From fully quantum thermodynamical identities to a second law equality

Alvaro Alhambra, Lluis Masanes, Jonathan Oppenheim, Chris Perry

Fluctuating States

Fluctuating Work
Thermodynamics is an information theory

$W = kT \log 2$

Maxwell
Szilard
Landauer
Bennett
What do we mean by $W=kT\log_2$? (consider the limit of perfect erasure)

A) $W=kT\log_2$ 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

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

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

\[
e^{\beta w_0} + e^{\beta w_1} = 1/(1 - \epsilon)
\]

\[
e^{\beta \tilde{w}_0} + e^{\beta \tilde{w}_1} = 1/\epsilon
\]
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 $\rightarrow$ 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 occurring. – 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

\[ \langle W \rangle \leq \Delta F \quad \text{In any cyclic process} \]
Free Energy

\[ F = \langle E \rangle - TS \]

\[ \langle W \rangle_{\text{rev}} = F(\rho_{\text{initial}}) - F(\rho_{\text{final}}) \]

\[ \rho_{\text{initial}} \rightarrow \rho_{\text{final}} \text{ iff } \langle W \rangle \leq \Delta F \]
Free Energy

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\[ \rho_{\text{initial}} \rightarrow \rho_{\text{final}} \text{ iff } \langle W \rangle \leq \Delta F \]

This is just the first order term of an equality!
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 $\rho_\beta$ and the measure is $F(\rho) - F(\rho_\beta)$.

But thermodynamics can also be irreversible.
What is Thermodynamics??

A resource theoretic approach: \( \Gamma \)

- \((\rho_s, H_s)\)
- adding **free states** \(\rho_B, H_B\)
- work system \(\rho_W, H_w\)

- 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 \(W\): \( [U, \Delta_w] = 0 \quad [\Delta_w, H_w] = i \)

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

- $H_{\text{int}}$
- $H(t)$
- Implicit battery: arbitrary $U$, and take $W = \text{tr} HP - \text{tr} HU p U^\dagger$
- 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? (2nd 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 $\rho$ to $\sigma$?
(2\textsuperscript{nd} law)

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

Many Second Laws
$H=0$ (Noisy Operations), no work

majorisation

$\rho \rightarrow \sigma \text{ iff } \rho > \sigma \quad p(1) \geq p(2) \geq p(3) \ldots \quad \sum_k p(k) \geq \sum_k q(k) \ \forall \ k$

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

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)

\[ q(s') = \sum_s P(s'|s)p(s) \]

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

\[ \sum_{s'} P(s'|s) = 1 \]
Fluctuating work

\[ \rho \rightarrow \sigma \text{ if f } \]

\[ \sum_{s,w} P(s',w|s) e^{\beta(E_s - E_w)} = 1 \]

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

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

\[ \sum_{s',s,w} P(s',w|s) e^{\beta(E_{s'} - E_s + w)} \frac{p(s)}{p(s')p(s')} = \sum_{s'} p(s') \]

\[ \langle e^{\beta(f_s - f_s + w)} \rangle = 1 \]

2nd law equality

Classical derivation: Seifert (2012)
Corrections to second law

\[ \langle e^{\beta (f_s' - f_s + w)} \rangle = 1 \]

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

\[ F = \langle f_s \rangle \]

\[ = \langle E \rangle - TS \]

\[ \langle f_s' - f_s + w \rangle \leq 0 \]

Standard 2\textsuperscript{nd} law

\[ W \leq \Delta F \]

\[ \sum_{k=1}^{N} \frac{\beta^k}{k!} \langle (f_s' - f_s + w)^k \rangle \leq 0 \]
Fluctuating work in erasure

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

\[ e^{\beta w_0} + e^{\beta w_1} = 1/(1 - \epsilon) \]

\[ e^{\beta \bar{w}_0} + e^{\beta \bar{w}_1} = 1/\epsilon \]

Same considerations apply to non-deterministic case
What do we mean by $W=kT \log_2$? (consider the limit of perfect erasure)

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no work to fluctuating work

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

doubly stochastic maps

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

majorisation

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

Gibbs-stochastic maps

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

thermo-majorisation

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

fluctuating work

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

linear program

\[
\sum_{s,w} P(s', w|s) e^{\beta(E_{s'} - E_s + w)} = 1
\]
Thermo-majorisation curves

\[ w(s, s') = \alpha_s - \gamma_{s'} \]
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Quantum identity

\[ tr_W \left[ \mathcal{F}_{H_s+H_w} \Gamma_{SW} \mathcal{F}_{H_s+H_w}^{-1} \right] 1_s \otimes \rho_W = 1_s \]

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

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

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

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

$$\text{tr}_W \left( J_{H_S'+H_W} \Gamma_{SW} J_{H_S+H_W}^{-1} \right) \left( 1_S \otimes \rho_W \right)$$

$$= \text{tr}_W J_{H_S'+H_W} \left( \text{tr}_B \left[ U J_{H_S+H_W}^{-1} \frac{e^{-\beta H_B}}{Z_B} (1_S \otimes \rho_W) U^\dagger \right] \right)$$

$$= \text{tr}_W J_{H_S'+H_W} \left( \frac{1}{Z_B} \text{tr}_B \left[ U J_{H_S+H_B+H_W}^{-1} (1_{SB} \otimes \rho_W) U^\dagger \right] \right)$$

$$= \text{tr}_W J_{H_S'+H_W} \left( \frac{1}{Z_B} \text{tr}_B \left[ J_{H_S'+H_B+H_W}^{-1} (U 1_{SB} \otimes \rho_W U^\dagger) \right] \right)$$

$$= \text{tr}_B W \left( \frac{-\beta H_B}{Z_B} U (1_{SB} \otimes \rho_W) U^\dagger \right)$$

$$= \text{tr}_B \left( \frac{-\beta H_B}{Z_B} 1_{SB} \right) = 1_S .$$

Masanes, JO (2014)
### Fully quantum identities

<table>
<thead>
<tr>
<th>Generalised Gibbs-stochastic</th>
<th>( \text{tr}<em>W \left( \mathcal{J}</em>{H_s' + H_W} \Gamma_{SW} \mathcal{J}_{H_s + H_W}^{-1} \right) (1_S \otimes \rho_W) = 1_S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Second Law equality</td>
<td>( \text{tr}<em>{SW} \left[ \left( \mathcal{J}</em>{T \ln \rho_s'} \mathcal{J}<em>{H_s' + H_W} \Gamma</em>{SW} \mathcal{J}<em>{H_s + H_W}^{-1} \mathcal{J}</em>{T \ln \rho_s}^{-1} \right) (\rho_s \otimes \rho_W) \right] = 1 )</td>
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<tr>
<td>Generalised Jarzynski equality</td>
<td>( \text{tr}<em>{SW} \left[ \left( \mathcal{J}</em>{H_W} \Gamma_{SW} \mathcal{J}<em>{H_s + H_W}^{-1} \mathcal{J}</em>{T \ln \rho_s}^{-1} \right) (\rho_s \otimes \rho_W) \right] = Z'_s )</td>
</tr>
<tr>
<td>Crooks equation(^1) (Petz recovery)</td>
<td>( \mathcal{J}<em>{H_s' + H_W} \Gamma</em>{SW} \mathcal{J}<em>{H_s + H_W}^{-1/2} = \Theta</em>{SW}^* )</td>
</tr>
</tbody>
</table>

\(^1\) 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
| Crooks equation (Petz recovery)| \[
\frac{p_{\text{forward}}(w, s, s')}{p_{\text{back}}(-w, s, s')} = e^{-\beta w} \frac{Z'_S}{Z_S}
\] |
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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

\[ \rho \xrightarrow{W} \sigma \]

\[ \rho \rightarrow \rho' = p^* \sigma + (1-p^*)X \]

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

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

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

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

\[ p^* = \min_{l \in 1, 2 \ldots n} \frac{V_l(\rho)}{V_l(\sigma)} \leq p^* \leq 2^{-W_{\sigma \Rightarrow \rho}} \leq 2^{W_{\rho \Rightarrow \sigma}} \]
Probabilistic state transformations

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

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

\[ \sum_s T(s'|s)p(s) \geq p^*p(s') \]

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

\[ t \geq \frac{1}{v} V^{1/d} \]

\[ t \geq \frac{1}{u} w_{max} \]

- Bath of volume V has sub-exponential density of states \( \Omega(E) \)
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