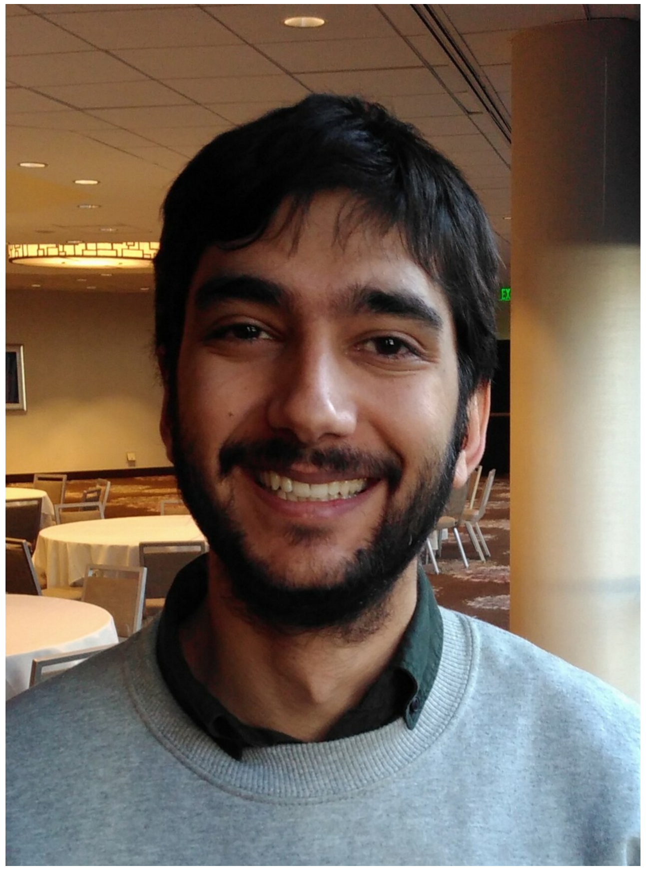
From fully quantum thermodynamical identities to a second law equality

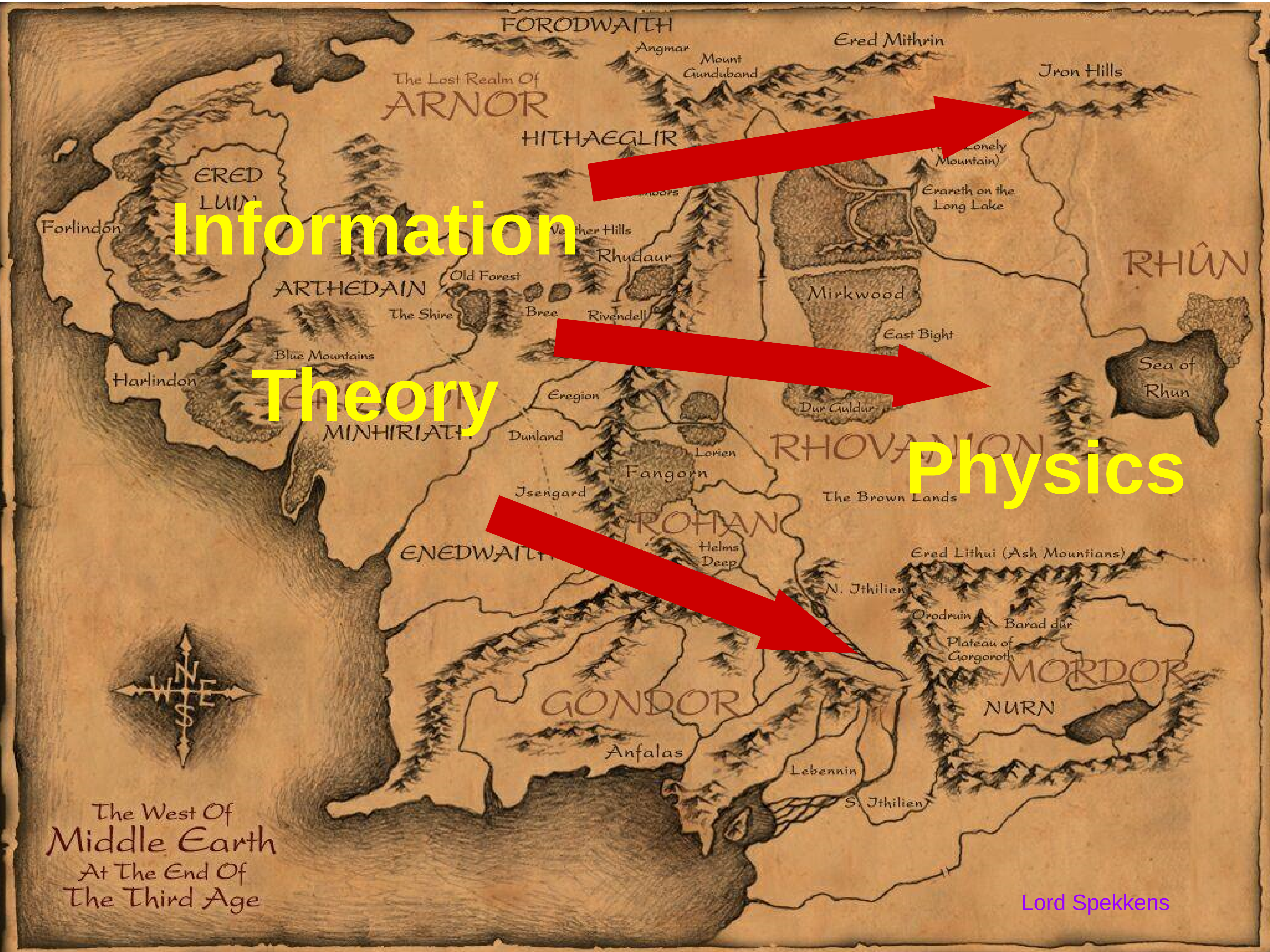
Alvaro Alhambra, Lluis Masanes, Jonathan Oppenheim, Chris Perry

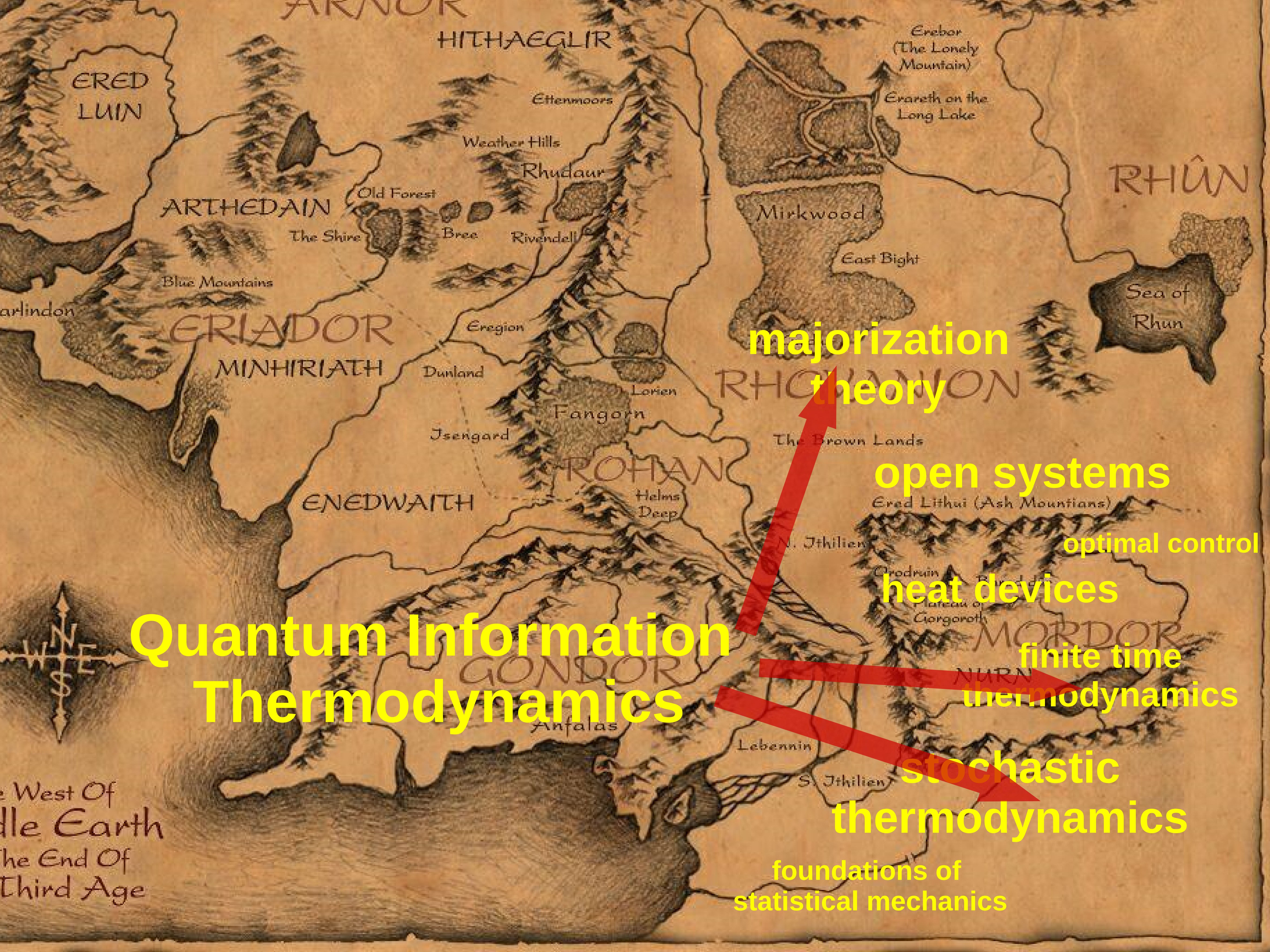
Fluctuating States
Phys. Rev. X 6, 041016 (2016)

Fluctuating Work
Phys. Rev. X 6, 041017 (2016)



UCL


Information
Theory
Physics
Lord Spekkens
FORODWAITH
Angmar
Mount Gunduband
Ered Mithrin
Iron Hills
The Lost Realm Of
ARNOR
HITHAEGLIR
ERED LUIN
Forlindon
Erareth on the Long Lake
RHÛN
Rhudaur
ARTHEDAIN
Old Forest
The Shire
Bree
Rivendell
Mirkwood
East Bight
Blue Mountains
Harlindon
Sea of Rhun
Eregion
Dur Guldur
MINHIRIATH
Dunland
Lorien
Fangorn
Isengard
The Brown Lands
ROHAN
Helms Deep
ENEDWAITH
Ered Lithui (Ash Mountians)
N. Ithilien
Orodruin
Barad dur
Plateau of Gorgoroth
MORDOR
NURN
GONDOR
Anfalas
Lebennin
S. Ithilien
The West Of
Middle Earth
At The End Of
The Third Age


Quantum Information
Thermodynamics
majorization
theory
open systems
optimal control
heat devices
finite time
thermodynamics
stochastic
thermodynamics
foundations of
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HITHAEGLIR
ERED
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MORDOR
NURN
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Third Age

Thermodynamics is an information theory

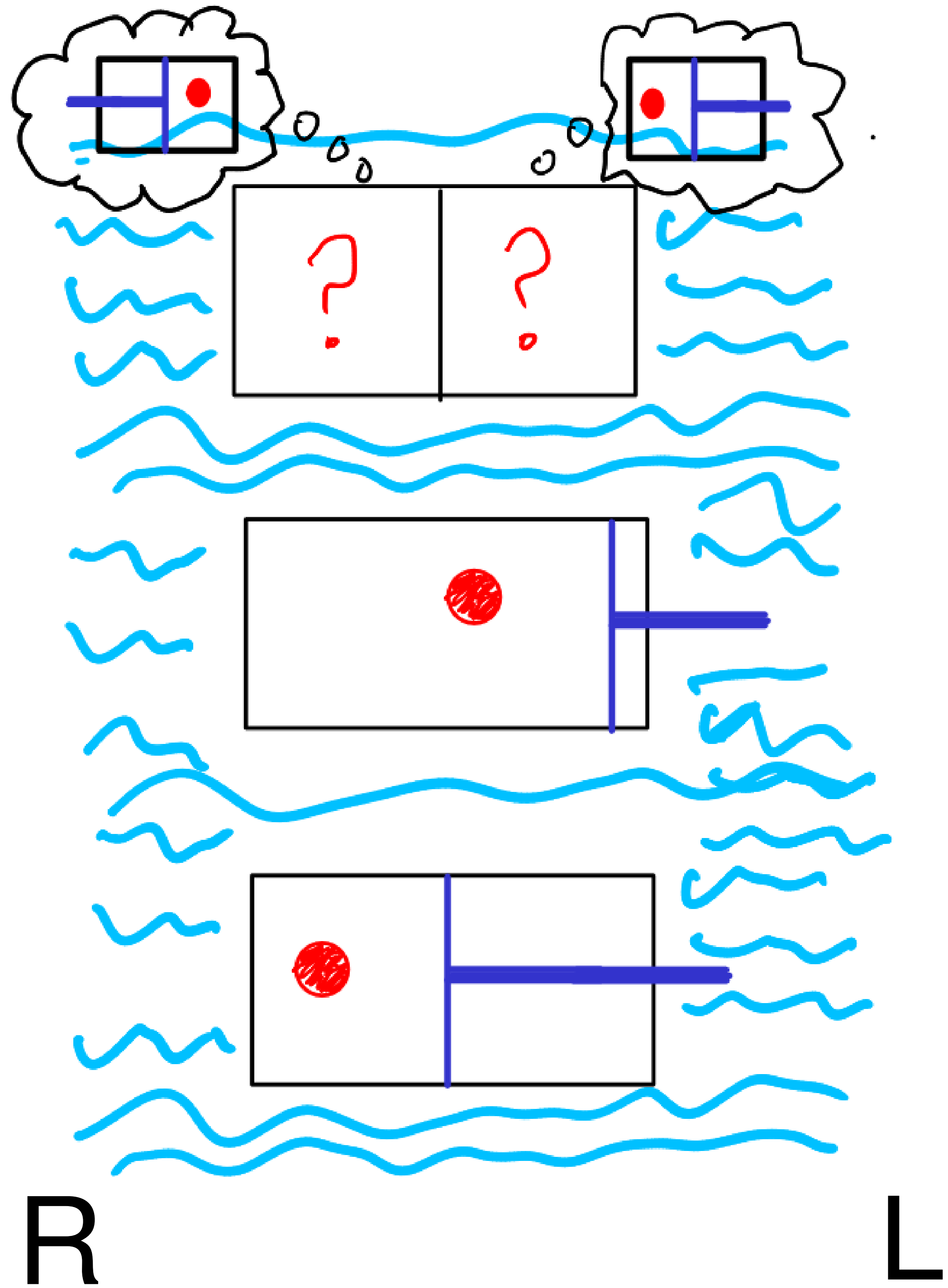
Maxwell

Szilard

Landauer

Bennett

$W = kT\log 2$



What do we mean by W=kTlog2?

(consider the limit of perfect erasure)

A) W=kTlog2 on average, but there will be fluctuations around this value.

B) We can achieve perfect erasure.

C) By using slightly more work on average, you can sometimes gain work when you erase.

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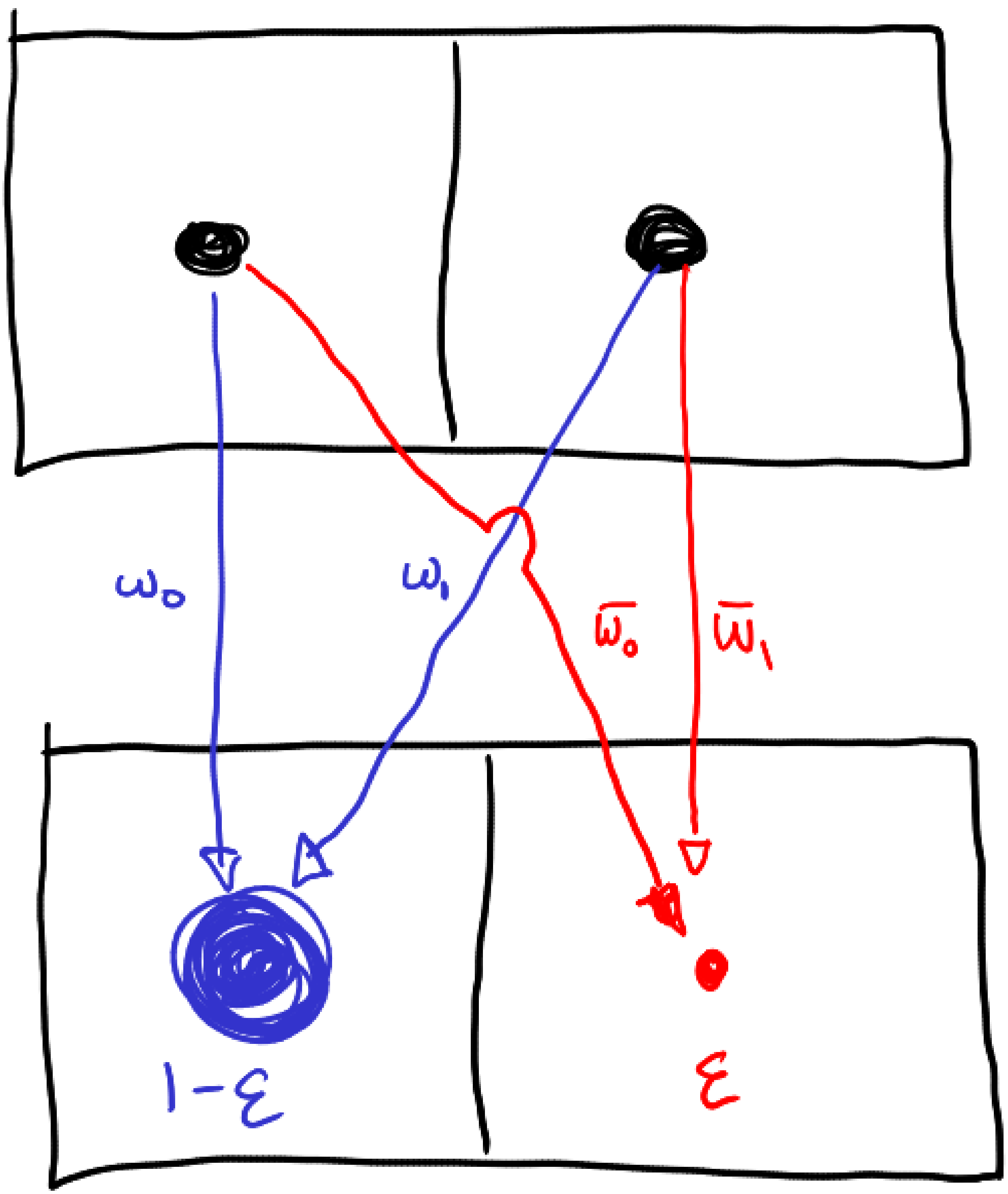
D) None of these statements are true.

E) This quiz is undecidable.

Fluctuating work in erasure

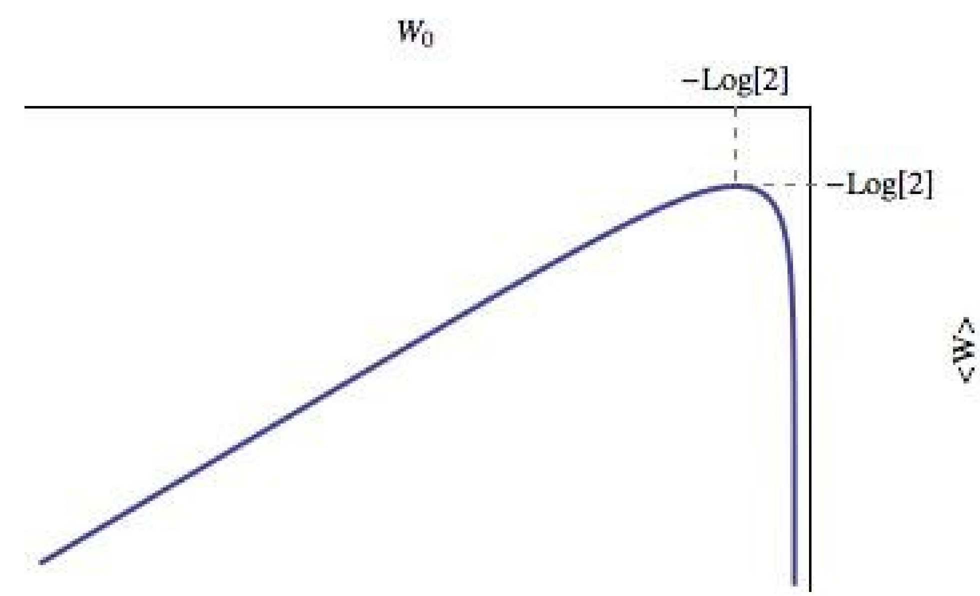


$$\sum_{s',w} P(s',w|s)=1$$

$$\sum_{s,w} P(s',w|s)\,e^{\beta(E_{s'}-E_s+w)}=1$$

$$e^{\beta w_o}+e^{\beta w_1}=1/(1-\epsilon)$$

$$e^{\beta \bar{w}_o}+e^{\beta \bar{w}_1}=1/\epsilon$$



Main Results

- **QIT strengthening of Stochastic Thermodynamics**
- Generalisations of doubly-stochastic maps, majorisation
- Second law of thermodynamics as an equality (fine grained free energy)
- Fully quantum identity $\longrightarrow$ Stochastic Thermodynamics
- Fluctuations of work and of states
- Proof and quantification of third law of thermodynamics

Outline

- Review of thermodynamics (Macroscopic, QIT)
- Equalities for work fluctuations
- Quantum identities
- Outlook

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3 laws of thermodynamics

0) If R_1 is in equilibrium with R_2 and R_3 then R_2 is in equilibrium with R_3

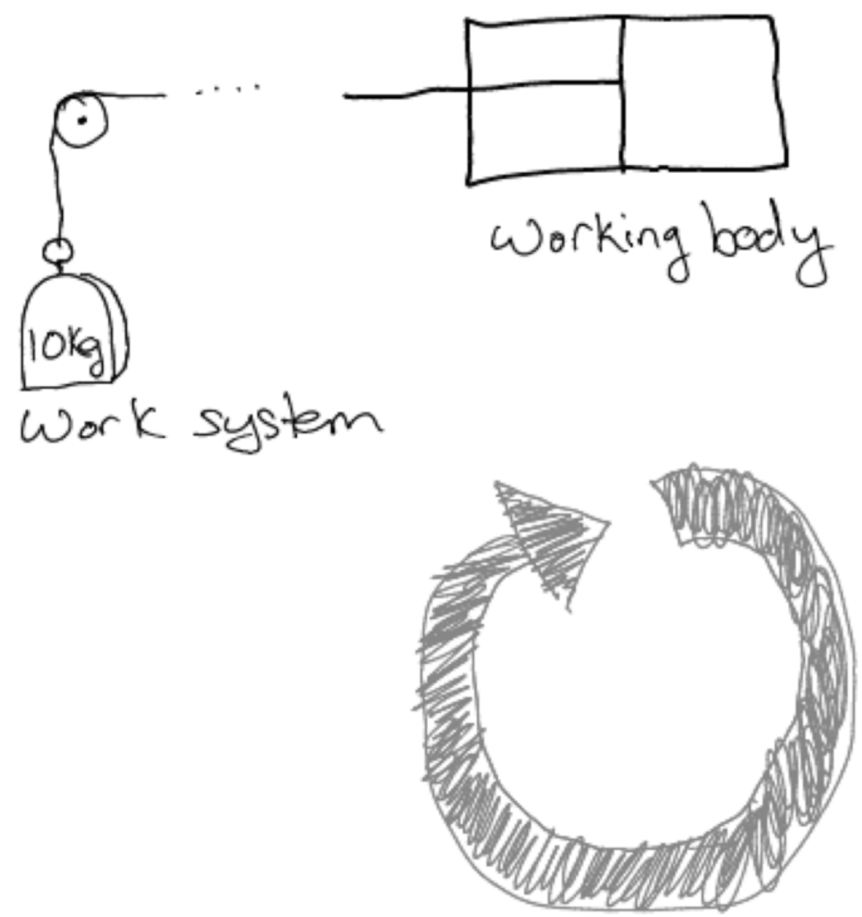
1) $dE = dQ - dW$ (energy conservation)

2) Heat can never pass from a colder body to a warmer body without some other change occuring. – Clausius

3) One can never attain T=0 in a finite number of steps

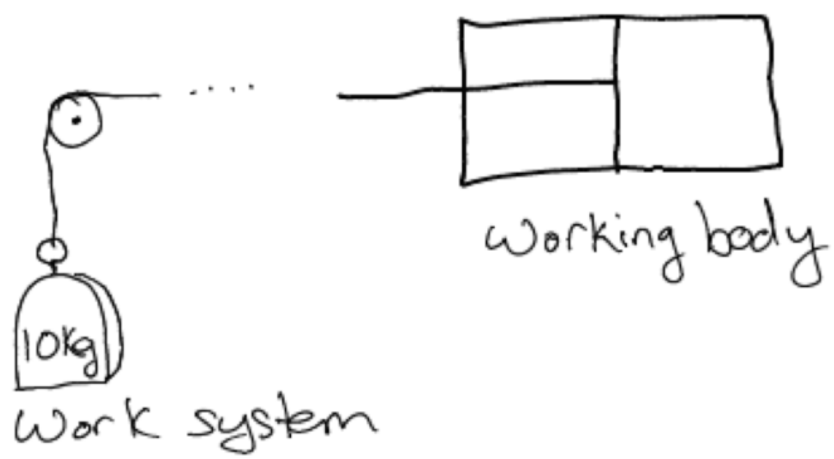
The second law

Heat can never pass from a colder body to a warmer body without some other change occurring – Clausius

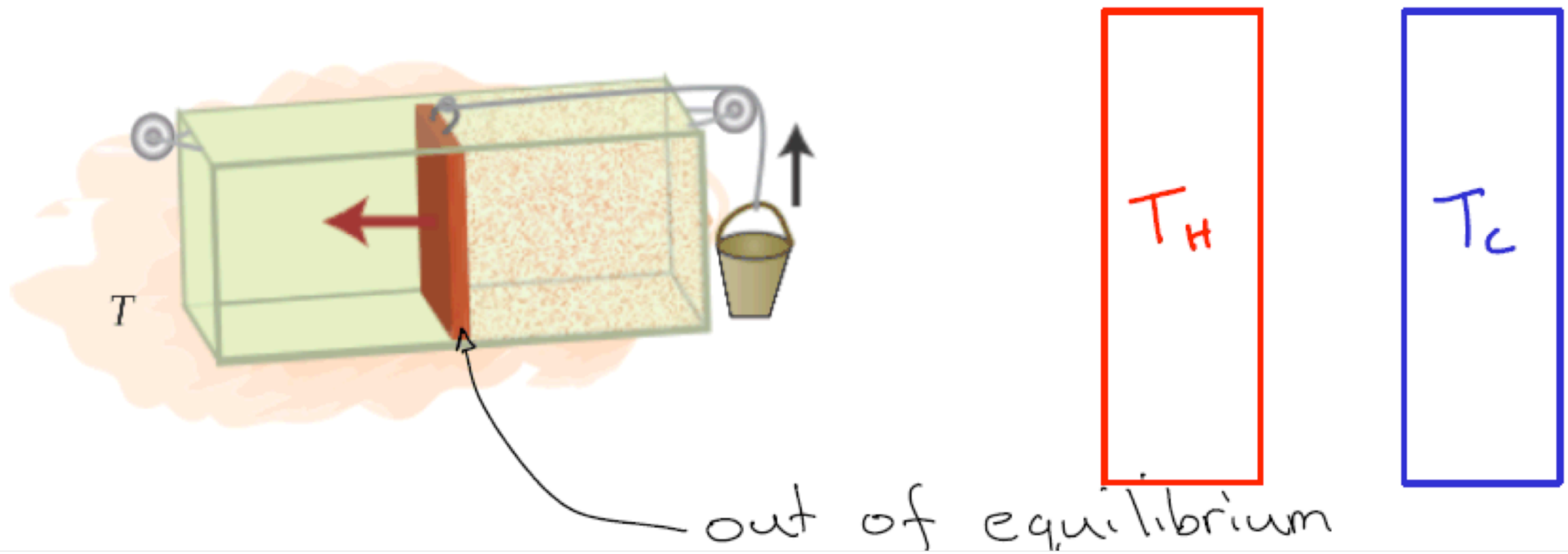


The second law

$$\langle W \rangle \leq \Delta F$$ In any cyclic process



Free Energy

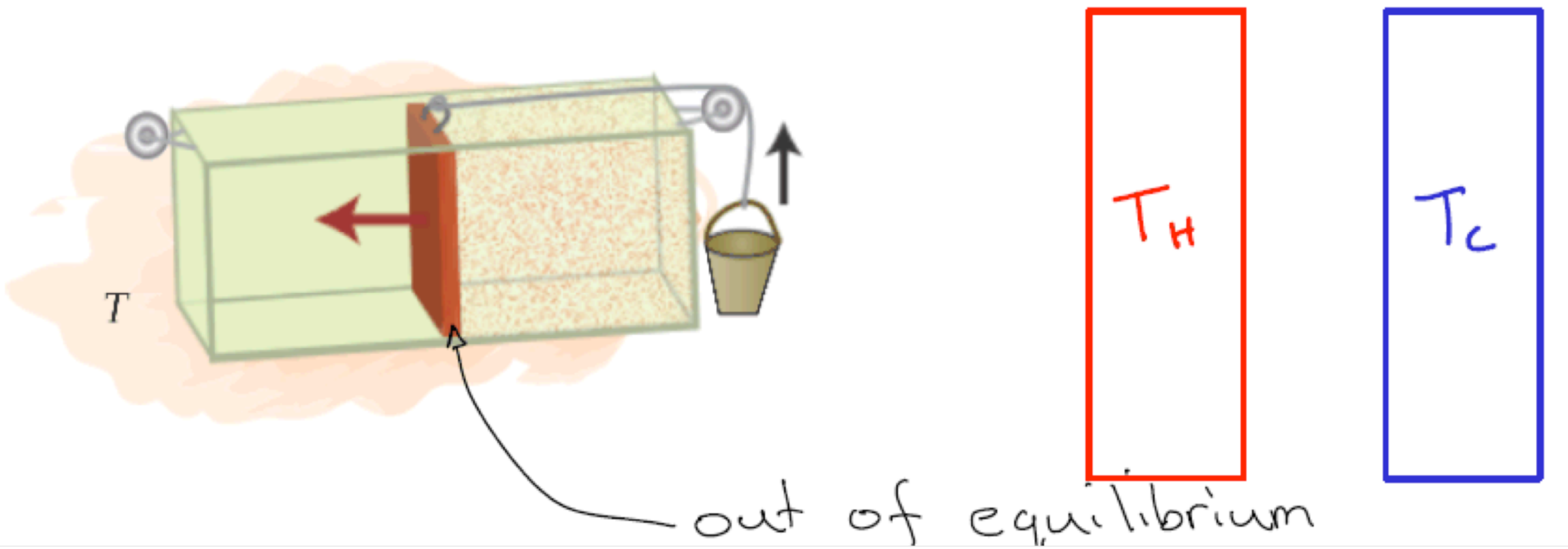


$$F = \langle E \rangle - TS$$

$$\langle W \rangle_{\mathrm{rev}} = F(\rho_{\mathrm{initial}}) - F(\rho_{\mathrm{final}})$$

$$\rho_{\mathrm{initial}} \rightarrow \rho_{\mathrm{final}} \quad \text{iff} \quad \langle W \rangle \leq \Delta F$$

Free Energy



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

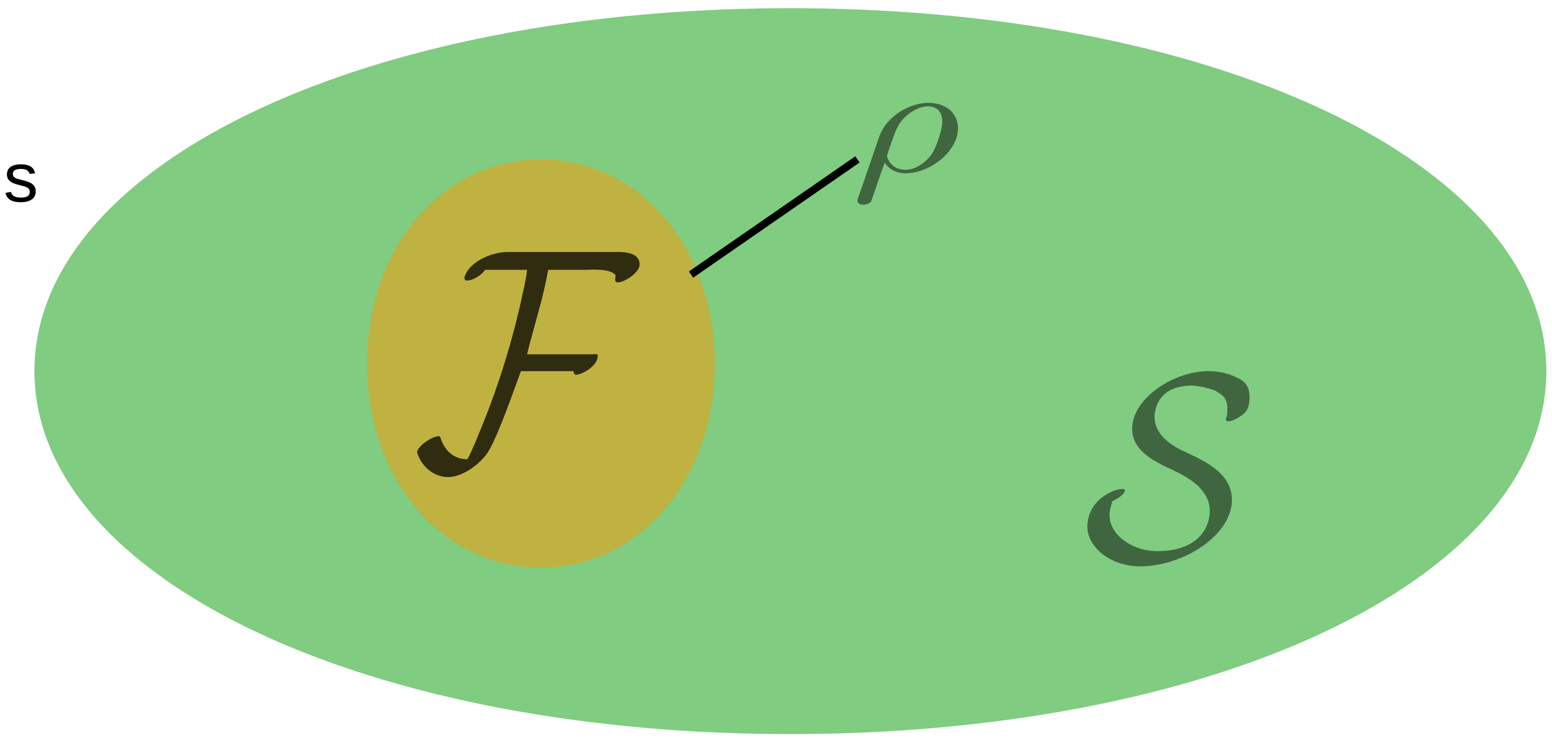
$$\langle W \rangle_{rev} = F(\rho_{initial}) - F(\rho_{final})$$

$$\rho_{initial} \rightarrow \rho_{final} \quad \text{iff} \quad \langle W \rangle \leq \Delta F$$

This is just the first order term of an equality!

Resource Theories

$\mathcal{C}$lass of operations



In reversible theories and under minor assumptions, relative entropy distance to free states $\mathcal{F}$ is the unique measure of the resource (Horodecki et. al. 2011)

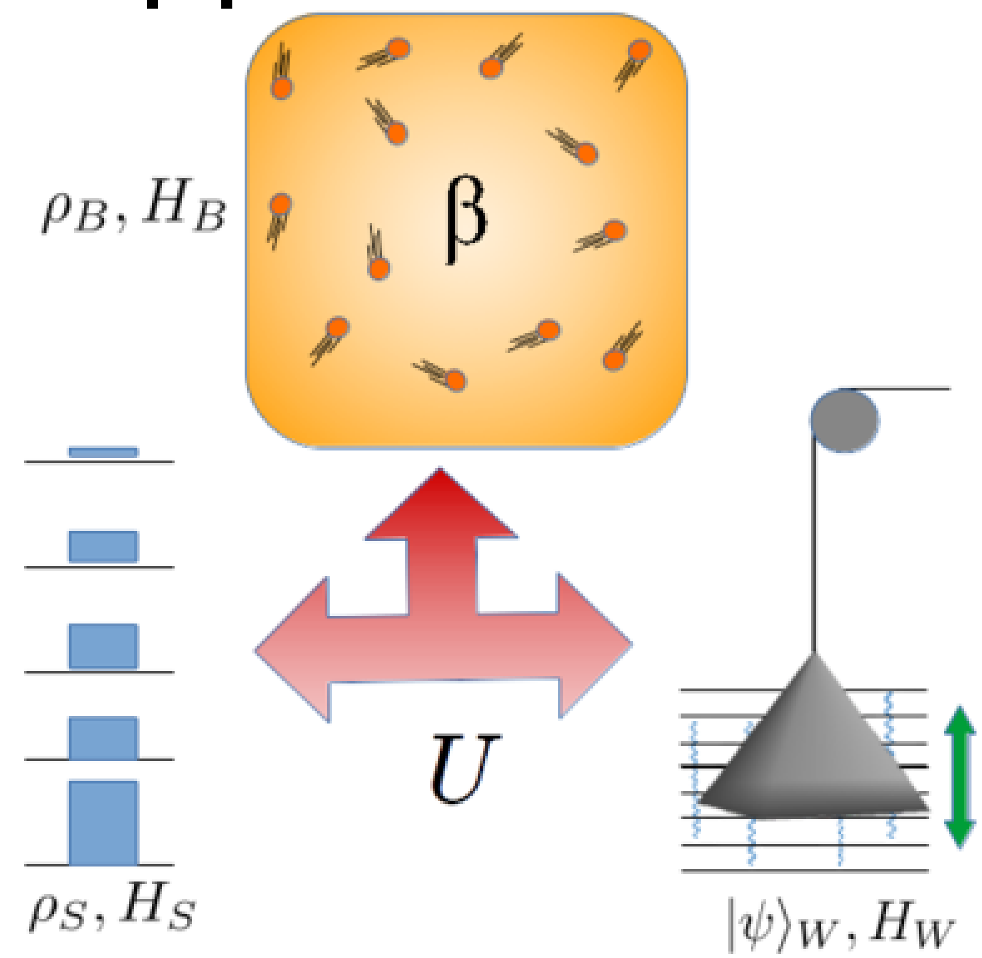
In thermodynamics, $\mathcal{F}$ will turn out to be the Gibbs state ρ_β and the measure is $F(\rho) - F(\rho_\beta)$

But thermodynamics can also be irreversible

What is Thermodynamics??

A resource theoretic approach: Γ

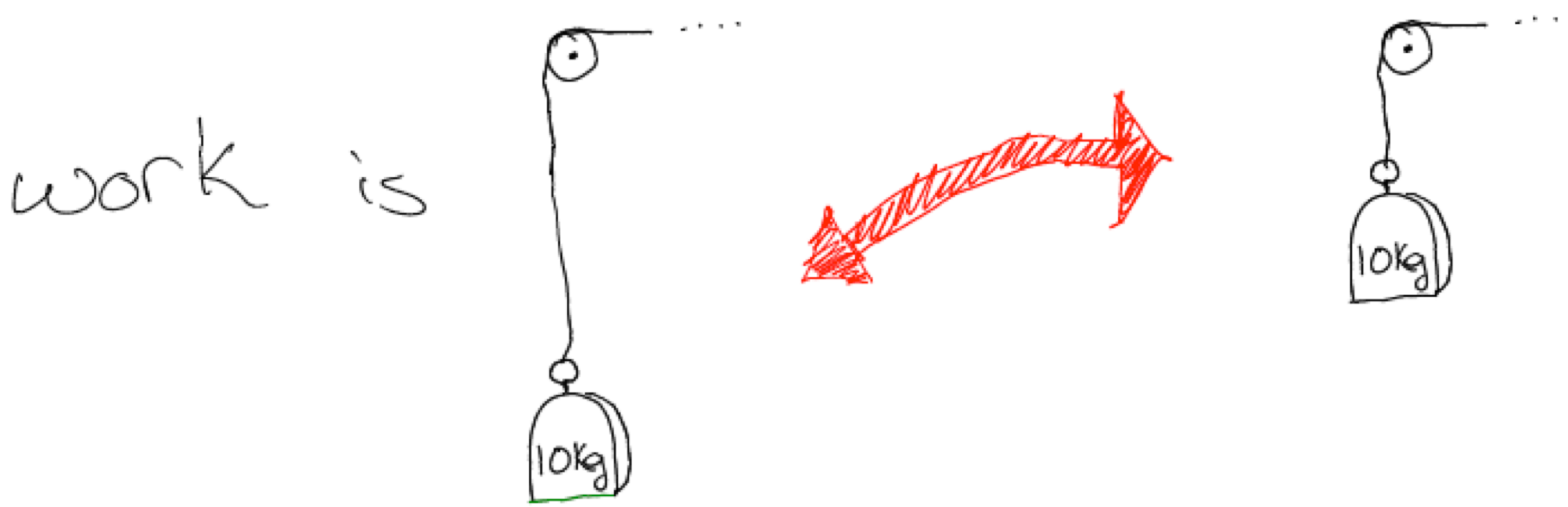
- (ρ_s, H_s)
- adding **free states** ρ_B, H_B
- work system ρ_W, H_w



- energy conserving unitaries U (**1st law**) $[U, H_s + H_w + H_B] = 0$
- tracing out
- *can allow changing Hamiltonian by adding switch bit*
- translation invariant on W: $[U,\Delta_W]=0$ $[\Delta_W,H_w]=i$

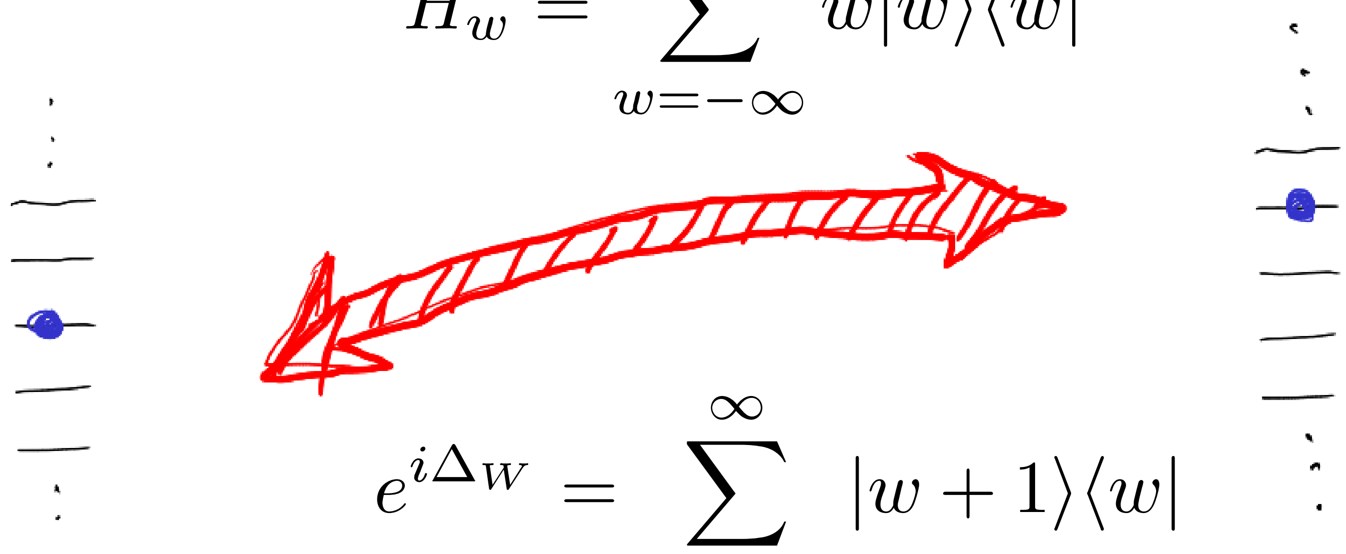
Streater (1995)
Janzig et. al. (2000)
Horodecki, JO (2011)
Skrzypczyk et. al. (2013)
Brandao et. al. (2015)

Work



or in the micro - regime

$$H_w = \sum_{w=-\infty}^{\infty} w|w\rangle\langle w|$$



$$e^{i\Delta W} = \sum_{w=-\infty}^{\infty} |w+1\rangle\langle w|$$

Broadest definition of thermo

Includes other paradigms (Brandao et. al. 2011)

- H_{int}
- $H(t)$
- implicit battery: arbitrary U, and take $W = \mathrm{tr}H\rho - \mathrm{tr}HU\rho U^\dagger$
- Implemented using very crude control (Perry et. al. 2016)
- c.f. catalytic transformations (Brandao et. al. 2015)

What is the cost of a state transformation? (2^{nd} law)

What do we mean by work?

- No work: Ruch, Mead (1975); Janzig (2000); Horodecki et. al. (2003); Horodecki, JO (2011)
- Deterministic or worst case work: Dahlsten et al. (2010); Del Rio et. al. (2011); Horodecki, JO (2011); Aaberg (2011); Faist et. al. (2013), Egloff (2015)
- Average work: Brandao et. al. (2011); Skrzypczyk et. al. (2013); Korzekwa et. al (2015)
- Fluctuating work: Jarzynski (1997); Crooks (1999); Tasaki (1999)

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When can we go from ρ to σ?
(2nd law)

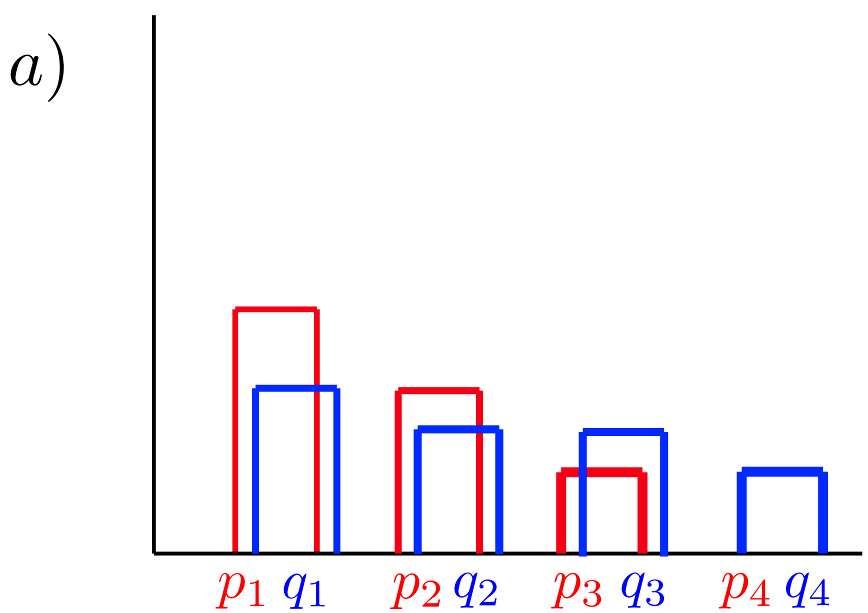
$$\langle W \rangle \leq F(\rho) - F(\sigma)$$

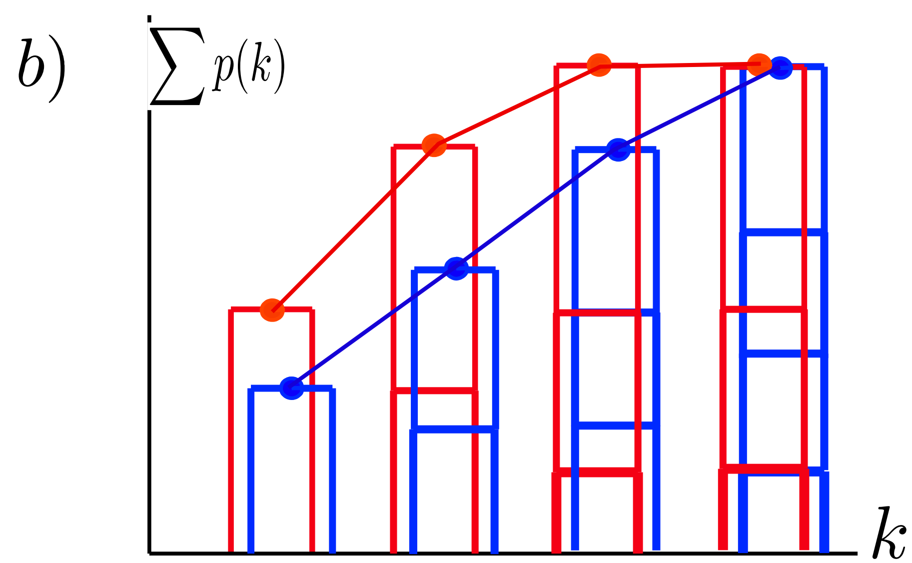
Many Second Laws

H=0 (Noisy Operations), no work

majorisation

$$\rho \rightarrow \sigma \; iff \; \rho \succ \sigma \qquad p(1) \geq p(2) \geq p(3) \ldots \qquad \sum_k p(k) \geq \sum_k q(k) \; \forall k$$





$$q(s') = \sum_s P(s'|s)p(s)$$

$$\sum_s P(s'|s) = 1$$

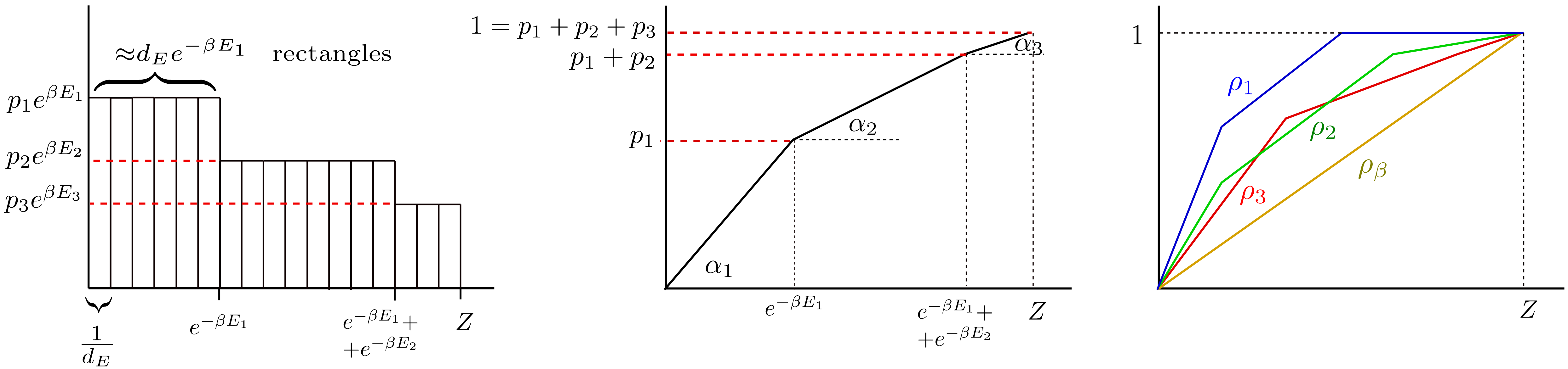
$$\sum_{s'} P(s'|s) = 1$$

Horodecki et. al. 2003

(Thermal Operations), deterministic work

thermo-majorisation

$$p(1)e^{\beta E_1} \geq p(2)e^{\beta E_2} \geq p(3)e^{\beta E_3}$$ (β-ordering)



$$q(s') = \sum_s P(s'|s)p(s)$$

$$\sum_s P(s'|s)e^{-\beta E_s} = e^{-\beta E_{s'}}$$

$$\sum_{s'} P(s'|s) = 1$$

Horodecki, JO (2011)
Ruch, Mead, (75)

Fluctuating work

$\rho \to \sigma \;\; iff$

$$\sum_{s,w} P(s',w|s)\, e^{\beta(E_{s'}-E_s+w)} = 1$$

$$\sum_{s',w} P(s',w|s) = 1$$

$$f_s := E_s + T\log p(s)$$

$$F = \langle f_s \rangle$$
$$= \langle E \rangle - TS$$

$$q(s',w) = \sum_s P(s'w|s)p(s)$$

$$\sum_{s'} \sum_{s,w} P(s',w|s) e^{\beta(E'_s - E_s + w)} \frac{p(s)}{p(s)} p(s') = \sum_{s'} p(s')$$

$$\langle e^{\beta(f_{s'} - f_s + w)} \rangle = 1$$

2nd law equality

Classical derivation: Seifert (2012)

Corrections to second law

$$\langle e^{\beta(f_{s'} - f_s + w)} \rangle = 1$$

$$f_s := E_s + T \log P(s)$$

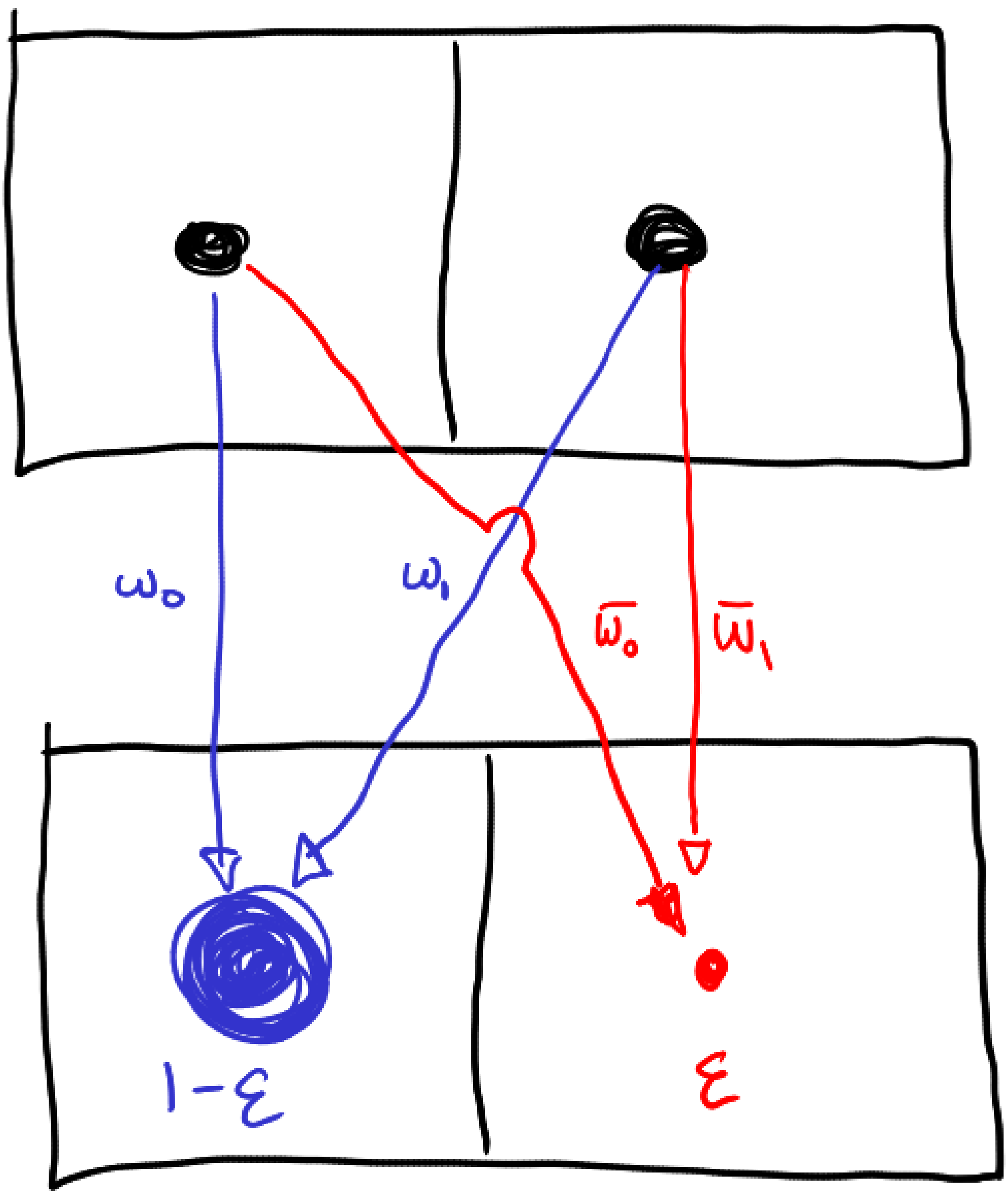
$$F = \langle f_s \rangle$$
$$= \langle E \rangle - TS$$

$$\langle f_{s'} - f_s + w \rangle \le 0$$

Standard 2nd law $W \le \Delta F$

$$\sum_{k=1}^{N} \frac{\beta^k}{k!} \langle (f_{s'} - f_s + w)^k \rangle \le 0$$

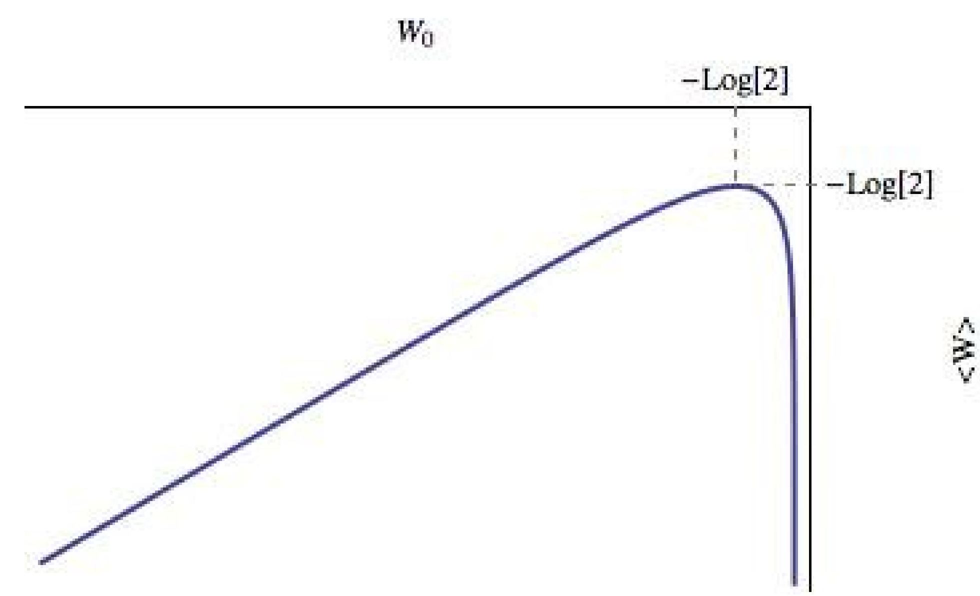
Fluctuating work in erasure



$$\sum_{s,w} P(s',w|s)\, e^{\beta(E_{s'}-E_s+w)}=1$$

$$e^{\beta w_o} + e^{\beta w_1} = 1/(1-\epsilon)$$

$$e^{\beta \bar{w}_o} + e^{\beta \bar{w}_1} = 1/\epsilon$$



Same considerations apply to non-deterministic case

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C) ~~By using slightly more work on average, you can sometimes gain work when you erase.~~

D) None of these statements are true.

E) This quiz is undecidable.

no work to fluctuating work

doubly stochastic maps

$$\sum_{s'} P(s'|s)=1$$

$$\sum_{s} P(s'|s)=1$$

majorisation

Gibbs-stochastic maps

$$\sum_{s'} P(s'|s)=1$$

$$\sum_{s} P(s'|s)e^{\beta(E_{s'}-E_s)}=1$$

thermo-majorisation

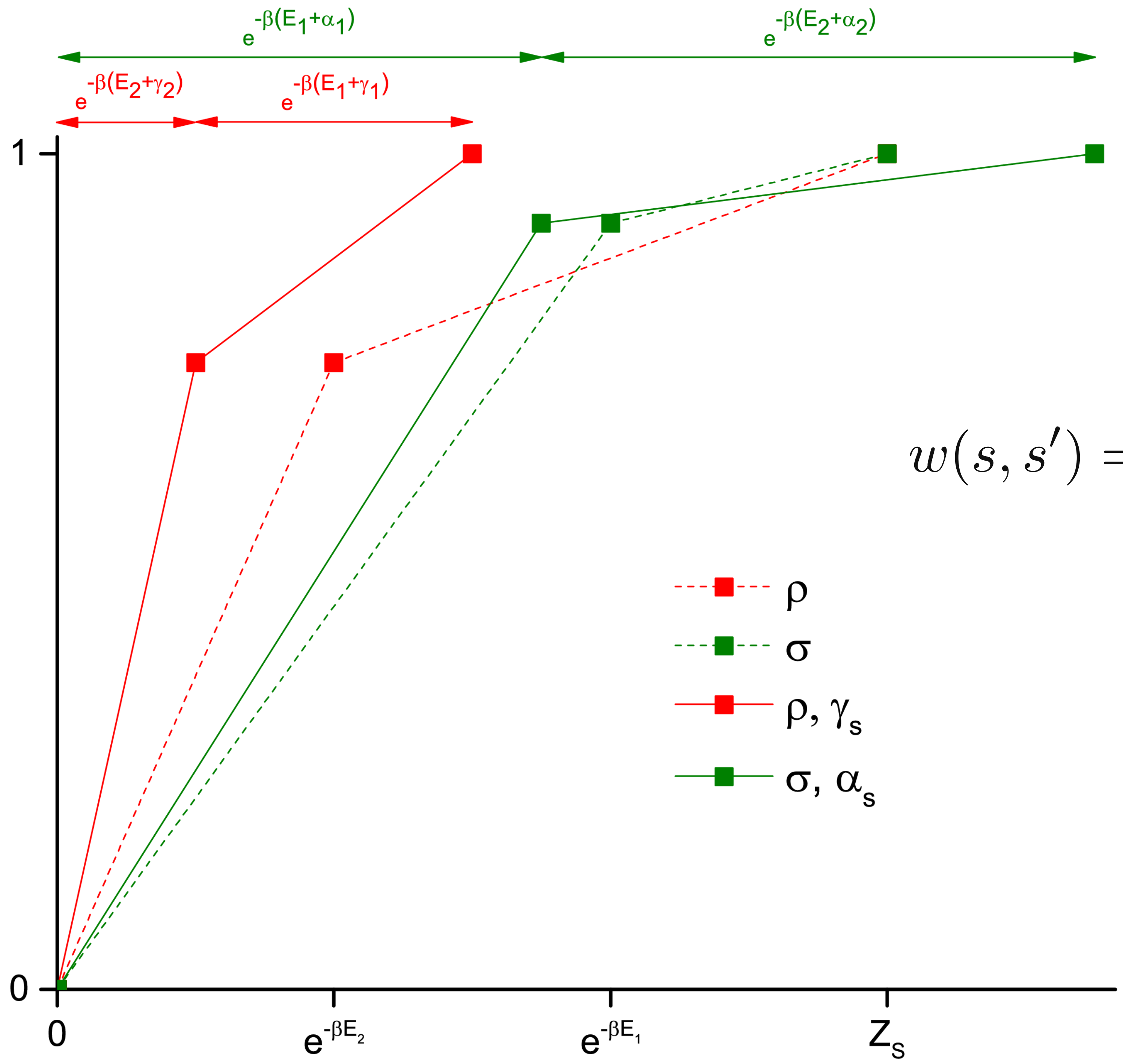
fluctuating work

$$\sum_{s'} P(s'|s)=1$$

$$\sum_{s,w} P(s',w|s)e^{\beta(E_{s'}-E_s+w)}=1$$

linear program

Thermo-majorisation curves



$$w(s,s') = \alpha_s - \gamma_{s'}$$

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Quantum identity

$$tr_W[\mathcal{F}_{H'_s+H_w}\Gamma_{SW}\mathcal{F}^{-1}_{H_s+H_w}]1_S\otimes\rho_W=1_S$$

$$\mathcal{F}_H(\rho):=e^{\frac{\beta}{2}H}\rho\, e^{\frac{\beta}{2}H}$$

$$\Gamma_{SW}=tr_B U\rho_{SWB}U^{\dagger}$$

$$\sum_{s,w}P(s',w|s)e^{\beta(E_{s'}-E_s+w)}=1$$

For classical states

$$P(s',w|s)=tr[|s'\rangle\langle s'|\otimes|w\rangle\langle w|\Gamma_{SW}(|s\rangle\langle s|\otimes|0\rangle\langle 0|)]$$

c.f. Aaberg (2016)

Quantum identity

$$
\begin{aligned}
& \mathrm{tr}_W \left(\mathcal{J}_{H'_S + H_W} \Gamma_{SW} \mathcal{J}^{-1}_{H_S + H_W} \right) (\mathbb{1}_S \otimes \rho_W) \\
= \quad & \mathrm{tr}_W \mathcal{J}_{H'_S + H_W} \left(\mathrm{tr}_B \left[U \mathcal{J}^{-1}_{H_S + H_W} \frac{e^{-\beta H_B}}{Z_B} (\mathbb{1}_S \otimes \rho_W) U^\dagger \right] \right) \\
= \quad & \mathrm{tr}_W \mathcal{J}_{H'_S + H_W} \left(\frac{1}{Z_B} \mathrm{tr}_B \left[U \mathcal{J}^{-1}_{H_S + H_B + H_W} (\mathbb{1}_{SB} \otimes \rho_W) U^\dagger \right] \right) \\
= \quad & \mathrm{tr}_W \mathcal{J}_{H'_S + H_W} \left(\frac{1}{Z_B} \mathrm{tr}_B \left[\mathcal{J}^{-1}_{H'_S + H_B + H_W} (U \mathbb{1}_{SB} \otimes \rho_W U^\dagger) \right] \right) \\
= \quad & \mathrm{tr}_{BW} \left(\frac{-\beta H_B}{Z_B} U (\mathbb{1}_{SB} \otimes \rho_W) U^\dagger \right) \\
= \quad & \mathrm{tr}_B \left(\frac{-\beta H_B}{Z_B} \mathbb{1}_{SB} \right) = \mathbb{1}_S \ .
\end{aligned}
$$

Masanes, JO (2014)

Fully quantum identities

Generalised Gibbs-stochastic	$\mathrm{tr}_W\left(\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\right)(\mathbb{1}_S\otimes\rho_W)=\mathbb{1}_S$
Second Law equality	$\mathrm{tr}_{SW}\left[\left(\mathcal{J}_{T\ln\rho'_S}\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\mathcal{J}^{-1}_{T\ln\rho_S}\right)(\rho_S\otimes\rho_W)\right]=1$
Generalised Jarzynski equality	$\mathrm{tr}_{SW}\left[\left(\mathcal{J}_{H_W}\Gamma_{SW}\mathcal{J}^{-1}_{H_S+H_W}\mathcal{J}^{-1}_{T\ln\rho_S}\right)(\rho_S\otimes\rho_W)\right]=Z'_S$
Crooks equation[1] (Petz recovery)	$\mathcal{J}_{H'_S+H_W}\Gamma_{SW}\mathcal{J}^{-1/2}_{H_S+H_W}=\Theta^*_{SW}$

[1] c.f. Åberg (2016)

Quantum identities w/ diagonal input

Generalised Gibbs-stochastic	$\sum_{s,w} P(s',w\|s)\, e^{\beta(E_{s'}-E_s+w)}=1$
Second Law equality	$\langle e^{\beta(f_{s'}-f_s+w)}\rangle=1$
Generalised Jarzynski equality	$\langle e^{\beta(w-f_s)}\rangle=Z'_S$ c.f. Sagawa, Ueda (2011) Schumacher (2014) Manzano (2015)
Crooks equation (Petz recovery)	$\frac{p_{\mathrm{forward}}(w,s,s')}{p_{\mathrm{back}}(-w,s,s')}=e^{-\beta w}\frac{Z'_S}{Z_S}$

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Outlook and open questions

- Fluctuations of states
  - Probabilistic transformation (LOCC: Vidal 1999, Jonathan & Plenio 1999), Alhambra et. al. (2014); Renes (2015); Narasimhachar, Gour (2016)
- Generalised third laws
  - Reeb, Wolf (2013)
  - Thermal machines: Masanes, JO (2014)
- Fully quantum fluctuations (non-commuting case)
- Recovery Maps
  - Alhambra et. al. (2015), Åberg (2016), Alhambra et.al. (2016)
- Embezzlement of work? (Brandao et. al. 2015)
- Autonomous machines and clocks
  - Horodecki et. al. (2011), Woods et. al. (2016)

Probabilistic state transformations

$\rho \xrightarrow{\;\;\not w\;\;} \sigma$

$\rho \longrightarrow \rho' = p^{*}\sigma + (1-p^{*})X$

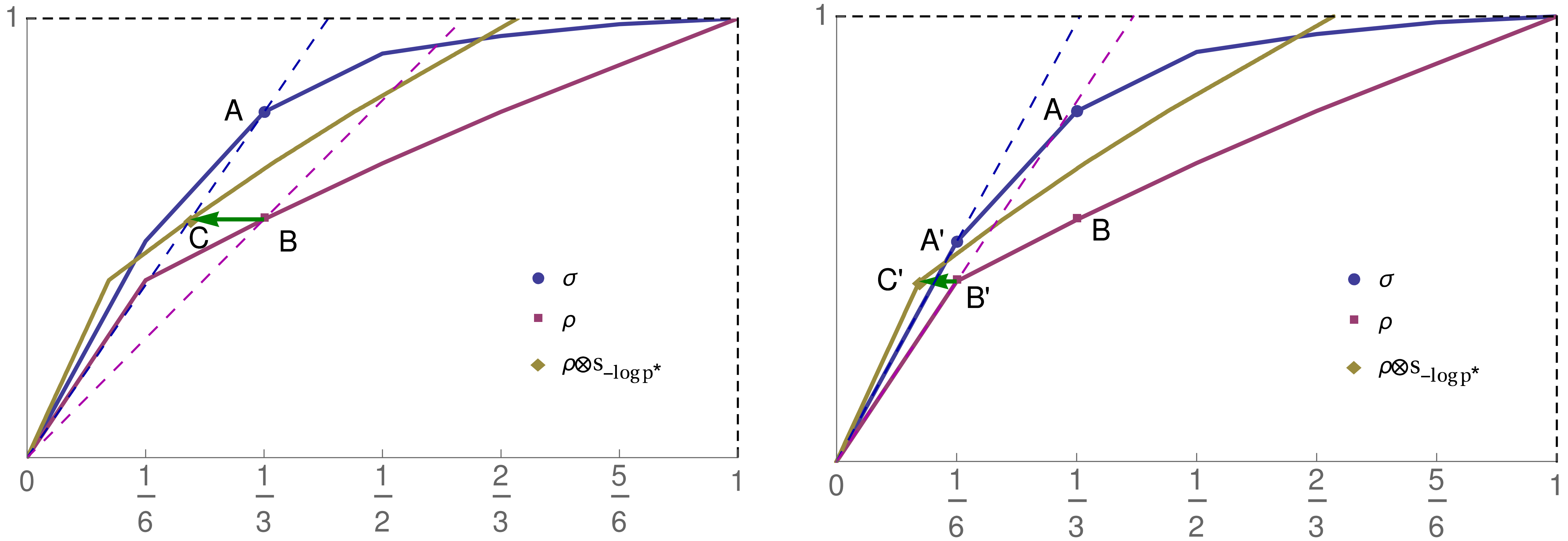
$$p^{*} = \min_{l \in 1,2 \ldots n} \frac{V_l(\rho)}{V_l(\sigma)}$$

$$V_l(\rho) = \sum_{s=1}^{l} p(s)$$

$$2^{W_{\rho \Rightarrow \sigma}} \leq p^{*} \leq 2^{-W_{\sigma \Rightarrow \rho}}$$

c.f. entanglement theory
G. Vidal (1999)
Jonathan, Plenio (1999)

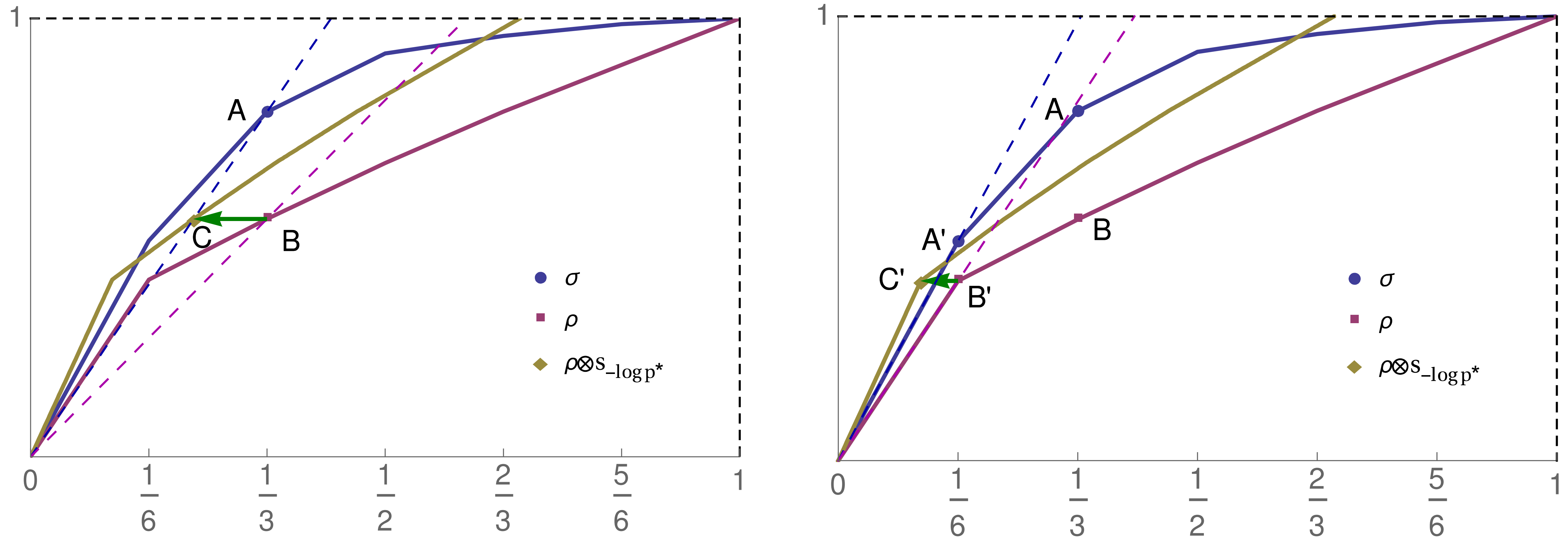
Probabilistic state transformations



$$p^* = \min_{l \in 1,2\ldots n} \frac{V_l(\rho)}{V_l(\sigma)}$$

$$2^{W_{\rho \Rightarrow \sigma}} \leq p^* \leq 2^{-W_{\sigma \Rightarrow \rho}}$$

Probabilistic state transformations



$$p^* = \min_{l \in 1,2\ldots n} \frac{V_l(\rho)}{V_l(\sigma)}$$

$$\sum_s T(s'|s)\, e^{-\beta E_s} \leq e^{-\beta E_{s'}}$$

$$\sum_s T(s'|s)\, p(s) \geq p^* p(s')$$

Renes (2015)

Quantitative third law
(Masanes, JO; to appear in Nat. Comm.)

Heat Theorem (Planck 1911): *when the temperature of a pure substance approaches absolute zero, its entropy approaches zero*

Unattainability Principle (Nernst 1912): *any thermodynamical process cannot attain absolute zero in a finite number of steps or within a finite time*

$$T' \geq \frac{\alpha T}{t^{2d+1}}$$

Thermal Machines

- Like Turing Machines
- In a finite time, they interact with a finite volume and inject a finite amount of work
- $t \geq \frac{1}{v} V^{1/d}$ $\qquad$ $t \geq \frac{1}{u} w_{max}$
- Bath of volume V has sub-exponential density of states Ω(E)

Outlook and open questions

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