Single-shot thermo, lecture 13

- This is the last blackboard-maths-lecture.
  Next time: with computer + projector → current research.

Recap last lecture:

Introduced Rényi divergences $D_\alpha(p\|q) = \frac{\operatorname{sgn}\alpha}{\alpha-1} \log \sum_{i=1}^{n} p_i^\alpha q_i^{1-\alpha}$.
Via thermal Lorenz curves, we derived the

- work of formation: $(|E\rangle\langle E|, H) \xrightarrow{\text{thermal}} (\rho, H') \Rightarrow$
  [redacted] $\frac{1}{\beta} D_\infty(\rho\|\gamma') - \frac{1}{\beta} \log Z =: W_{form}$

- extractable work: $(\rho[\text{redacted}], H') \xrightarrow{\text{thermal}} (|E\rangle\langle E|, H) \Rightarrow$
  $E \leq \frac{1}{\beta} D_0(\rho\|\gamma') - \frac{1}{\beta} \log Z =: W_{extr}$.

Allowing small probability $\varepsilon > 0$ of error basically replaces these quantities by $D^\varepsilon_{[\text{redacted}]}(\rho\|\gamma')$ ("smoothed").

3.11. Catalytic thermal operations and the "second laws" of quantum thermodynamics

Recall: [redacted] $(\rho_S, H_S) \xrightarrow{\text{thermal}} (\rho'_{S'}, H'_{S'})$ iff for every $\varepsilon > 0$ there exists ρ'_ε with $\|\rho' - \rho'_\varepsilon\| < \varepsilon$ and a thermal operation $\mathcal{D}_\varepsilon$ with $\mathcal{D}_\varepsilon(\rho) = \rho'_\varepsilon$.

Now: allow additional catalyst that is not altered by the operation (cf. catalysts in the resource theory of nonuniformity).

<u>Def</u>: $(p_S, H_S) \xrightarrow{\text{cat-thermal}} (p'_{S'}, H'_{S'})$ iff for every $\varepsilon > 0$ there is p'_ε, $(r_\varepsilon, H_\varepsilon)$ with $\| p' - p'_\varepsilon \| < \varepsilon$ and a thermal op. D_ε with

$$D_\varepsilon(p \otimes r_\varepsilon) = p'_\varepsilon \otimes r_\varepsilon$$ [redacted]

catalyst (with its own Hamiltonian H_ε; we will see: can always choose $H_\varepsilon = 0$).

How can we decide whether $(p, H) \xrightarrow{\text{cat-thermal}} (p', H')$?

<u>Lemma</u>: Given prob. distr. p, p', q, q', where q and q' have full rank, the following conditions are equivalent:

(i) $D_\alpha(p \| q) \geq D_\alpha(p' \| q')$ for all $\alpha \in \mathbb{R}$

(ii) For every $\varepsilon > 0$ there exist prob. dist. r_ε, s_ε of full rank, a prob. dist. p'_ε and a stochastic map Λ_ε such that

1. $\Lambda_\varepsilon(p \otimes r_\varepsilon) = p'_\varepsilon \otimes r_\varepsilon$
2. $\Lambda_\varepsilon(q \otimes s_\varepsilon) = q' \otimes s_\varepsilon$
3. $\| p' - p'_\varepsilon \| \leq \varepsilon$.

Moreover, we can always have $s_\varepsilon = \eta$ for all ε (the max. mixed state)

Apply this to [redacted] q, q', s_ε Gibbs states corresponding to H, H', H_ε, and apply equivalences of previous lectures.

$\Longrightarrow$

$$\boxed{(p, H) \xrightarrow{\text{cat-thermal}} (p', H') \iff D_\alpha(p \| \gamma) \geq D_\alpha(p' \| \gamma') \ \forall \alpha \in \mathbb{R}}$$

Gibbs states

Special case $\alpha=1$ (cf. exercise sheet 1):

$$D(\rho\|\gamma) \geq D(\rho'\|\gamma') \Rightarrow$$

$$F(\rho)-F(\gamma) \geq F(\rho')-F(\gamma') \quad \text{free energy}$$

Motivates to define the α-free energies

$$\boxed{F_\alpha(\rho) := \frac{1}{\beta} D_\alpha(\rho\|\gamma) - \frac{1}{\beta}\log Z}$$

inv. temp. — Gibbs state, depends on Hamiltonian — partition function $\sum_i e^{-\beta E_i} = Z$

Cf. last lecture: F_∞: work of formation

F_0: extractable work

Now: $\boxed{(\rho, H) \xrightarrow{\text{cat-therm}} (\rho', H') \text{ if and only if } F_\alpha(\rho)-F_\alpha(\gamma) \geq F_\alpha(\rho')-F_\alpha(\gamma') \;\; \forall \alpha\in\mathbb{R}.}$

"Second laws of quantum thermodynamics", Brandão et al., arXiv:1305.5278 (2013)

$\alpha=1$: standard "second law": free energy must go down

(trivial Hamiltonians $H=H'=0$: entropy must go up).

<u>Proof sketch of lemma above</u>:

(ii) $\Rightarrow$ (i): Monotonicity: $D_\alpha(\phi(x)\|\phi(y)) \leq D_\alpha(x\|y)$

$$\Rightarrow D_\alpha(\rho'_\varepsilon \otimes r_\varepsilon \| q' \otimes s_\varepsilon) \leq D_\alpha(\rho\otimes r_\varepsilon \| q\otimes s_\varepsilon)$$

Homework: additivity

$$\Rightarrow D_\alpha(\rho'_\varepsilon\|q') + D_\alpha(r_\varepsilon\|s_\varepsilon) \leq D_\alpha(\rho\|q) + D_\alpha(r_\varepsilon\|s_\varepsilon)$$

Check finiteness of $D_\alpha(r_\varepsilon \| s_\varepsilon)$

$\Rightarrow D_\alpha(p'_\varepsilon \| q') \leq D_\alpha(p\|q)$

Continuity of D_α $\Rightarrow$ $D_\alpha(p'\|q') \leq D_\alpha(p\|q)$.

(i) $\Rightarrow$ (ii): Consider only the case that q, q' are <u>rational</u> (otherwise, approximation scheme).
and also that $D_\alpha(p\|q) \underset{\substack{\uparrow \\ \text{strictly larger}}}{>} D_\alpha(p'\|q')$ $\underline{\forall \alpha \in \mathbb{R}\setminus\{0\}}$.

assume this from now on.

Choose $N \in \mathbb{N}$ such that

$q = \left(\frac{d_1}{N}, \dots, \frac{d_k}{N}\right)$, all $d_i \in \mathbb{N}$. Similarly $q' = \left(\frac{d_1'}{N}, \dots, \frac{d_k'}{N}\right)$.

$\Gamma(p) := \bigoplus_i p_i \eta_i$, $\quad \eta_i = \left(\frac{1}{d_i}, \dots, \frac{1}{d_i}\right) \in \mathbb{R}^{d_i}$.

$\tilde{p} := \Gamma(p)$.

$\tilde{p}' := \Gamma'(p') = \bigoplus_i p_i' \eta_i'$. $\quad \eta_i' = \left(\frac{1}{d_i'}, \dots, \frac{1}{d_i'}\right) \in \mathbb{R}^{d_i'}$.

cf. <u>Gibbs rescaling</u>, exercise sheet 10.

$$D_\alpha(\tilde{p} \| \underset{\substack{\parallel \\ \left(\frac{1}{N}, \dots, \frac{1}{N}\right)}}{\eta_N}) \underset{\substack{\uparrow \\ \text{direct calculation}}}{=} D_\alpha(p\|q) > D_\alpha(p'\|q') = D_\alpha(\tilde{p}'\|\eta_N).$$

Problem 38 $\Rightarrow$ $H_\alpha(\tilde{p}) < H_\alpha(\tilde{p}')$.

Recall resource theory of nonuniformity / lecture 8:

Check also H_{Burg} $\Rightarrow$ $\tilde{p} \succ_T \tilde{p}'$.

$\Rightarrow \exists$ full-rank r, bistochastic ϕ:

$$\phi(\tilde{p} \otimes r) = \tilde{p}' \otimes r.$$

Set $\Lambda := (\Gamma'^{*} \otimes \mathbb{1}) \circ \phi \circ (\Gamma \otimes \mathbb{1})$,

where Γ'^{*} is the pseudoinverse of Γ':

$$\Gamma'^{*} \circ \underbrace{\Gamma'}_{\substack{\text{linear + injective,} \\ \text{but not bijective / no square matrix}}} = \mathbb{1}$$

ϕ stochastic $\Rightarrow \Lambda$ stochastic.

$$\begin{aligned}\Lambda(p \otimes r) &= \Gamma'^{*} \otimes \mathbb{1} \left(\phi(\Gamma(p) \otimes r) \right) \\ &= \Gamma'^{*} \otimes \mathbb{1} \left(\phi(\tilde{p} \otimes r) \right) \\ &= \Gamma'^{*} \otimes \mathbb{1} \left(\tilde{p}' \otimes r \right) = p' \otimes r.\end{aligned}$$

Similarly, $\Lambda(q \otimes \eta) = q' \otimes \eta$. $\square$

4. Recent generalizations

4.1. Grandcanonical resource theories

A system S is characterized by

- resource theory of nonuniformity: a state ρ_S
- res. th. of athermality: state ρ_S, Hamiltonian H_S
- "grand potential" res. th.: state ρ_S, Hamiltonian H_S, [redacted] particle number operator N_S.

Simplifying assumptions: $[H_S, N_S] = [S_S, H_S] = [S_S, N_S] = 0$. 6

Free states are of the form $\gamma = e^{-\beta(H - \mu N)}/Z$, (necessarily!),

free operations: • perform unitaries U on $S+E$, where

$$[U, H_S + H_E] = [U, N_S + N_E] = 0$$

• trace out subsystems,

• bring in free states.

ε-work value of a resource $R = (r, H_R, N_R)$: greatest W for which (state)

$$R + B_E \xrightarrow[\varepsilon]{\beta,\mu} B_{E+W}$$

free operation; accuracy of result in trace dist.

"battery" $B_E = (|E\rangle\langle E|, H, N)$ — finely spaced energies

ε-work cost of R: the least W such that

$$B_{E+W} \xrightarrow[\varepsilon]{\beta,\mu} R + B_E$$

Thm (Yunger-Halpern, Renes, 2014):

$$W^{\varepsilon}_{gain}(R) = \frac{1}{\beta} D^{\varepsilon}_{H}(r \| g_R)$$

grand canon. ensemble on R

$$\max_{\delta \in (0, 1-\varepsilon]} \left[\frac{1}{\beta} D_H^{1-\varepsilon-\delta}(r \| g_R) - \frac{1}{\beta} \log \frac{1}{\delta} \right] \leq W^{\varepsilon}_{cost}(R)$$

$$\leq \frac{1}{\beta} D_H^{1-\varepsilon}(r \| g_R) - \frac{1}{\beta} \log \frac{1-\varepsilon}{\varepsilon}$$

where $D^{\varepsilon}_{H}(S \| \gamma) = \min_{\substack{0 \leq Q \leq \mathbb{1} \\ tr(QS) \geq 1-\varepsilon}} tr(Q\gamma)$ is the "hypothesis-testing relative entropy"

This satisfies an "asymptotic equipartition property" (7)

$$\lim_{n\to\infty} \frac{1}{n} D_H^{\varepsilon}\left(r^{\otimes n} \| s^{\otimes n}\right) = D(r\|s) \quad \forall\, \varepsilon \in (0,1).$$

In fact,

$$\boxed{\begin{aligned} W^{\varepsilon}_{gain}\left(R^{\otimes n}\right) &= \frac{1}{\beta}\left[n \cdot D(r\|g_R) - O(\sqrt{n})\right] \\ W^{\varepsilon}_{cost}\left(R^{\otimes n}\right) &= \frac{1}{\beta}\left[n \cdot D(r\|g_R) + O(\sqrt{n})\right] \end{aligned}}$$

"onset of the thermodynamic limit"

4.2. Attempts of unification with fluctuation-dissipation theorems

Crooks' Theorem:

- forward protocol: parameter $\lambda(t)$ determines $H(\lambda(t))$ (time-dependent Hamiltonian).
  At $t=-\tau$: start in state $\gamma_{-\tau} = e^{-\beta H_{-\tau}}/Z$.
  Interaction with heat bath, satisfying certain assumptions.
  Stop at $t=\tau$; then let thermalize to γ_τ.

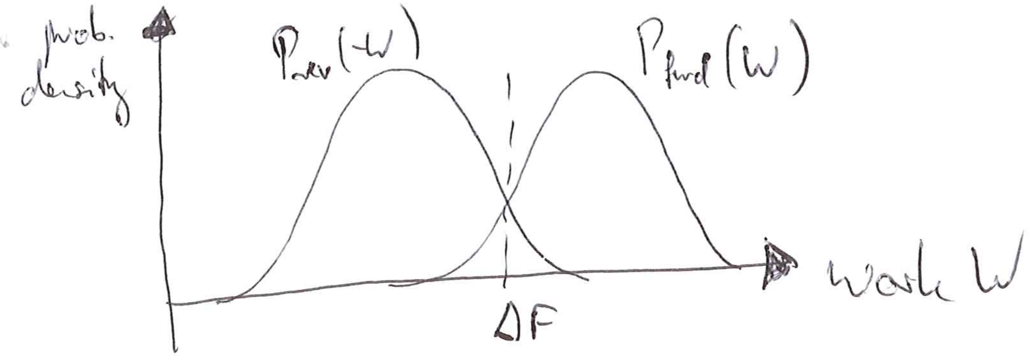
e.g. forward: compression; reverse: expansion.

- [redacted] Reverse protocol: run backwards.

Repeat many times $\Rightarrow$ prob. density $P_{fwd}(W)$ over [redacted] required work [redacted]
$P_{rev}(W)$ over gained work W.

$$\boxed{\frac{P_{fwd}(W)}{P_{rev}(-W)} = e^{\beta(W-\Delta F)}}.$$

$\Delta F = F(\gamma_\tau) - F(\gamma_{-\tau})$.



"Distribution over work": cf. our success prob. $\geq 1-\varepsilon$, Landauer erasure etc.

Lemma: $\frac{1}{\beta} D\left(P_{rev}(-W) \,\|\, P_{fwd}(W)\right) = \Delta F - \langle W \rangle_{rev}$,

where $\langle W \rangle_{rev}$ = average work gain from reverse process.

Note: $D(\cdot \| \cdot) \geq 0 \Rightarrow \langle W \rangle_{rev} \leq \Delta F$;

one obtains less work if $P_{rev}(-W)$ and $P_{fwd}(W)$ are more distinguishable (irreversibility).

Lemma: W_{min} := the least work that any reverse trial can output. Then

$$\frac{1}{\beta} D_\infty\left(P_{rev}(-W) \,\|\, P_{fwd}(W)\right) = \Delta F - W_{min}.$$

See the conceptual similarity to the results from the previous lecture...

More details: arXiv:1409.3878