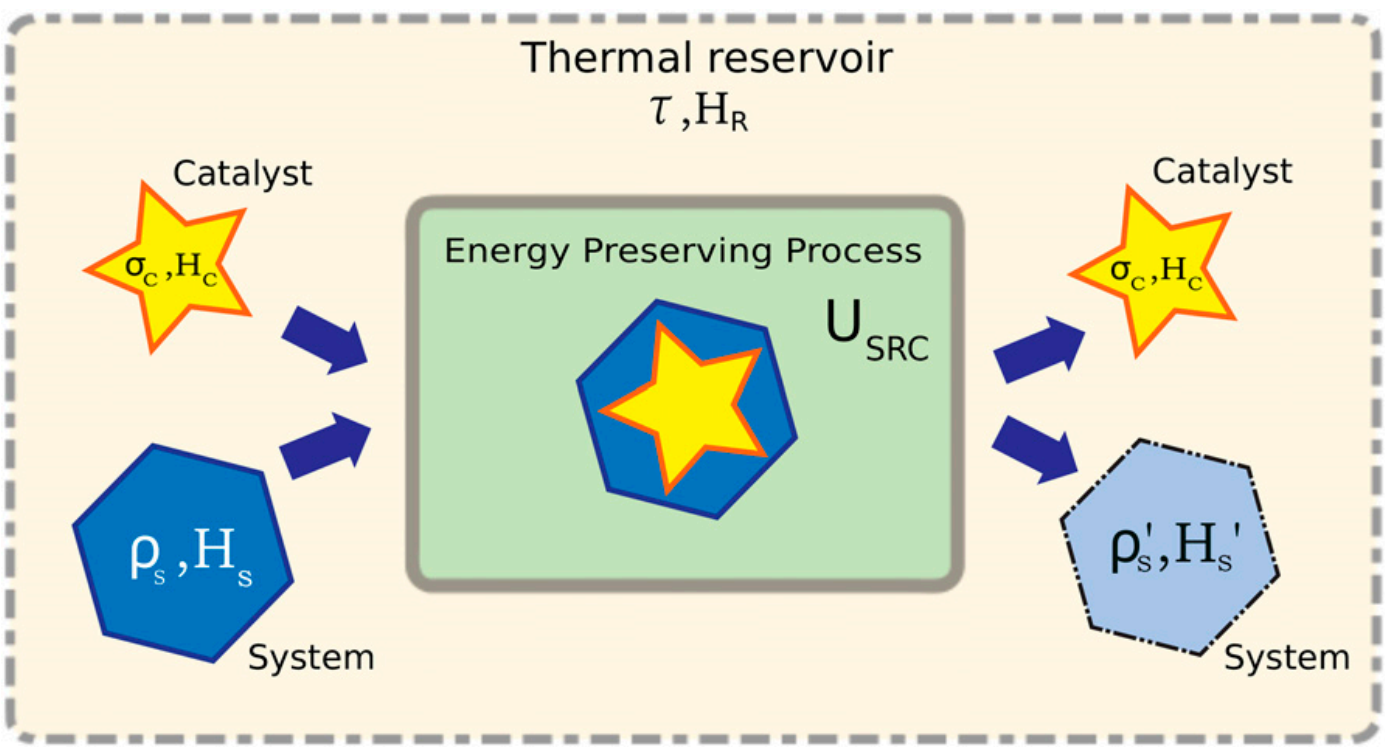

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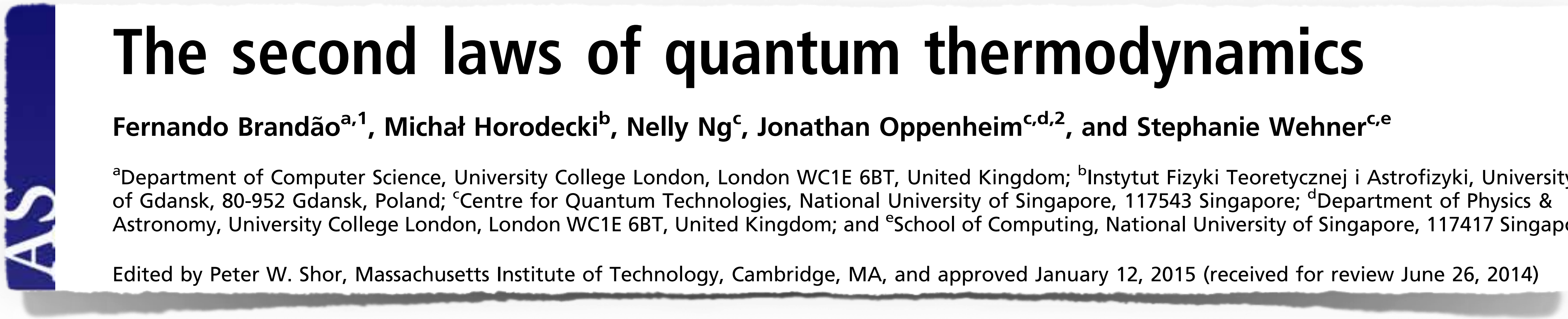

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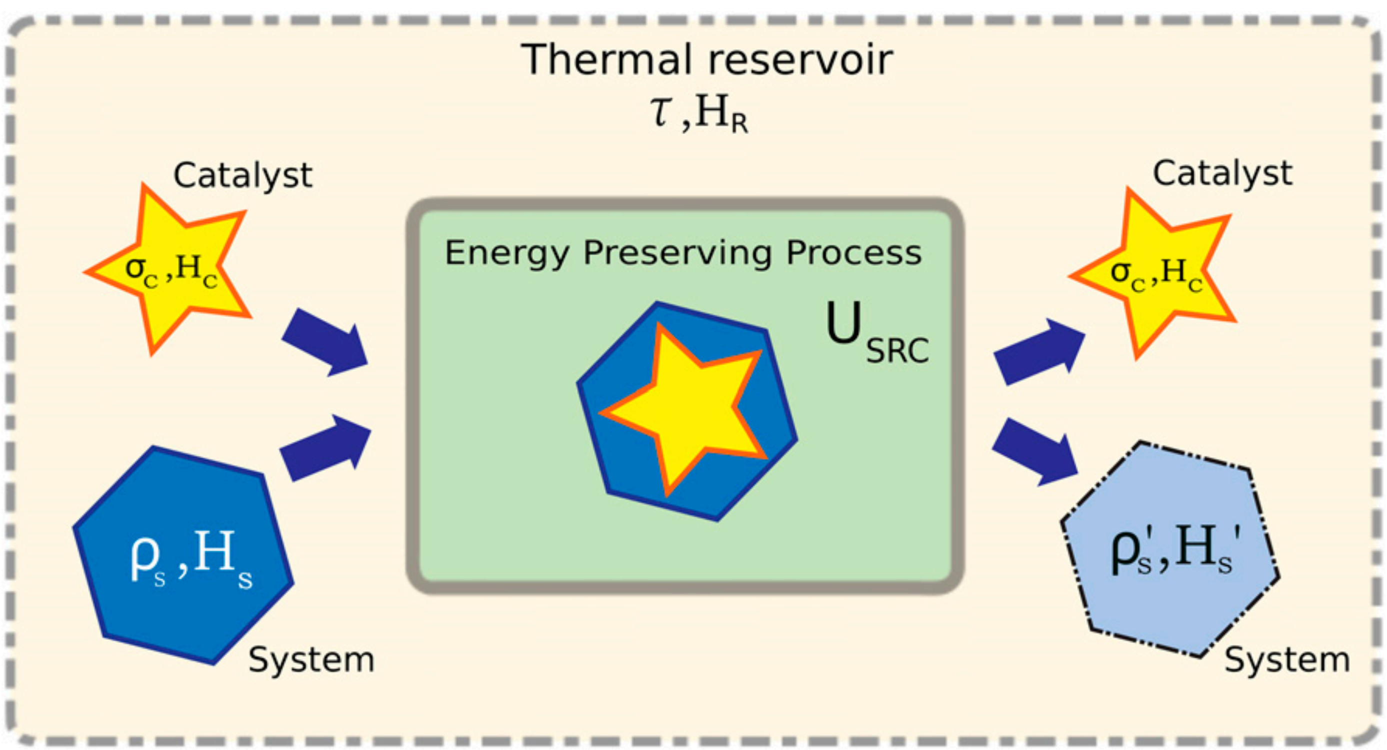

$$\mathrm{Tr}_R\left[U_{SRC}(\rho_S\otimes\sigma_C\otimes\gamma_R)U_{SRC}^\dagger\right]$$
$$=\rho_S'\otimes\sigma_C$$

thermal reservoir

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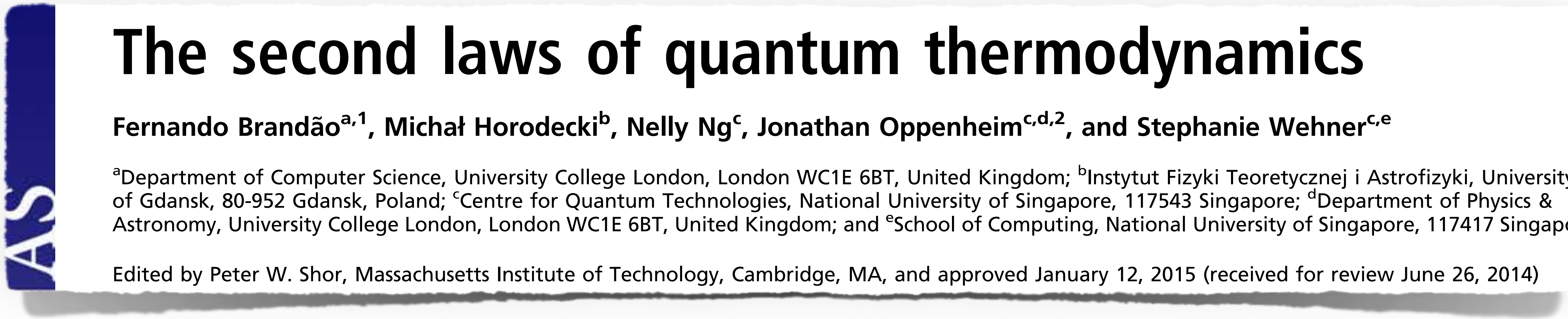

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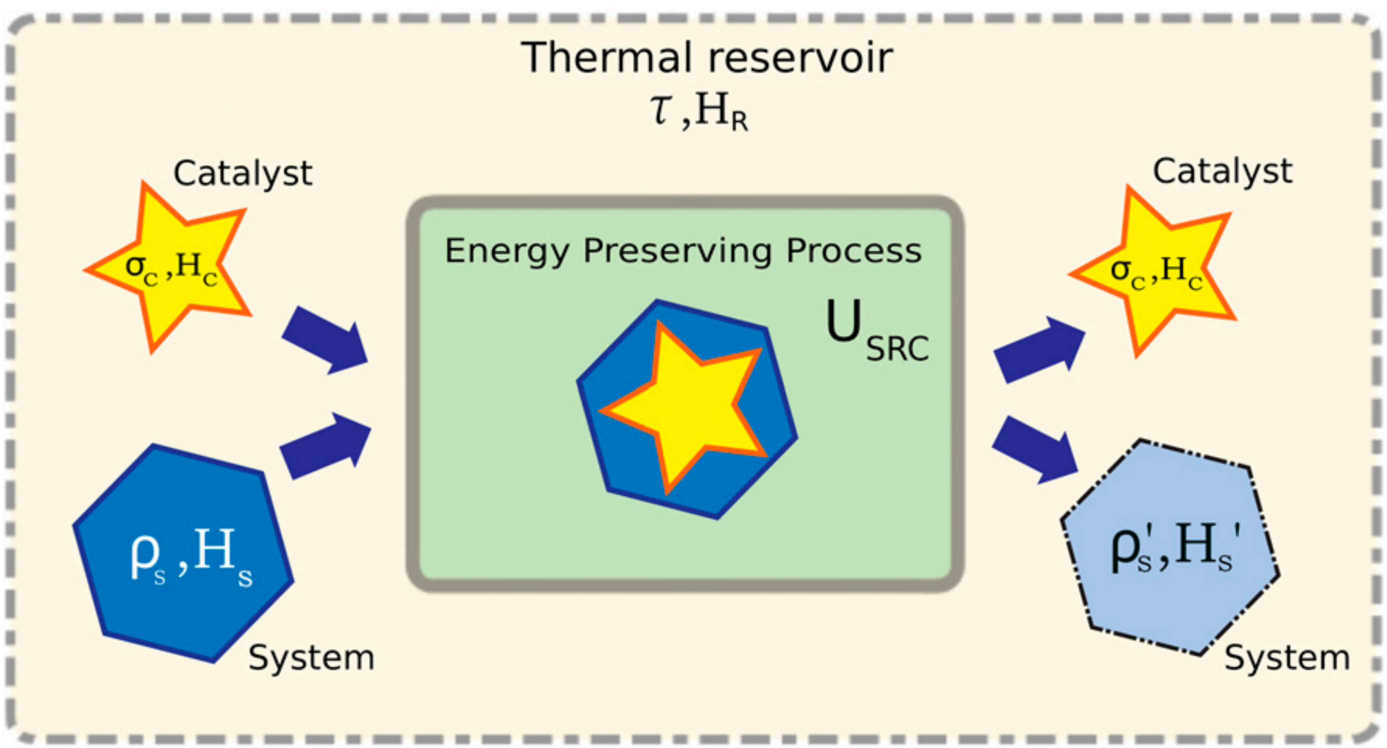

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$$=\rho'_S\otimes\sigma_C$$

thermal reservoir

$$[U_{SRC}, H_S+H_R+H_C]=0$$

(energy strictly preserved).

Thermodynamics as a "game" played by an agent against nature:

Thermodynamics as a resource theory

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- It is "free" to bring in any system *B* in its thermal state $\gamma_B = \exp(-H_B/(k_B T))$,
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they subsume the agent's knowledge or beliefs about the system.
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But other interpretations are possible, too.

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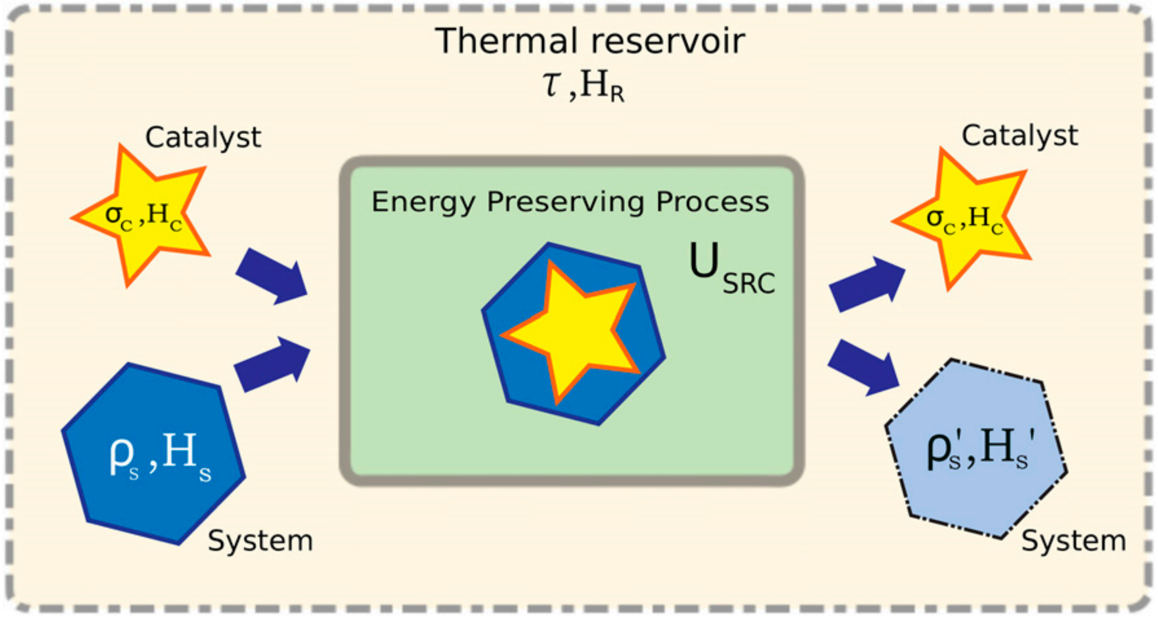

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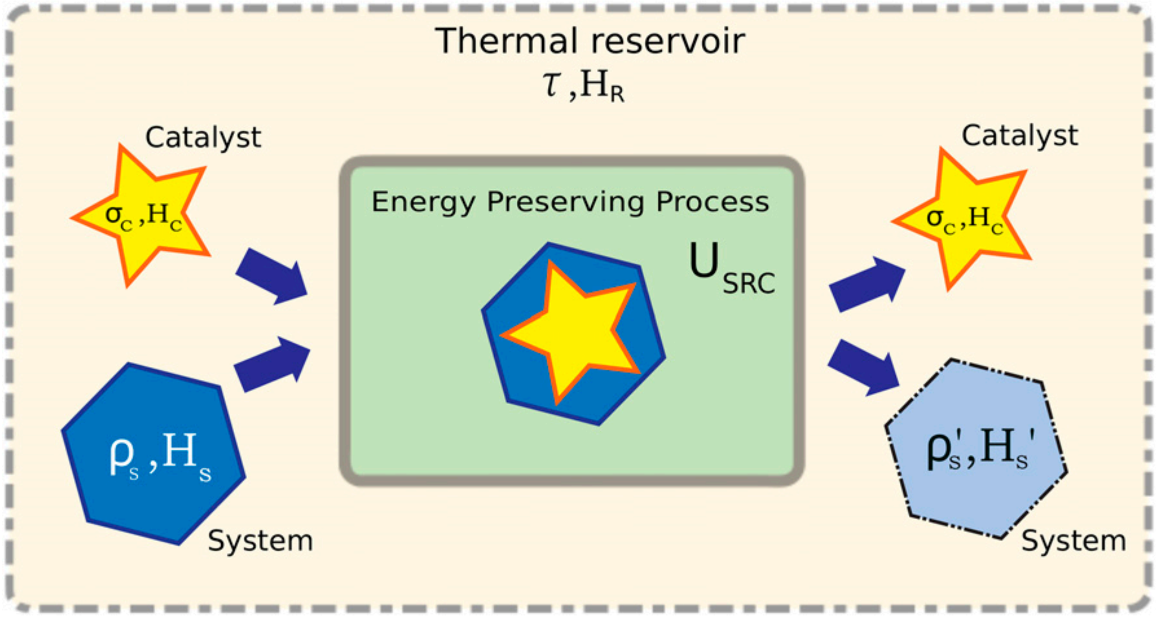

Theorem: For ("classical") states that are blockdiagonal in energy, $\rho \to \rho'$ is possible if and only if

$$F_\alpha(\rho) \geq F_\alpha(\rho') \text{ for all } \alpha$$

("Rényi-α-free energies").

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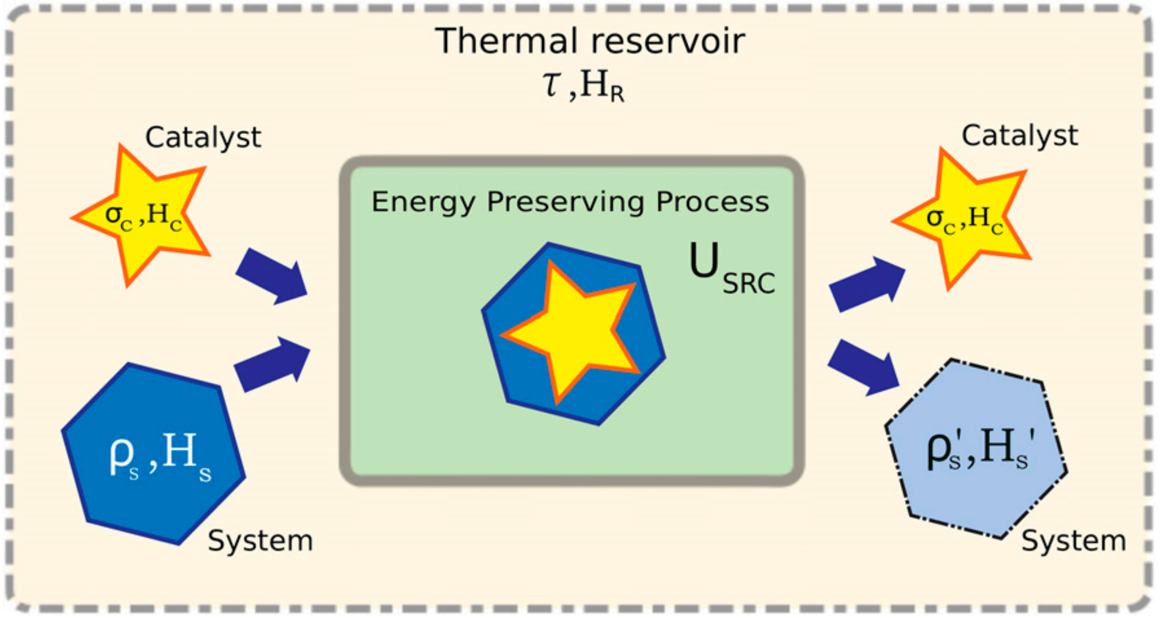

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$$F(\rho_A) \equiv F_1(\rho) = \mathrm{tr}(\rho_A H_A) - k_B T S(\rho_A),$$

$$F_\alpha(\rho) = k_B T S_\alpha(\rho \| \gamma) + F_\alpha(\gamma).$$

Rényi divergence

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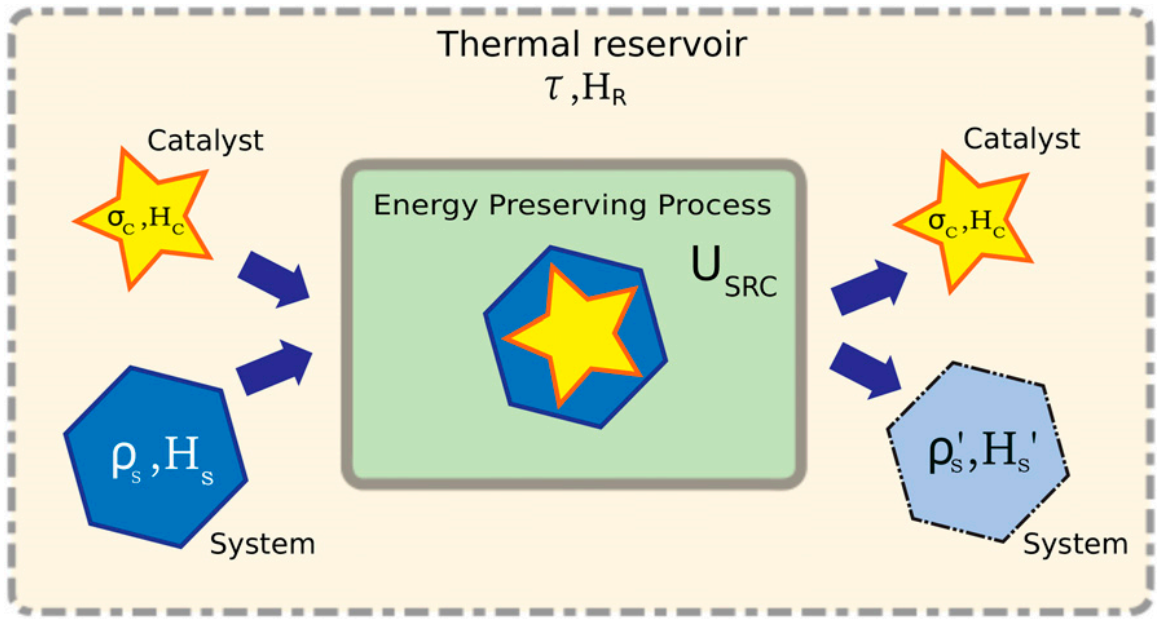

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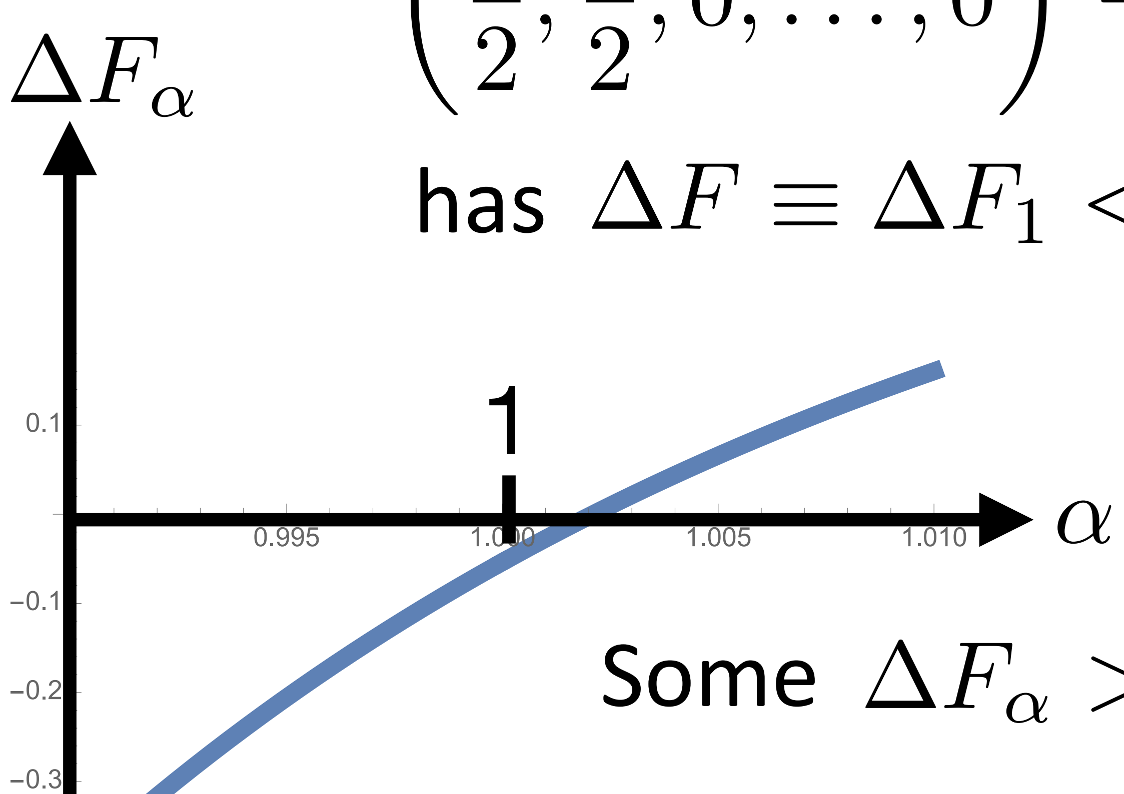
has $\Delta F \equiv \Delta F_1 < 0$ so why is this not possible?

$$\epsilon = \frac{1}{100}, \quad N = 10^{30}.$$



Some $\Delta F_\alpha > 0$, hence it **must be impossible.**

Extractable work / work cost

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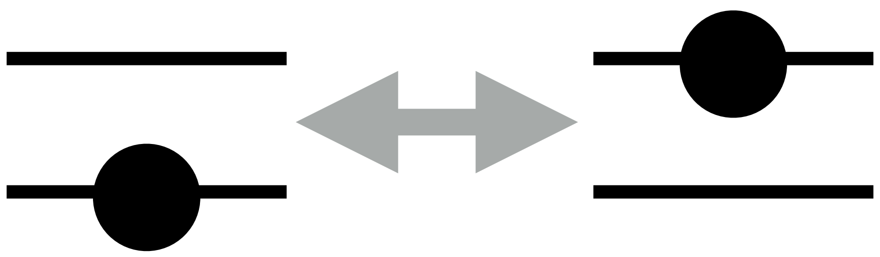
- work cost: $F_\infty^\varepsilon(\rho) - F(\gamma)$



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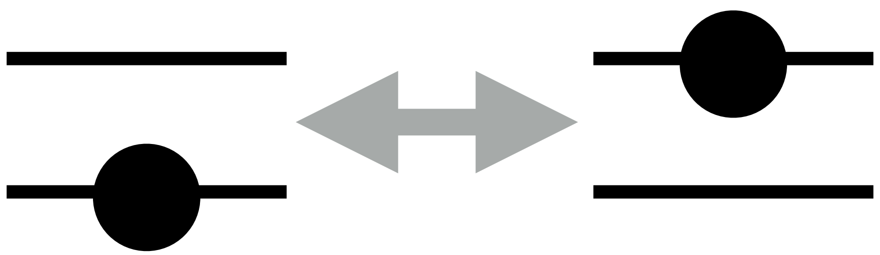

$F_0 \ll F \ll F_\infty$. Fundamental irreversibility.

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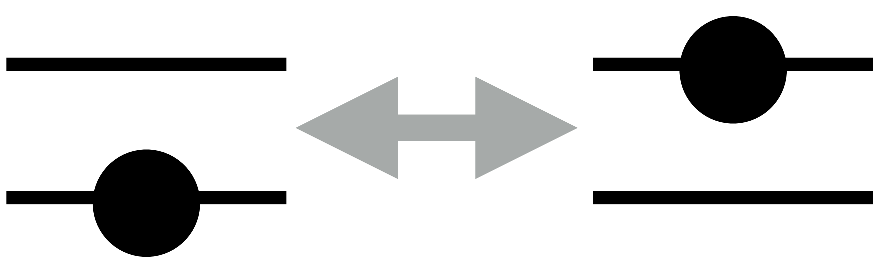

$F_0 \ll F \ll F_\infty$. Fundamental irreversibility.

$$\lim_{n\to\infty} \frac{1}{n} F_{0/\infty}^\varepsilon(\rho^{\otimes n}) = F(\rho) \equiv \mathrm{tr}(\rho H) - k_B T\, S(\rho).$$

(Only) in the thermodynamic limit, (the rates of) extractable work and work cost become equal. **Emergent reversibility.**

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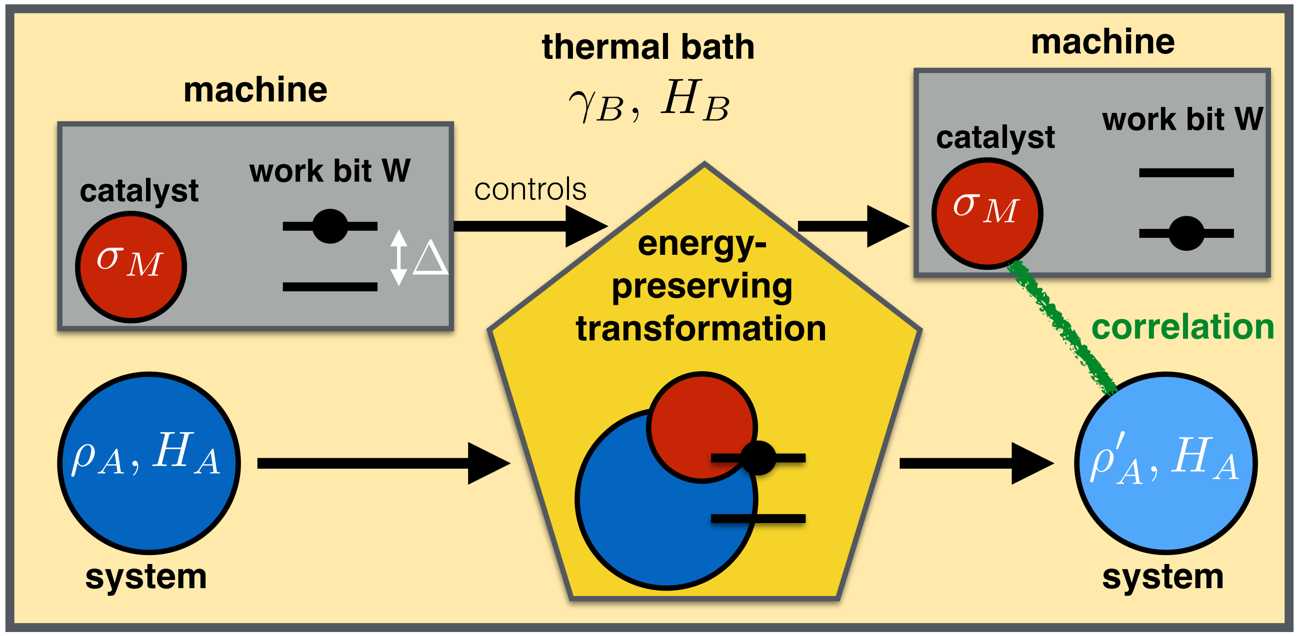

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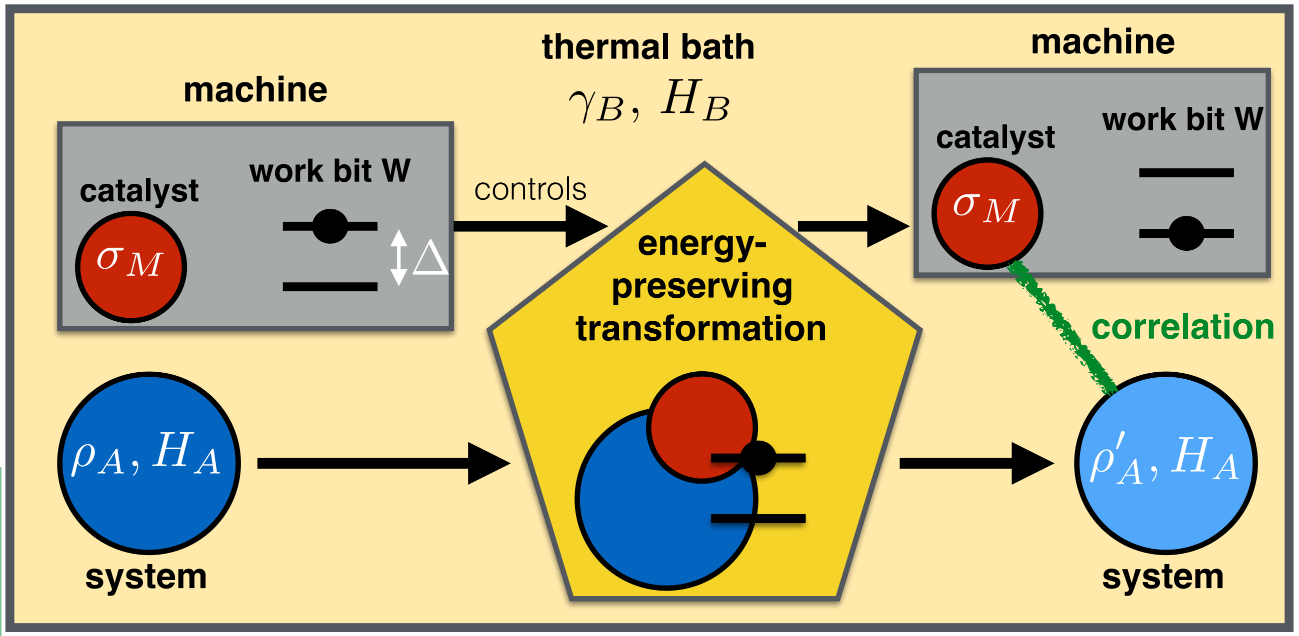

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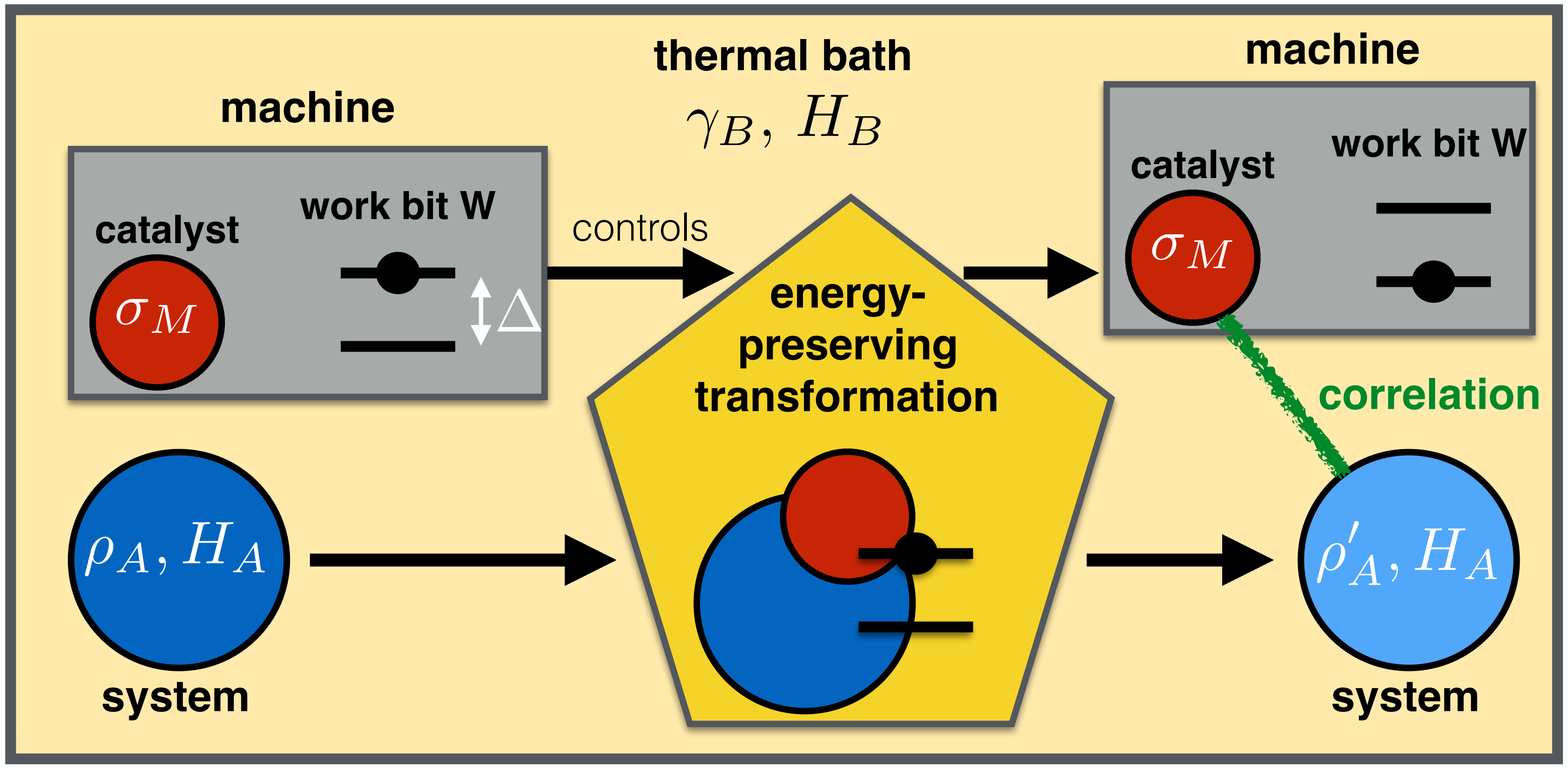

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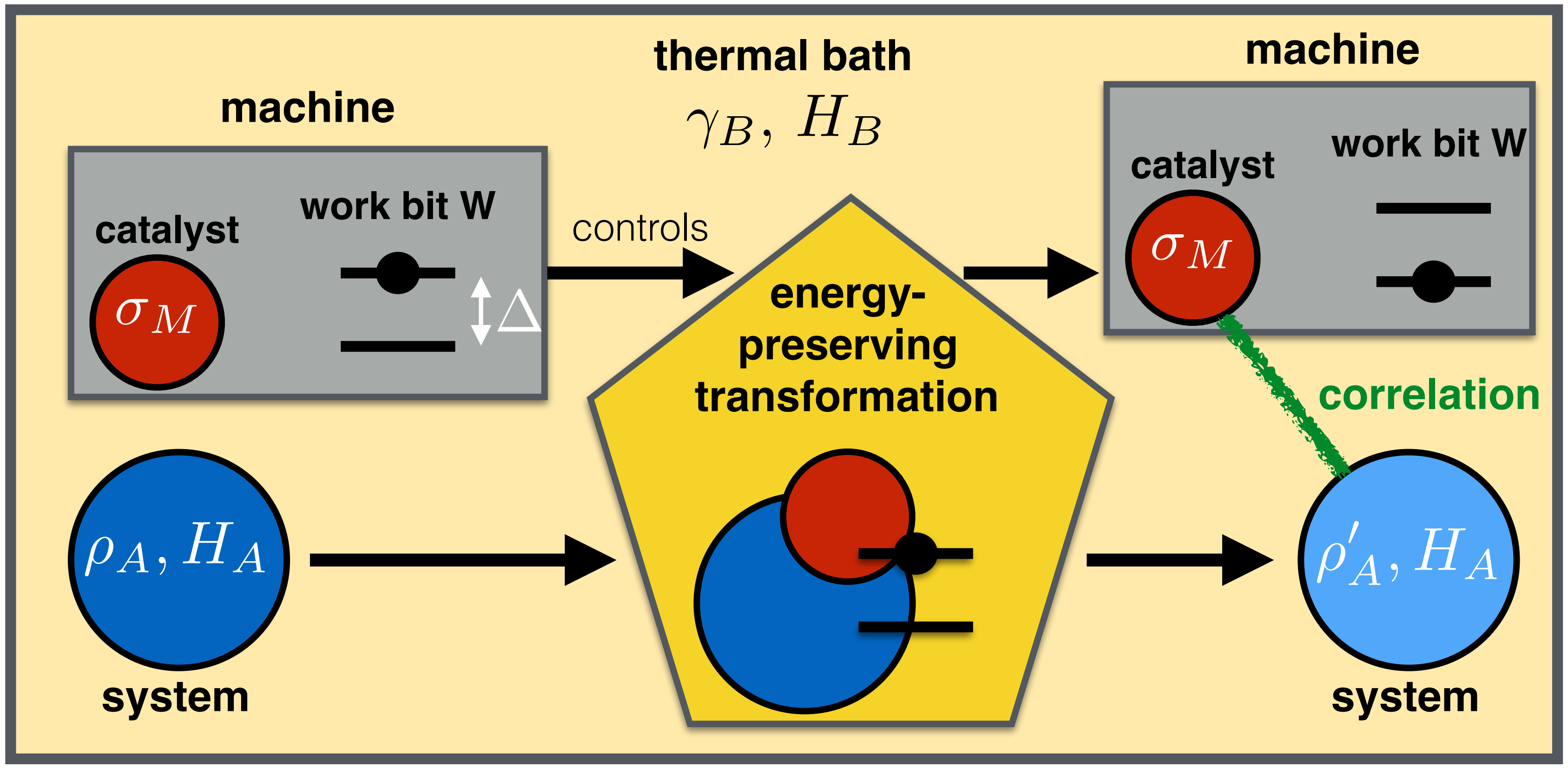

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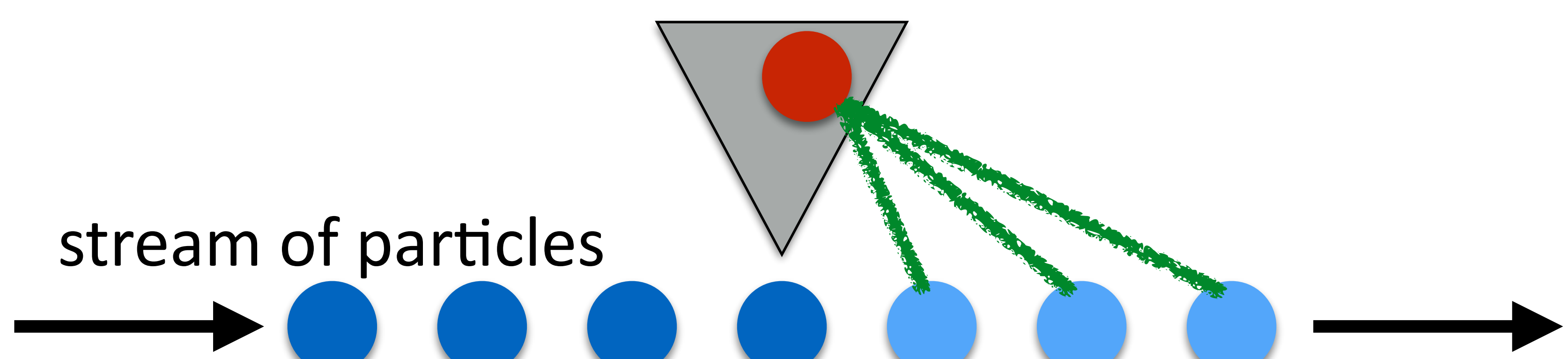
Okay for situations like these:

thermal machine,
acting on one system at a time,
not encountering systems again



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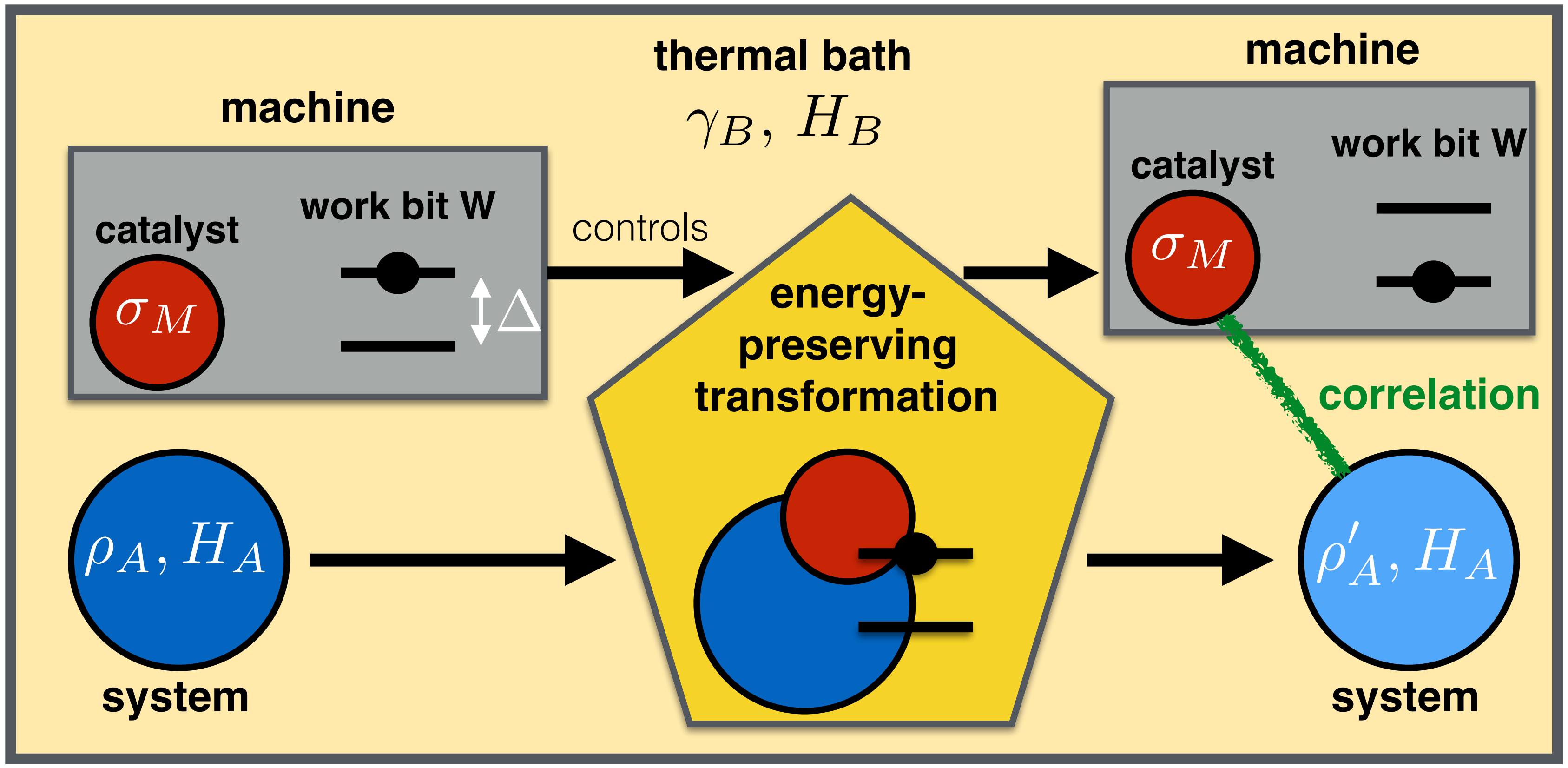
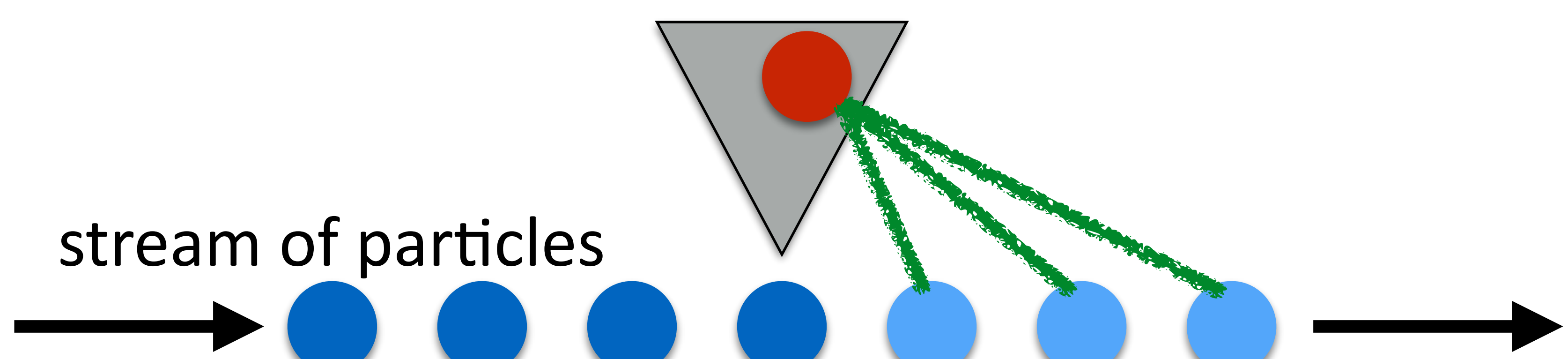


Preserve catalyst exactly, but allow **correlations** to build up.

Okay for situations like these:

thermal machine,
acting on one system at a time,
not encountering systems again



Can this help?
Yes!

Creating correlations can help: **example**

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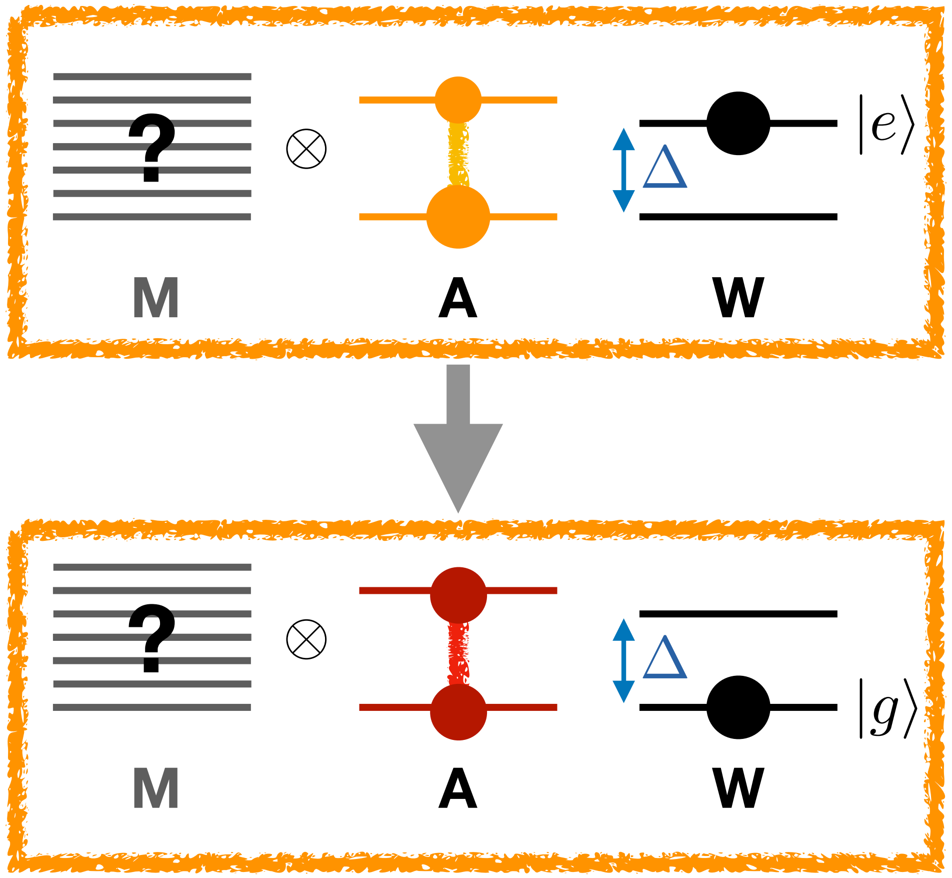

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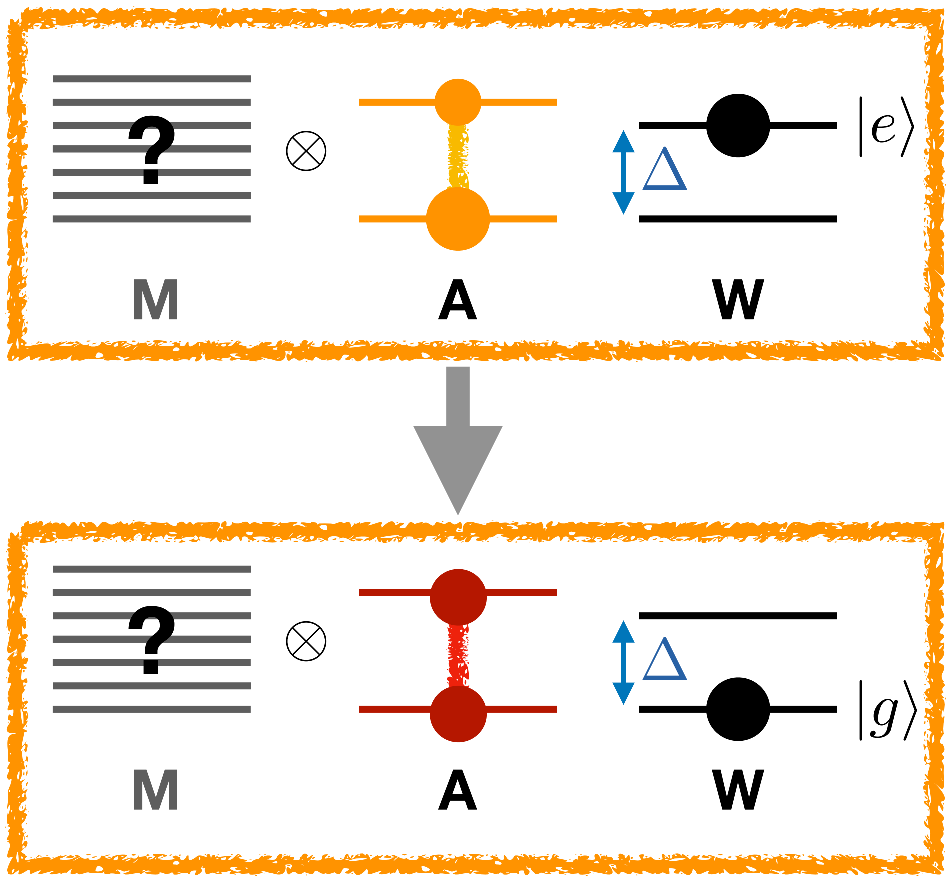

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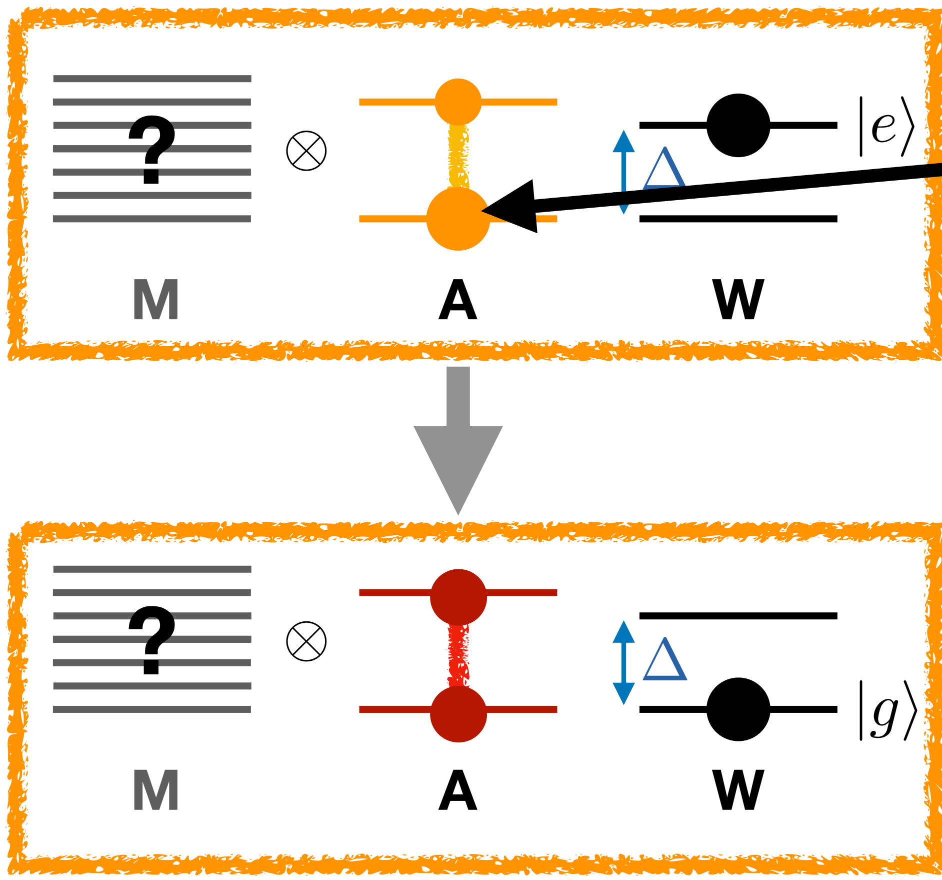

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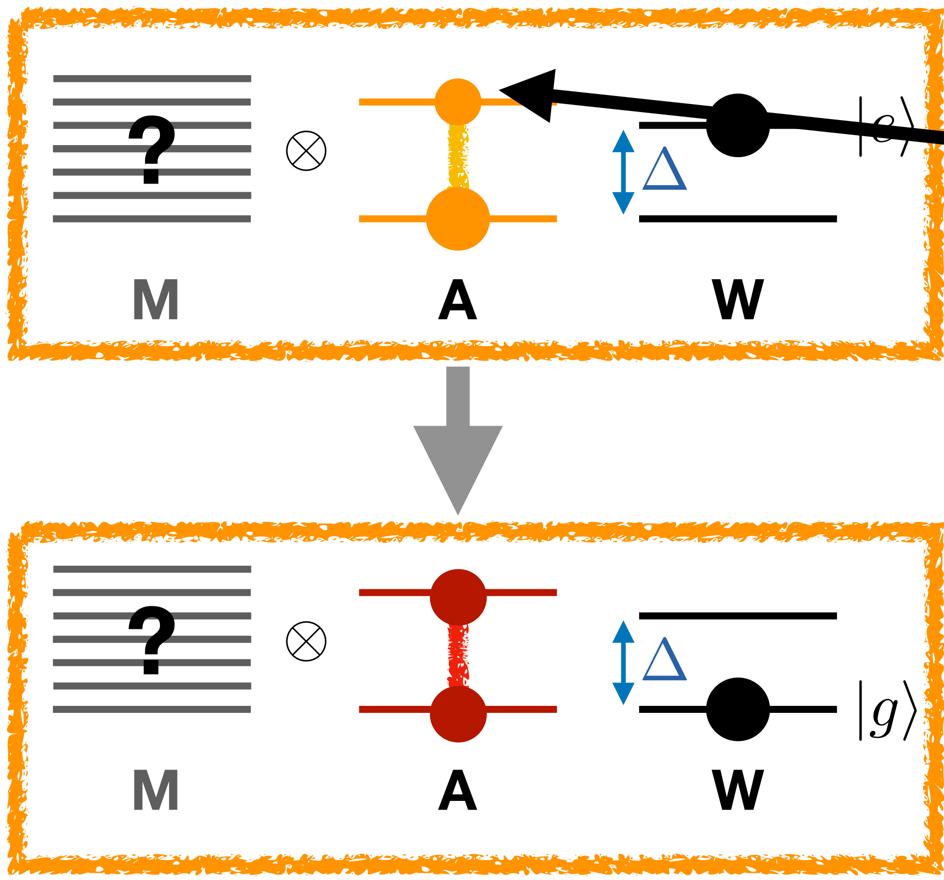

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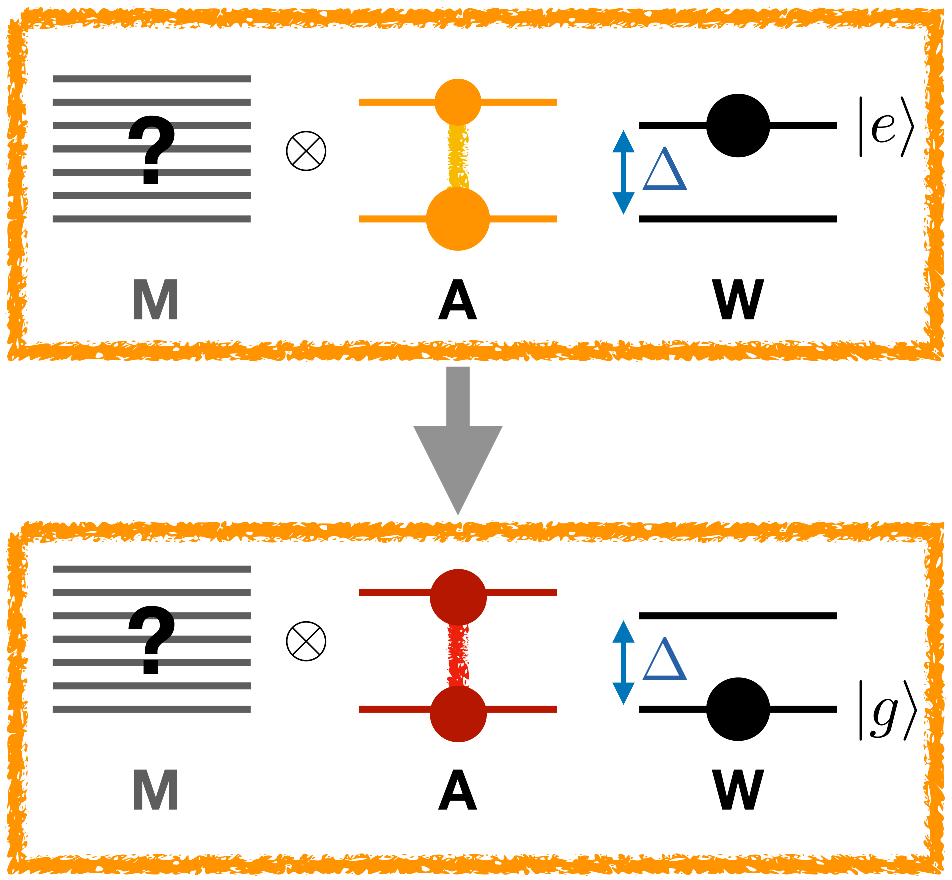

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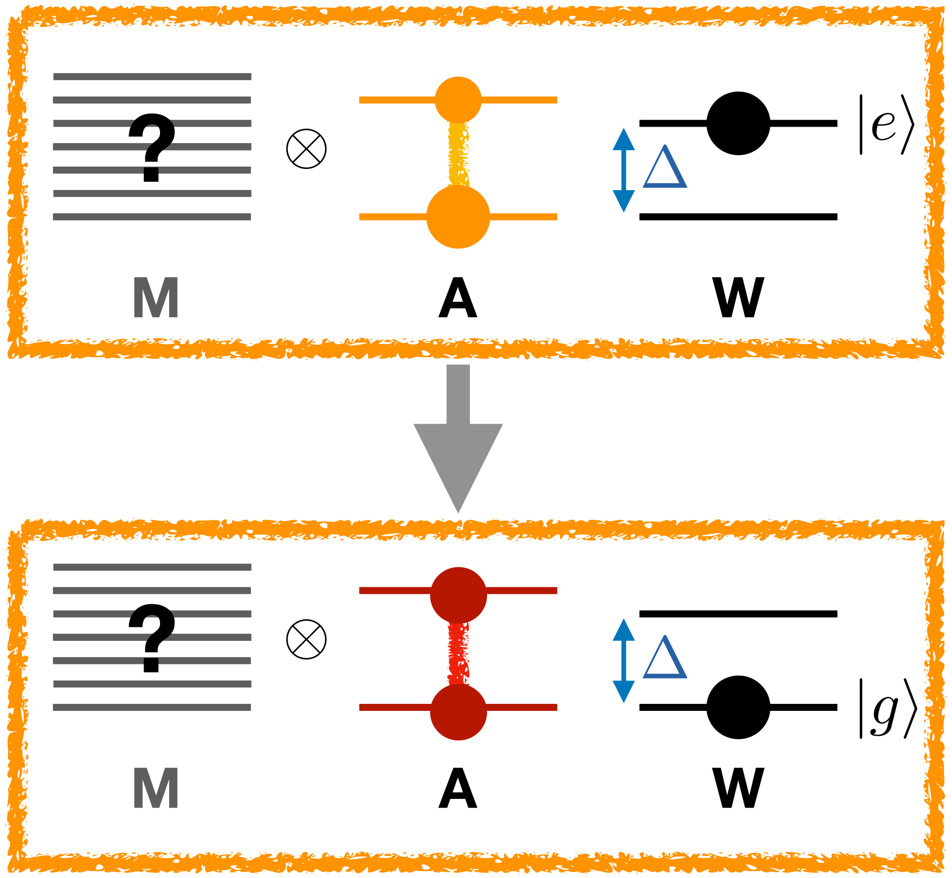

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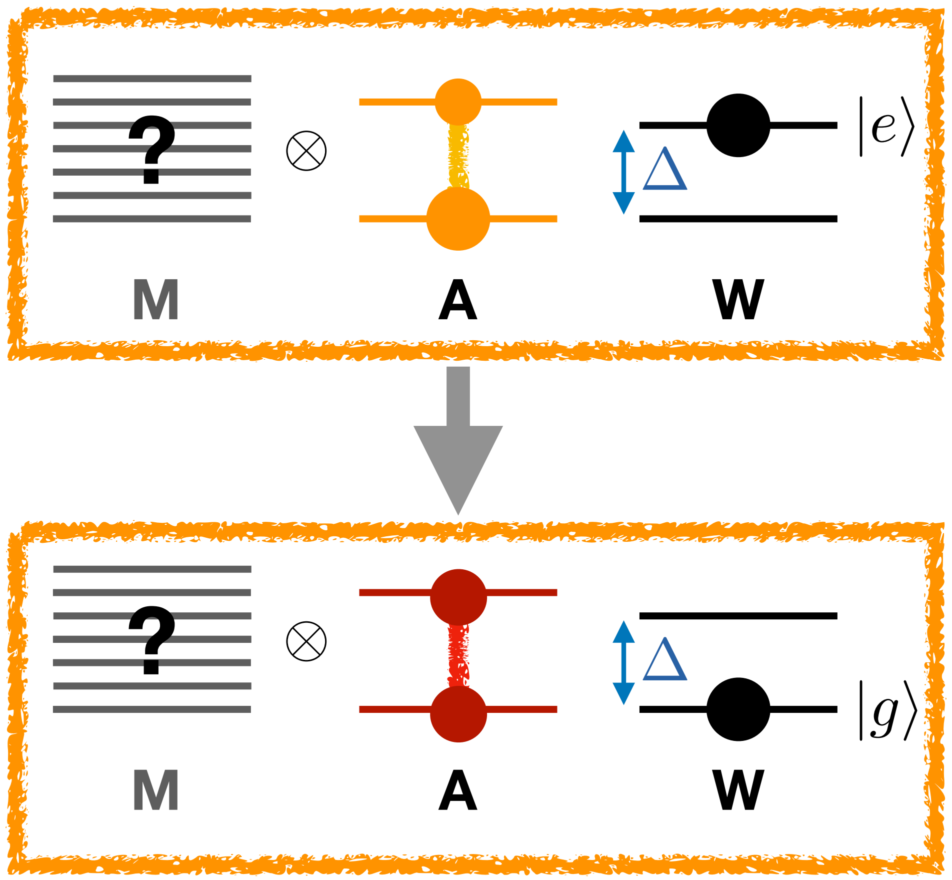

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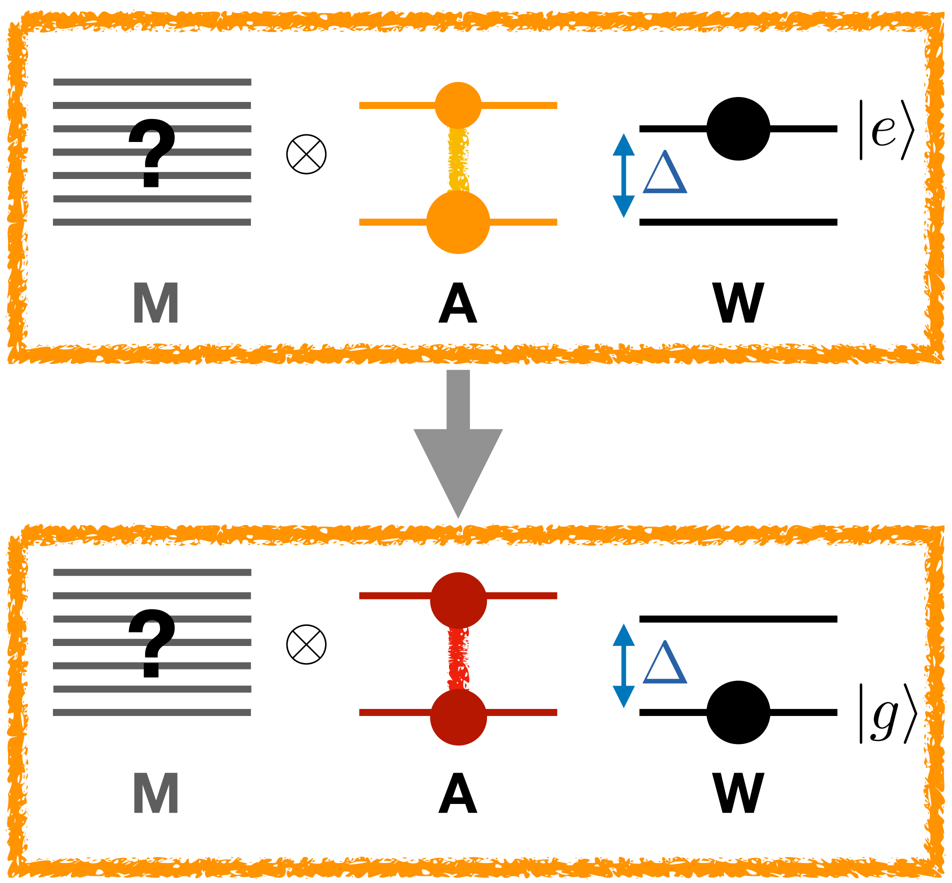

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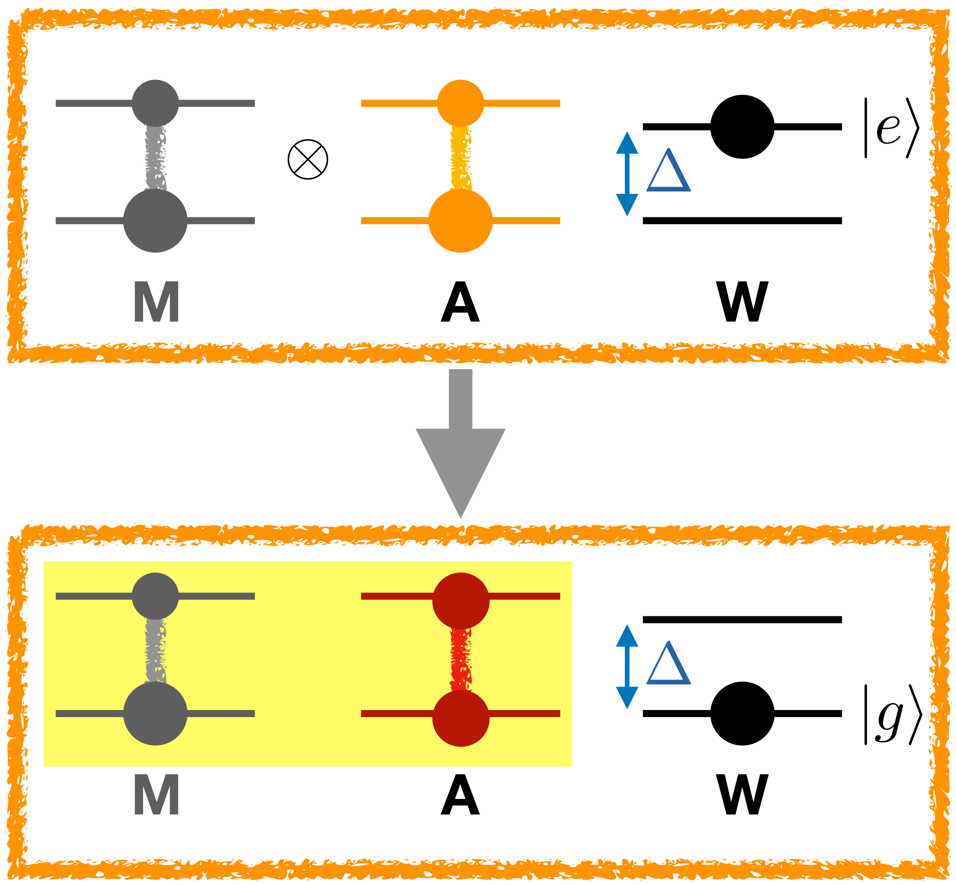

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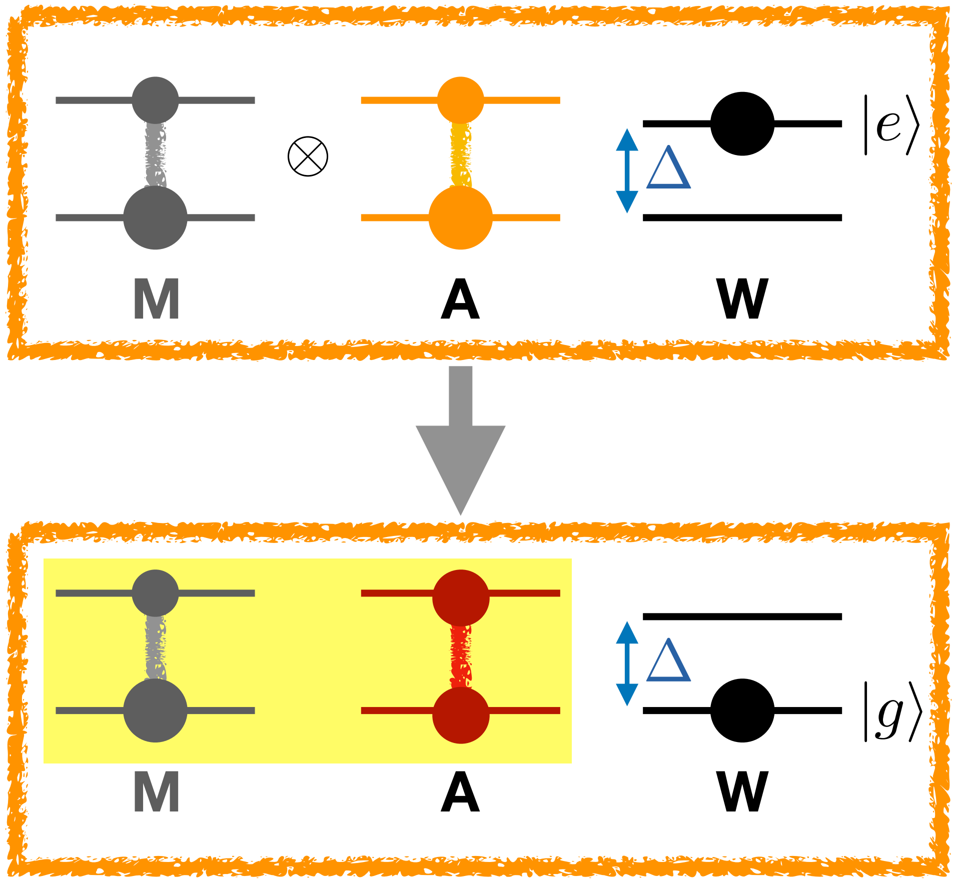

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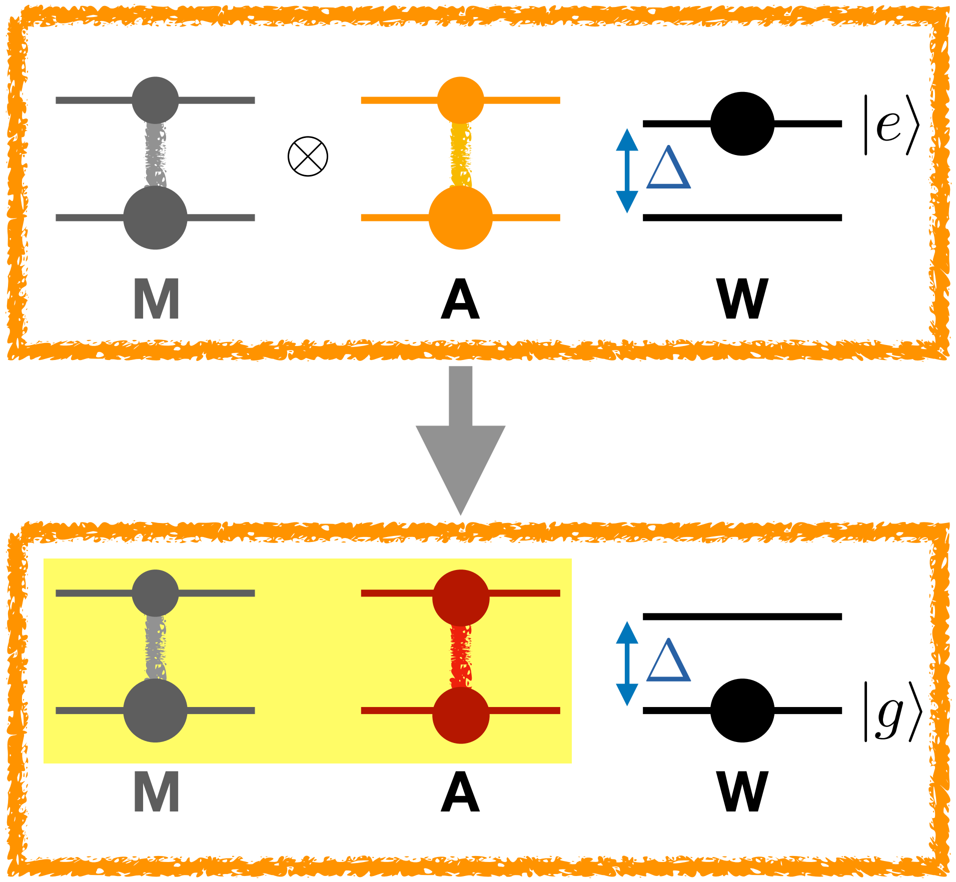

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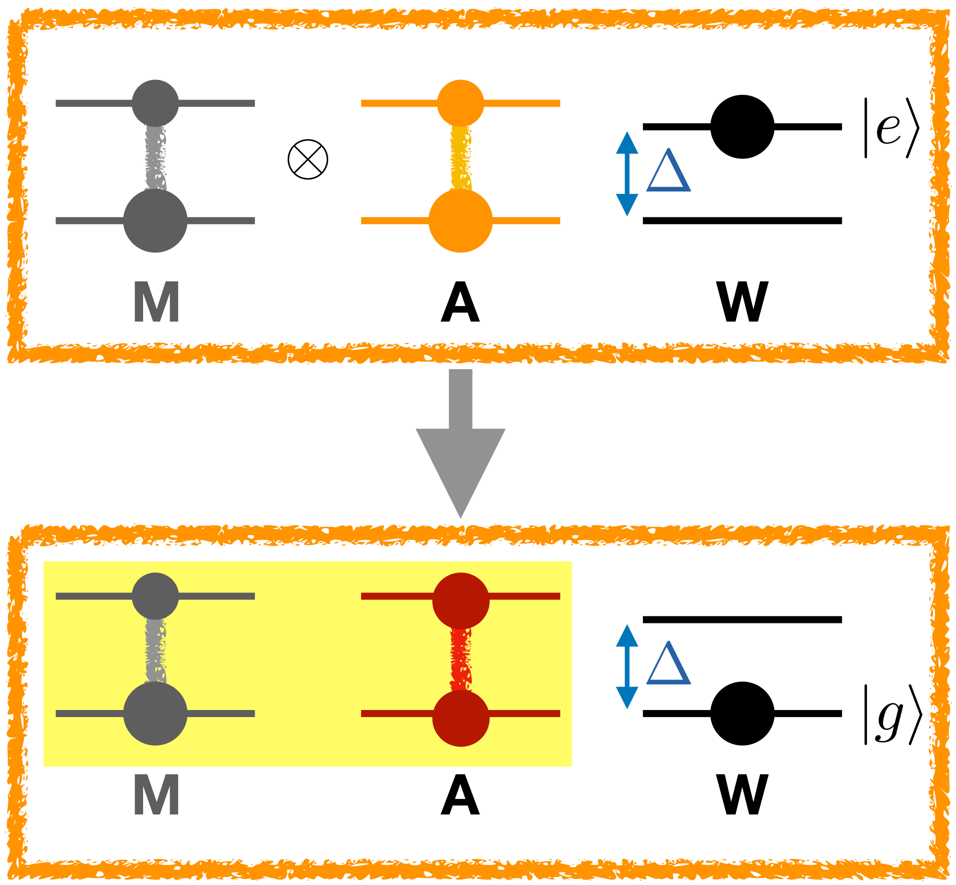

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Turns out: there is a thermal operation that achieves this transition,
and it only needs $\Delta \geq .26 k_B T$ (before it was $.4 k_B T$).

$\gamma_A \otimes \sigma_M$

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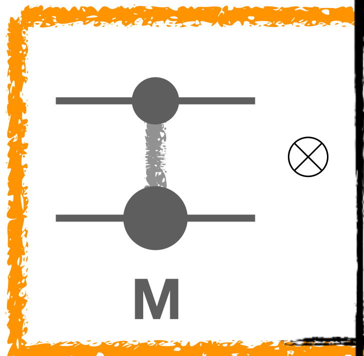
MM, ... e, PRX **8** (2018).

Two-l... 2.

Goal: ... ature.



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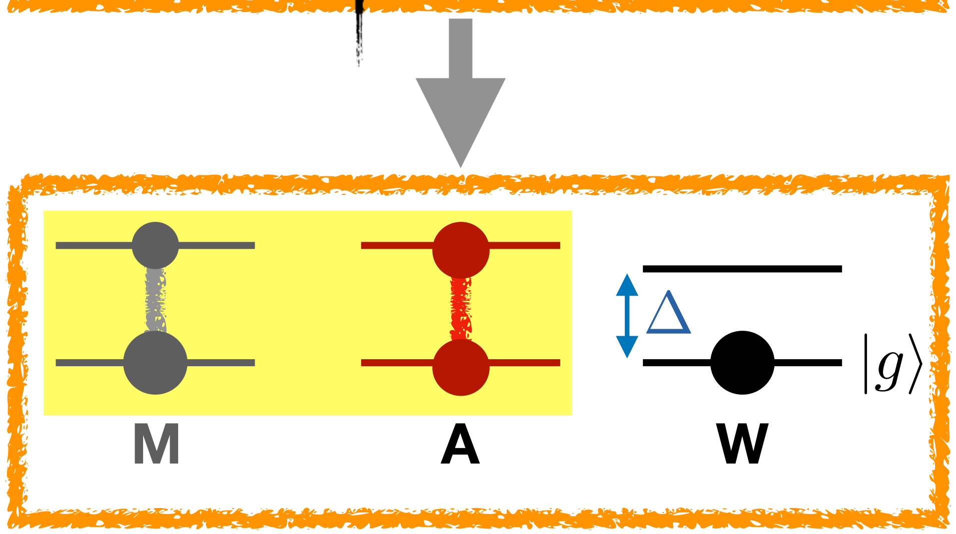

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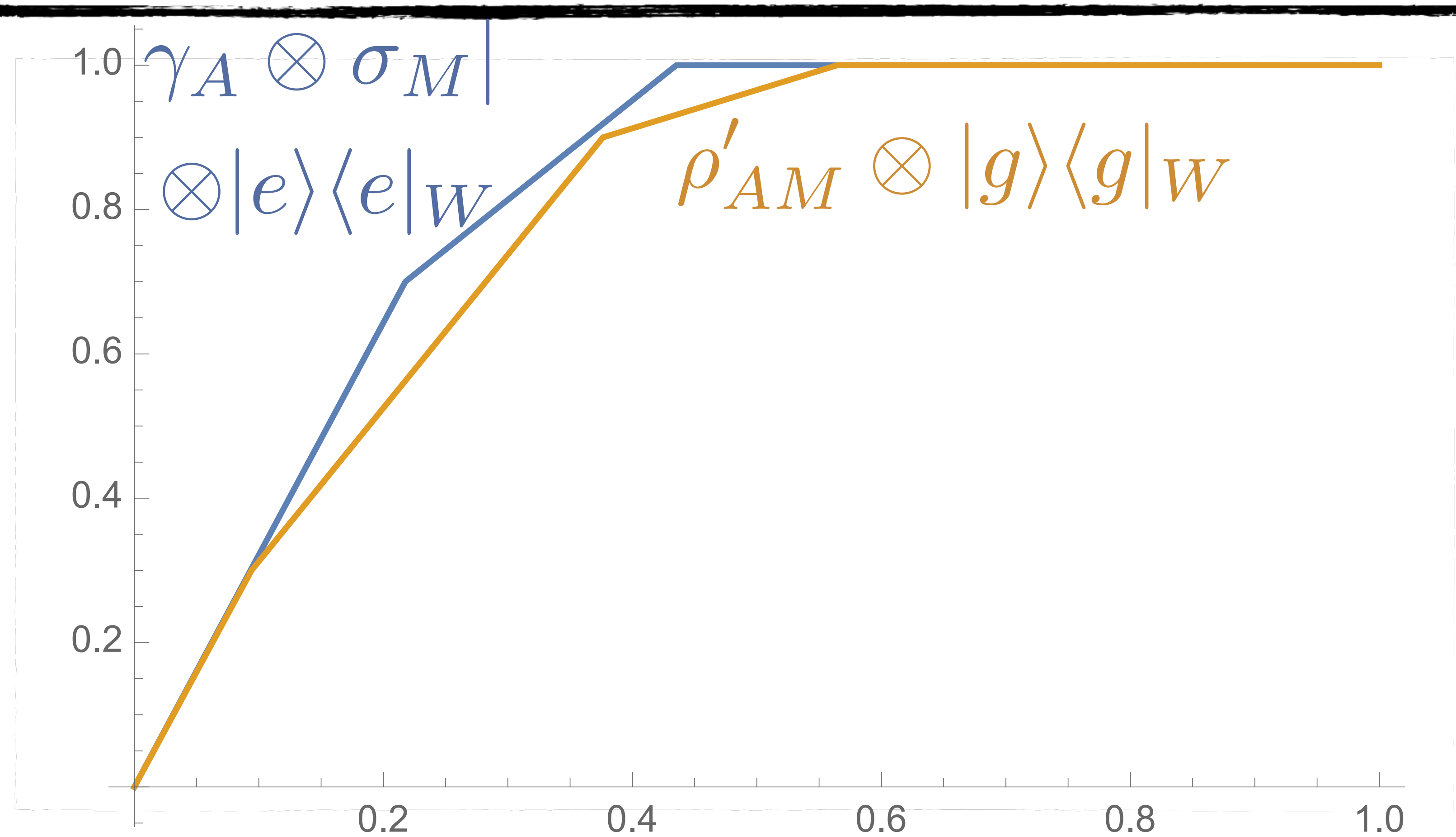

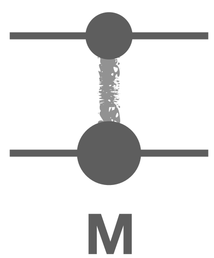

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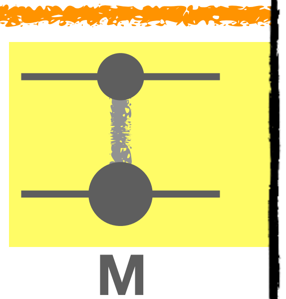

Q: Given arbitrary (larger) catalysts *M*, how far can we go?

A: Down to $\Delta F = .06 k_B T$, but not further!

M

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Main theorem

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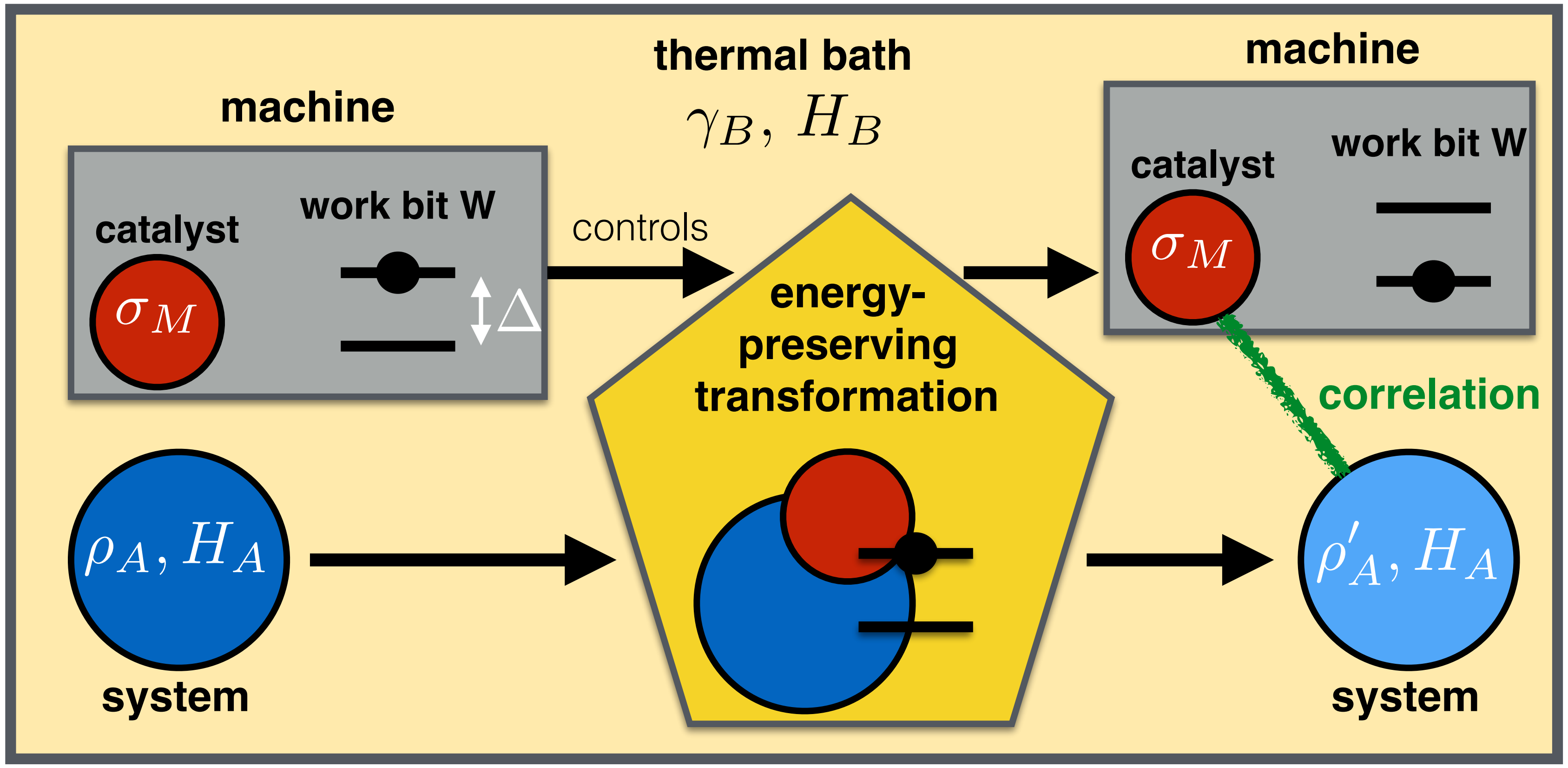

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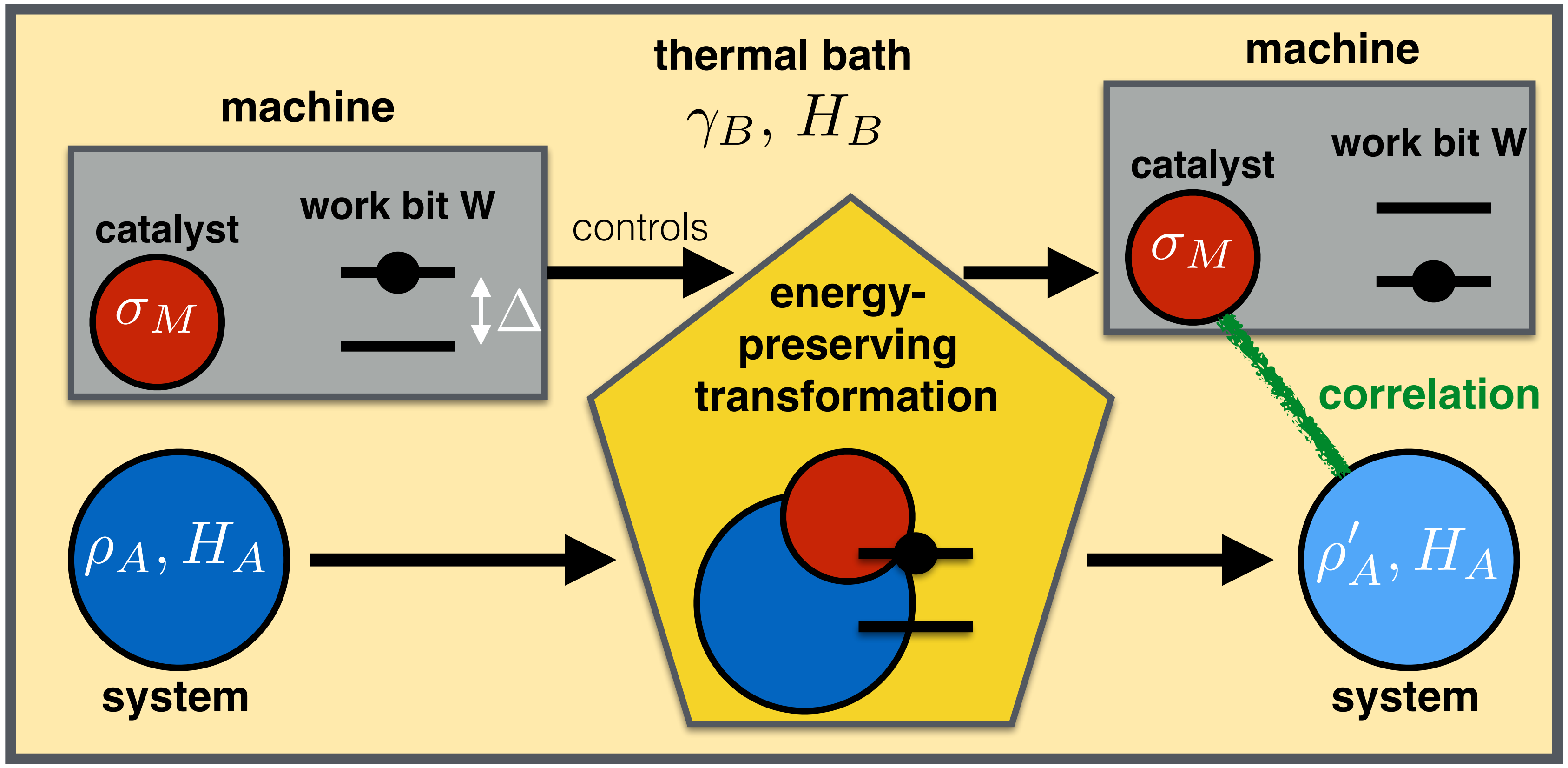

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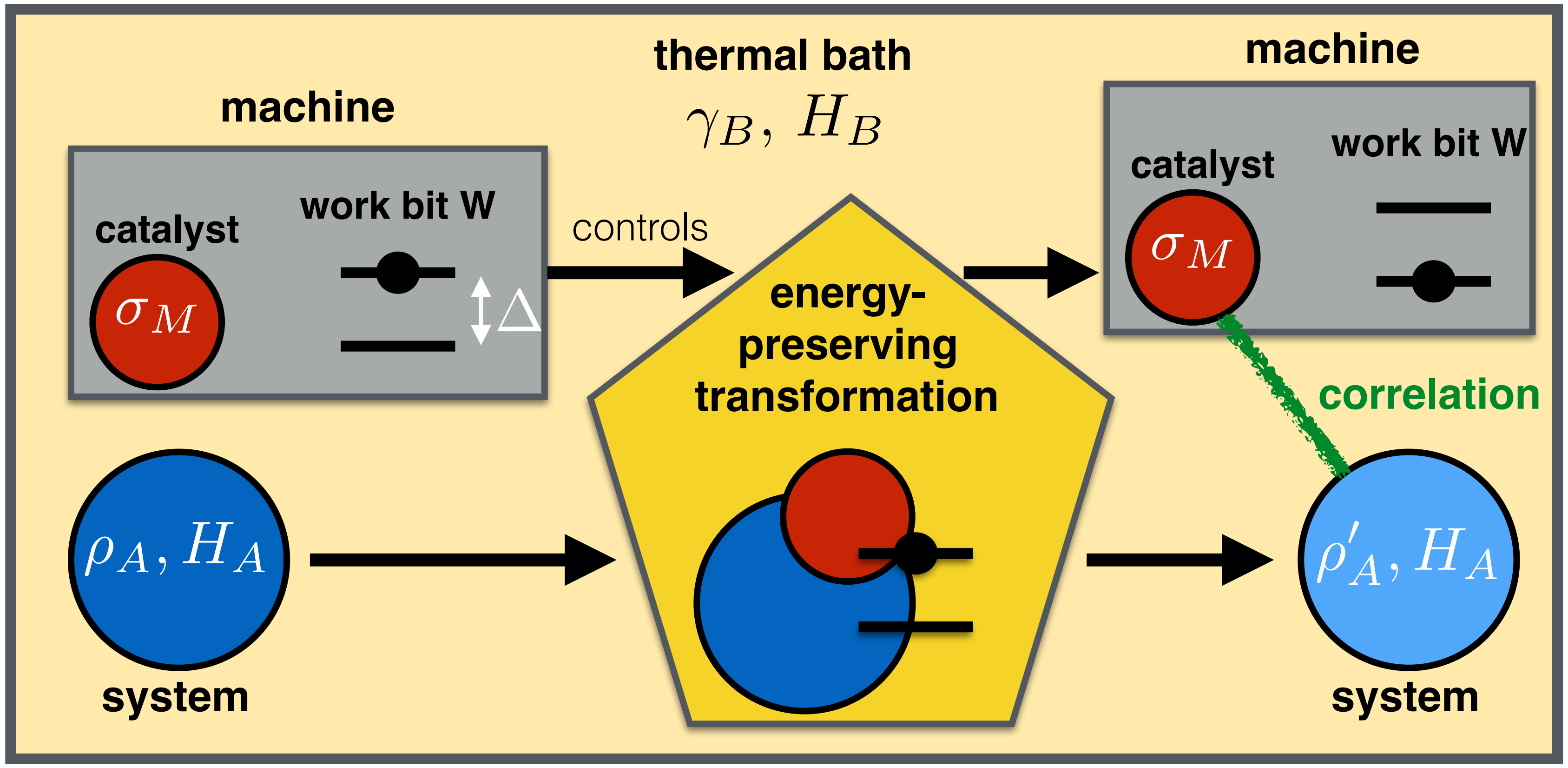

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With work bit W: The **work cost** is exactly $\Delta F = F(\rho') - F(\rho)$, resp. we can extract work arbitrarily close to $|\Delta F|$.

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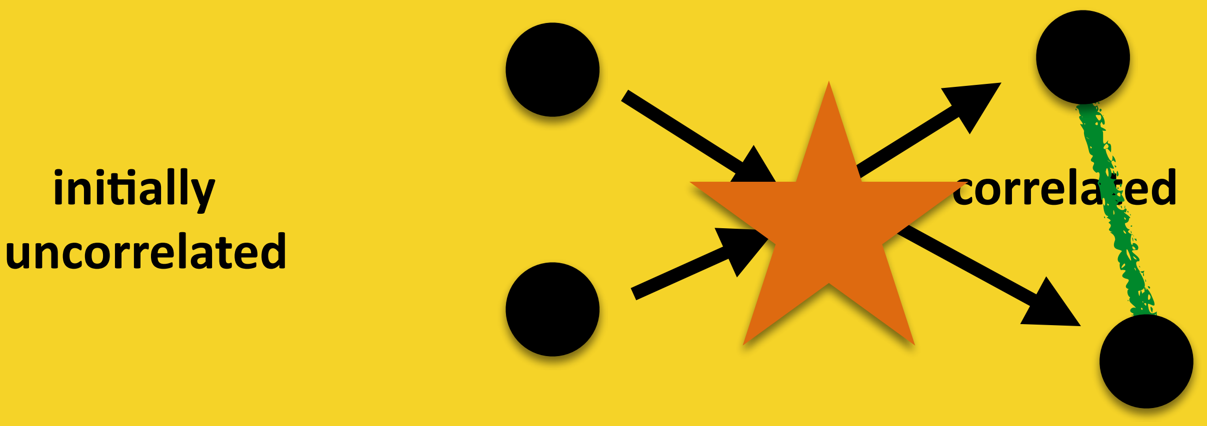
Somewhat reminiscent of the assumptions in Boltzmann's **Stoßzahlansatz** (1896):



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Exact characterization of the Helmholtz free energy *F* without thermodynamic limit or averaging.

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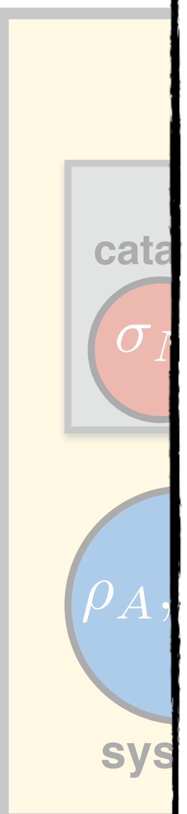

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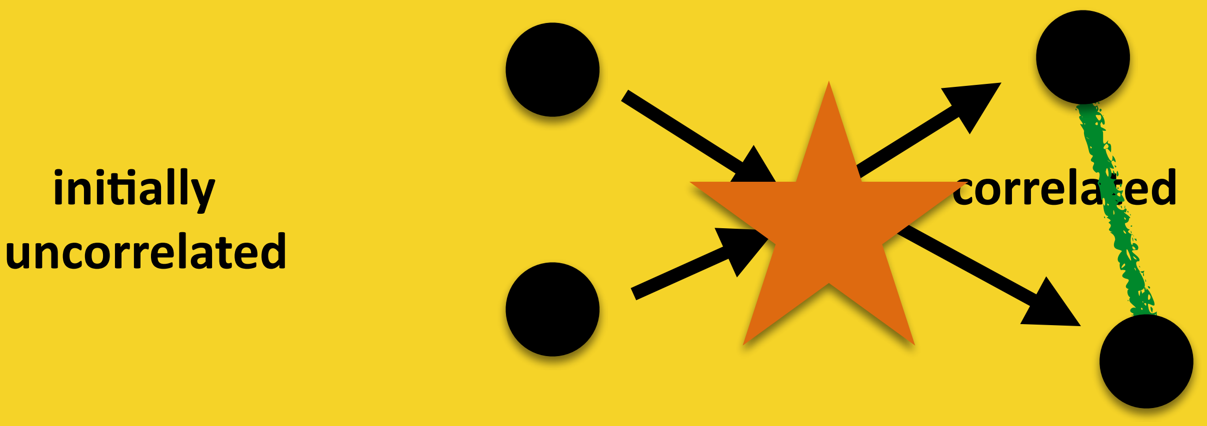

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Question: what happens in the case of **coherence** between the energy levels?

Exact … without thermodynamic limit or averaging.

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MM, *Correlating thermal machines and the second law at the nanoscale*, PRX **8** (2018).

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Main Theorem. Let $p, p' \in \mathbb{R}^m$ be probability distributions with $p^\downarrow \neq p'^\downarrow$. Then there exists an extension p'_{XY} of $p' \equiv p'_X$ such that

$$p_X \otimes p'_Y \succ p'_{XY} \tag{6}$$

if and only if $H_0(p) \leq H_0(p')$ and $H(p) < H(p')$. Moreover, for every $\varepsilon > 0$, we can choose Y and p'_{XY} such that the mutual information is $I(X:Y) \equiv S(p'_{XY} \| p'_X \otimes p'_Y) < \varepsilon$.

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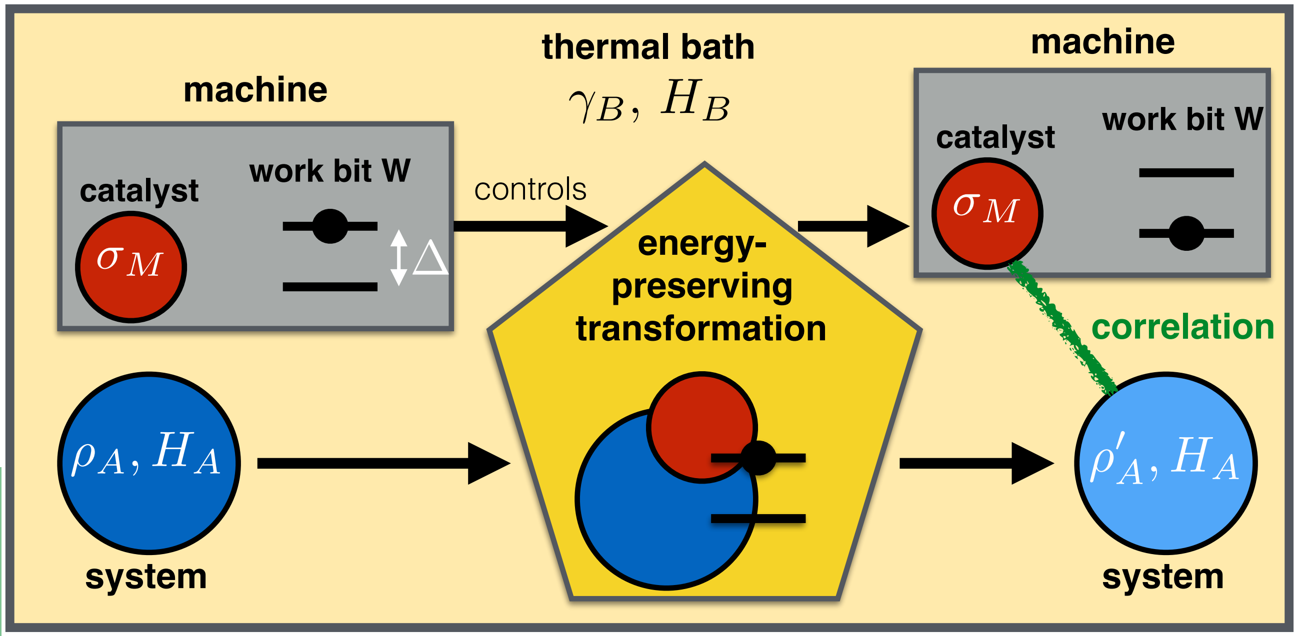
Majorization: prob. vectors $\quad p = (p_1, \ldots, p_n), \quad q = (q_1, \ldots, q_n)$

$$p \succ q \quad \Leftrightarrow \quad \sum_{i=1}^k p_i^\downarrow \geq \sum_{i=1}^k q_i^\downarrow \qquad (k = 1, \ldots, n).$$

Overview

1. Standard view: thermodynamic limit

2. Thermodynamics as a resource theory



3. Characterization of *F* and *S* without thermodynamic limit

4. How about coherence? A no-broadcasting theorem

5. Consequences for quantum information theory

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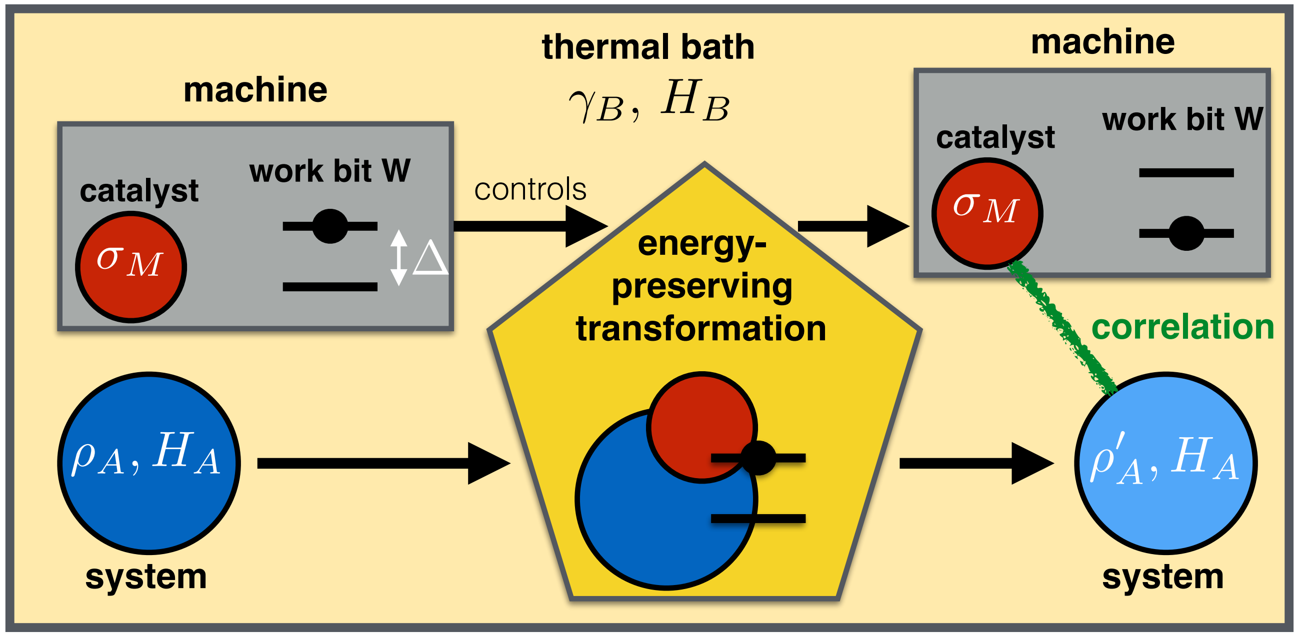

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What if we have coherence between energy levels?

Theorem. Let ρ_A, ρ'_A be block-diagonal states. Then, for every $\varepsilon > 0$, there is a thermal operation $\mathcal{T}_\varepsilon$, a state $\rho'_A(\varepsilon)$ with $\|\rho'_A - \rho'_A(\varepsilon)\| < \varepsilon$ and a finite-dimensional catalyst σ_C such that

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Note that thermal operations are **time-translation-symmetric**:

$\mathcal{T}_\varepsilon(\mathcal{U}_t(\rho_{AC})) = \mathcal{U}_t(\mathcal{T}_\varepsilon(\rho_{AC}))$, where $\mathcal{U}_t = e^{-itH} \bullet e^{itH}$.

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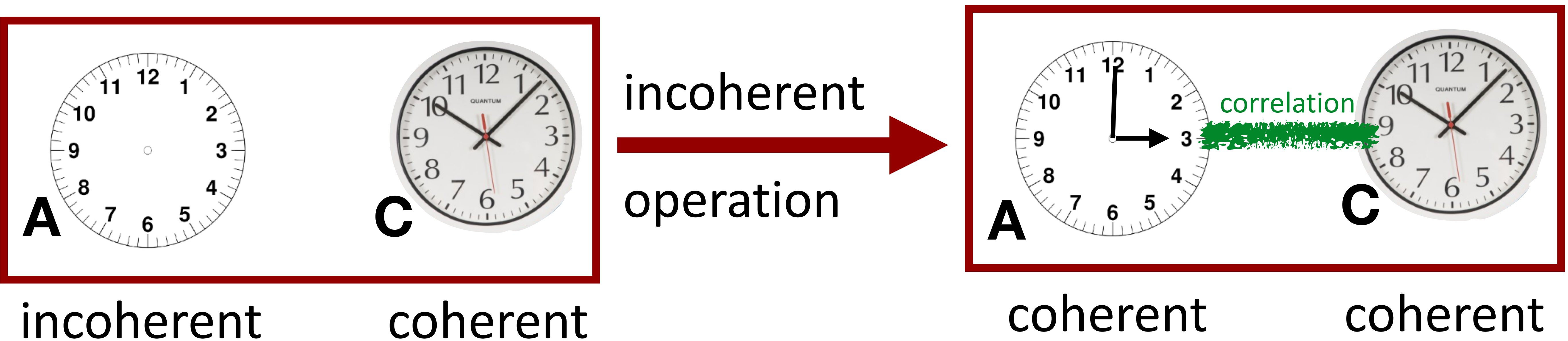

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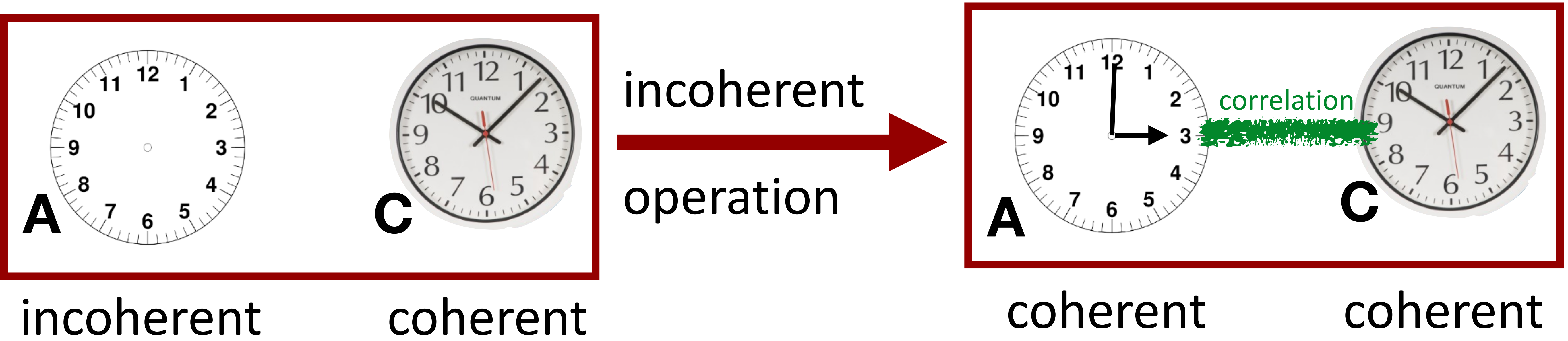

M. Lostaglio and MM, *Coherence and Asymmetry Cannot be Broadcast,* Phys. Rev. Lett. **123**, 020402 (2019).

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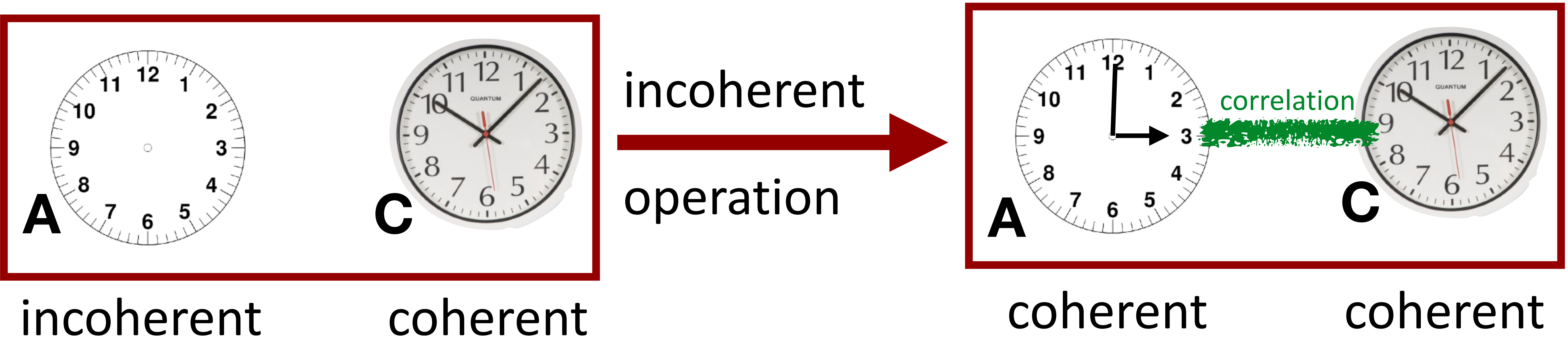

M. Lostaglio and MM, *Coherence and Asymmetry Cannot be Broadcast,* Phys. Rev. Lett. **123**, 020402 (2019).

Theorem: This is impossible.

Special case of a general no-broadcasting theorem for asymmetry.

What if we have coherence between energy levels?

Is it possible to have $\mathcal{T}(\rho_A \otimes \sigma_C) = \rho_A' \sigma_C$,

where $\mathcal{T}$ is **time-translation-symmetric**, and also ρ_A is time-translation symmetric, but ρ_A' isn't?

C identical to before.

A

incoherent

C

coherent

Consequence: The characterization of *F* that I've presented cannot remain valid in the presence of coherences between energy levels. 😕

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PRL **113,** 150402 (2014) PHYSICAL REVIEW LETTERS week ending 10 OCTOBER 2014

Catalytic Coherence

Johan Åberg*
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(Received 10 December 2013; revised manuscript received 30 July 2014; published 7 October 2014)

Because of conservation of energy we cannot directly turn a quantum system with a definite energy into a superposition of different energies. However, if we have access to an additional resource in terms of a system with a high degree of coherence, as for standard models of laser light, we can overcome this

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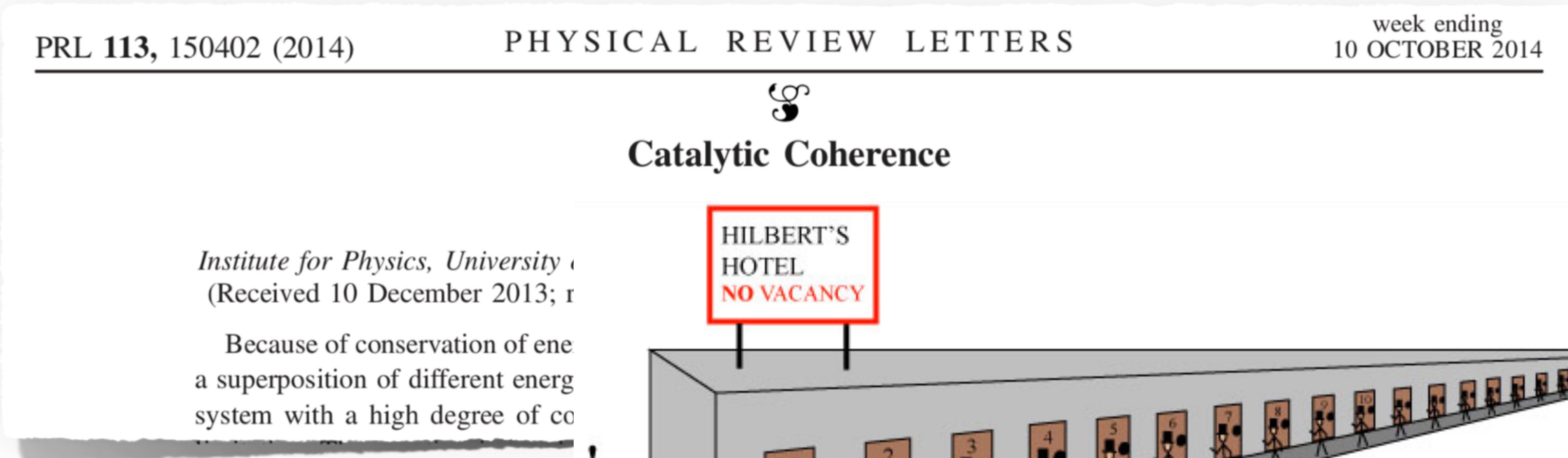
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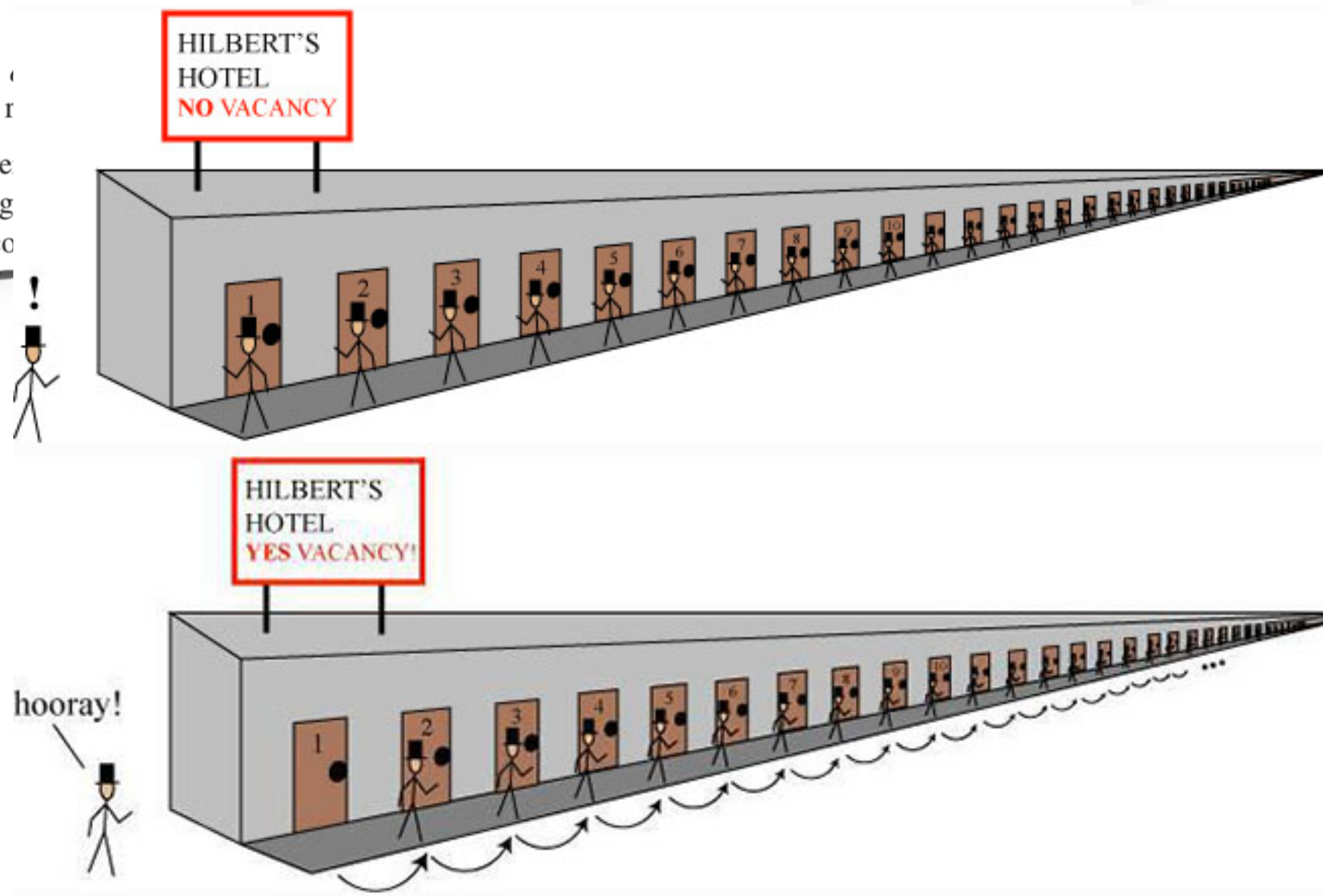
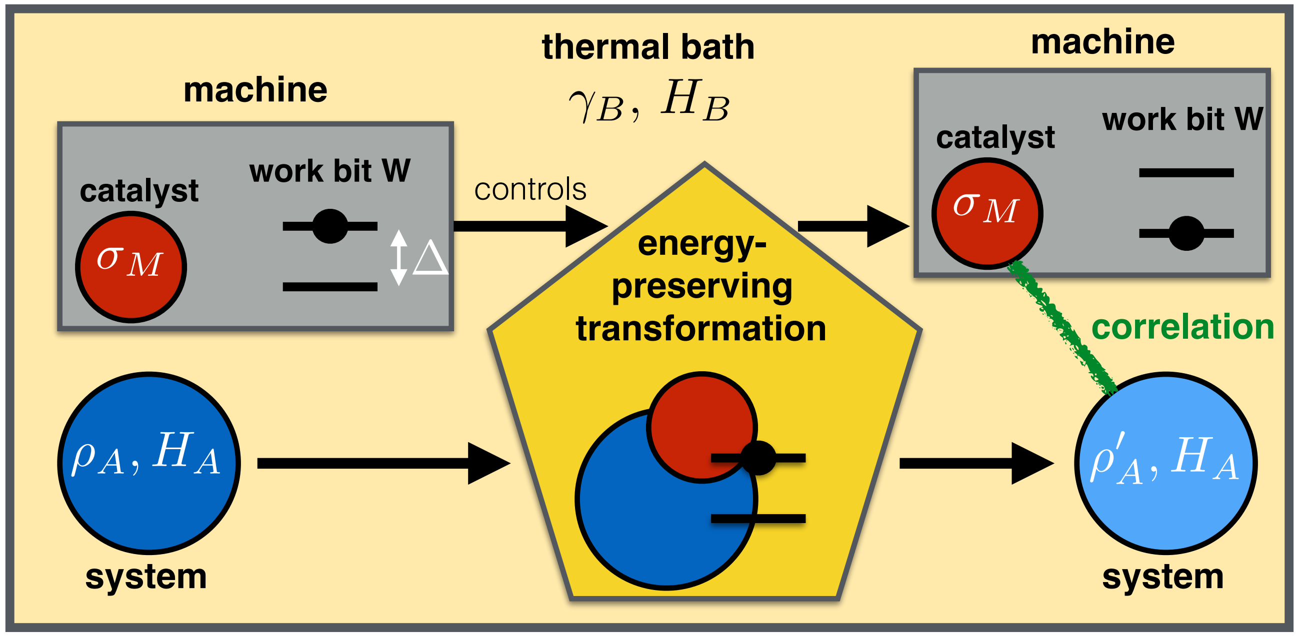


However, we showed that even this weak version is **impossible** for finite-dimensional catalysts.

Overview

1. Standard view: thermodynamic limit

2. Thermodynamics as a resource theory



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5. Consequences for quantum information theory

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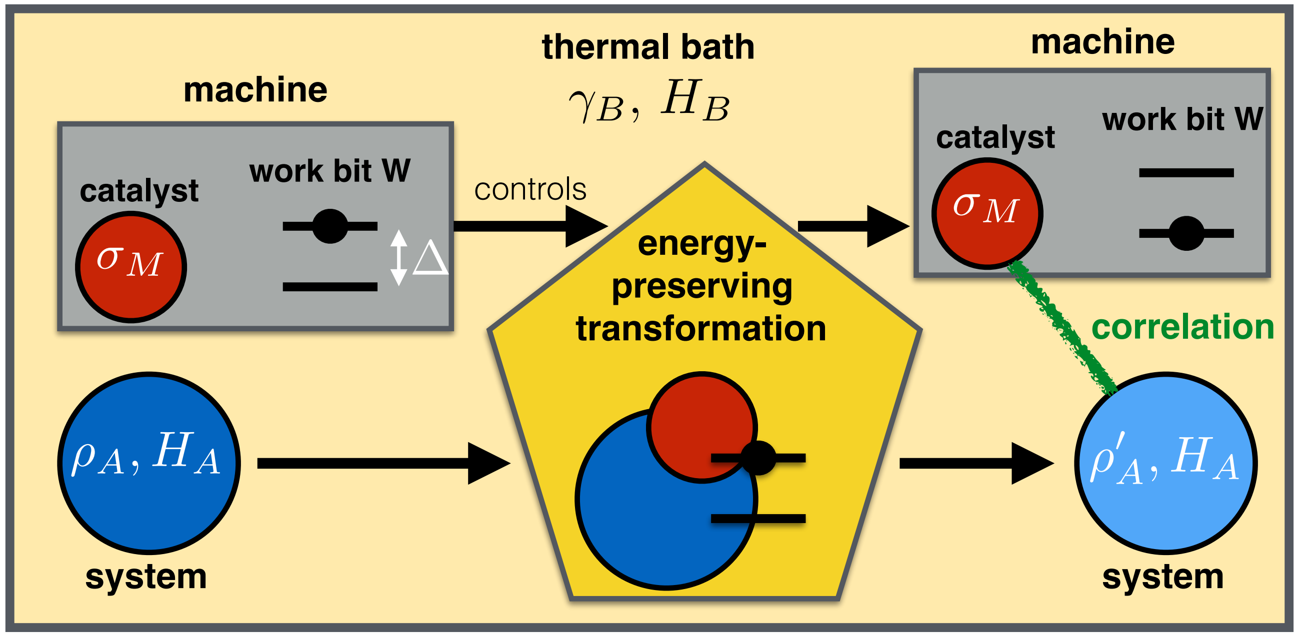

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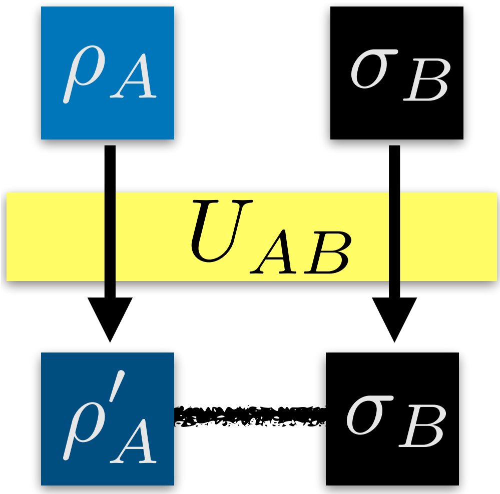

Theorem. Let ρ_A and ρ'_A be two quantum states with non-identical spectra on a finite-dimensional Hilbert space *A*. Then the following are equivalent:

- There exists another finite-dimensional system *B*, a unitary U_{AB} and a state σ_B such that

$$U_{AB}(\rho_A \otimes \sigma_B)U_{AB}^\dagger = \rho'_A \sigma_B.$$

- $\mathrm{rank}(\rho_A) \leq \mathrm{rank}(\rho'_A)$ and $S(\rho_A) < S(\rho'_A)$, where $S(\rho) = -\mathrm{tr}(\rho \log \rho)$ is von Neumann entropy.

H. Wilming, *Entropy and Reversible Catalysis*, Phys. Rev. Lett. **127**, 260402 (2021).

Consequences for quantum information theory

This is perhaps relevant in contexts like holographic duality, where entropy has a **dual spacetime interpretation**:

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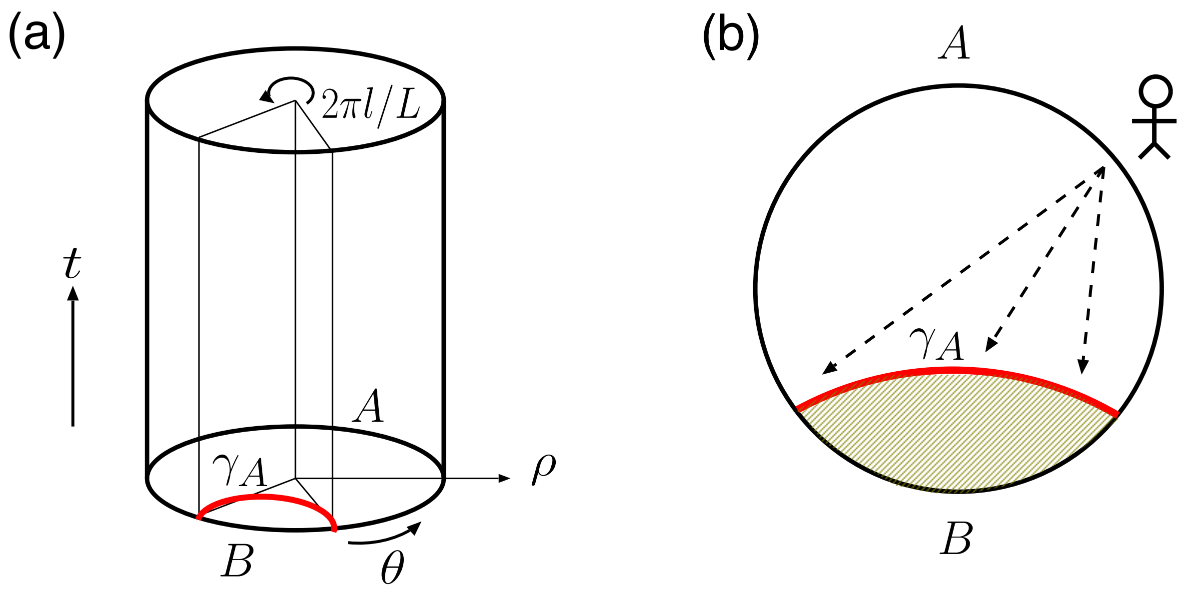
S. Ryu and T. Takayanagi, *Holographic Derivation of Entanglement Entropy from AdS/CFT*, Phys. Rev. Lett. **96**, 181602 (2006).

$$S_A = \frac{\text{Area of } \gamma_A}{4G_N^{(d+2)}}$$



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One interesting but random recent example:

Consequences for quantum information theory

Many more results in the last few years by colleagues.
One interesting but random recent example:

Quantum thermodynamics with coherence: Covariant Gibbs-preserving operation is characterized by the free energy

Naoto Shiraishi*
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3-8-1 Komaba, Meguro-ku, Tokyo 153-8902, Japan

A map $\mathcal{E} : S \to S$ is called a covariant Gibbs-preserving operation (CGPO) if (i) $\mathcal{E}(\rho_{\mathrm{Gibbs}}) = \rho_{\mathrm{Gibbs}}$ and (ii) $\mathcal{E}(e^{-iHt}\rho e^{iHt}) = e^{-iHt}\mathcal{E}(\rho)e^{iHt}$ for any t are satisfied. Here, $\rho_{\mathrm{Gibbs}} := e^{-\beta H}/Z$ is a Gibbs state with a given inverse temperature β We define the free energy $F(\rho) := S(\rho||\rho_{\mathrm{Gibbs}})$ with the relative entropy S. The CGPO is also called enhanced thermal operation in Ref. [7].

We investigate the correlated-catalytic conversion with CGPO in this Letter. We say that ρ is convertible to ρ' through CGPO with a correlated-catalyst if for any $\varepsilon > 0$ there exist an auxiliary system C called a catalyst, its state c, and a CGPO $\mathcal{E} : S \otimes C \to S \otimes C$ such that $\tau = \mathcal{E}(\rho \otimes c)$ with $\mathrm{Tr}_S[\tau] = c$ and $|\mathrm{Tr}_C[\tau] - \rho'|_1 < \varepsilon$. If the last condition is replaced by $\mathrm{Tr}_C[\tau] = \rho'$, we say this conversion *exact*.

Theorem 1. *Consider two states ρ and ρ' in S. We assume that the shortest period of ρ is $2\pi/\Delta$ (i.e., all modes are coherent). Then, ρ is convertible to ρ' through CGPO with correlated-catalyst if and only if $F(\rho) \geq F(\rho')$. In addition, if $F(\rho) > F(\rho')$ and ρ' is full-rank, then this conversion is exact.*

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- **Resource-theoretic** approach to thermodynamics: generalizes thermo. to small and strongly correlated systems. **Conceptually**, a different approach: restrictions for an agent who acts under reversibility and energy conservation.

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Thank you! Paper etc.: https://mpmueller.net