3. The resource theory of quantum states out of thermal equilibrium ("resource theory of atehorality")

From now on, every quantum system $S$ has a state $\rho_S$ and a Hamiltonian $H_S$.

There are several well-known characterizations of Gibbs states (thermal states): $\rho_\beta = \exp(-\beta H_S)/Z$, $\beta = 1/(k_B T)$, $Z$ such that $\text{Tr}[\rho_\beta] = 1$:

- Textbook derivation (also of Boltzmann distribution): couple a small system to a large heat bath, and consider the microcanonical ensemble on the joint system.
- Jaynes' maximum entropy principle: $\rho_\beta$ maximizes von Neumann entropy $S(\rho)$ among all $\rho$ with fixed inner energy $U = \text{Tr}(\rho H_S)$.
- Past and Woronowicz, Lenard (1978): the Gibbs (and ground) states are exactly the completely passive states.

3.1. Passive and completely passive states

Note that we can draw work from excited states via unitary transformations:

$1\text{E}\rightarrow 1\rightarrow 1\text{E} = U(1\text{E})$
Def. A state $S_s$ on a system with Hamiltonian $H_s$ is passive if it is impossible to draw any work (on average) from the system via any unitary transformation, i.e.

$$\text{tr} (S_s H_s) \leq \text{tr} (U S_s U^\dagger H_s) \text{ for all } U \text{ unitary.}$$

Homework: it turns out that there are state $S_s$ that are passive, but such that $S_s \otimes S_s$ is not passive!

Def. $S_s$ is completely passive if $S_s \otimes n$ is passive for every $n \in \mathbb{N}$ (with respect to the Hamiltonian $H = H_s + \ldots + H_s$).

Theorem: $S_s$ is passive if and only if $[S_s, H_s] = 0$, i.e. $S_s = (p_1 \ldots p_m)$ in the Hamiltonian's eigenbasis (some eigenbasis of $H_s$), and $E_i > E_j \Rightarrow p_i < p_j$.

Interpretation: Passivity means that there are no coherences between distinct energy levels, and there is no “overpopulation” of levels.

Proof sketch: Choose a basis such that $E_1 \leq E_2 \leq \ldots \leq E_m$. $S_s = (E_1 \ldots E_m)$. 

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Consider $G = U S U^t$. We have to show that the energy $H(G H S)$ is minimal if and only if

$$G = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_m \end{pmatrix},$$

where we use the ordering $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$.

For any $G = U S U^t$, we can consider the diagonal elements $G_{ii} = \langle i | G | i \rangle$. The Schur-Horn Theorem tells us that

$$\left( \lambda_1, \ldots, \lambda_m \right) \succeq \left( G_{11}, \ldots, G_{mm} \right),$$

("the eigenvalues of a Hermitian matrix majorize its diagonal elements").

Suppose $a_1 > a_2 > \cdots > a_m > 0$ is a set of numbers, and we compare $\sum i \cdot a_i$ and $\sum G_{ii} \cdot a_i$. Since

$$\sum_{i=1}^m i \cdot a_i = a_m + \sum_{k=1}^{m-1} \left( \sum_{i=k}^m 2i \right) \left( a_k - a_{k+1} \right),$$

and similarly for $\sum G_{ii} \cdot a_i$, this proves

$$\sum_{i=1}^m G_{ii} \cdot a_i \leq \sum_{i=1}^m i \cdot a_i.$$

Use this for $a_i := E_m - E_i$, and set

$$A := E_m H - H S = \text{diag} (a_1, \ldots, a_m).$$
\[ \begin{align*}
\text{\( \Rightarrow \) } & \quad \text{Tr}(U_S U^+) = \text{Tr}(S S_S) = \text{Tr}(S E_S U U^+) - \text{Tr}(G_A) \\
& = E_m - \sum_{i=1}^{m} \langle q_i | a_i \rangle \geq E_m - \sum_{i=1}^{m} \langle q_i | a_i \rangle \\
& = \text{Tr} [ \text{diag} (d_1, \ldots, d_m) N_S ] .
\end{align*} \]

One can show that equality holds only if \([G_S, N_S] = 0\). \qed

**Theorem (Proof not here):**

\(S_S\) is completely passive if and only if

- either there is some \(\beta > 0\) such that \(S_S = \exp(-\beta H_S)/Z\),
- or \(S_S\) is a ground state, i.e.
\[ \text{Tr}(S_S H_S) \leq \text{Tr}(S_S' H_S) \forall S_S' . \]

3.2. **Definition of the resource theory of otherness**

Fix some inverse temperature \(\beta = 1/(k_B T) > 0\).
The agent is given some quantum state \(S_S\) on a finite-dimensional Hilbert space \(H_S\) with Hamiltonian \(H_S\).

Then be may

- introduce any extra system \(H_X\) with any Hamiltonian \(H_E\) in the thermal state \(E = \exp(-\beta H_E)/Z\);
- apply any energy-preserving unitary on any subsystem \(X\), i.e. unitaries \(U\) with \([U, H_X] = 0\);
- disregard subsystems, i.e. trace over/marginalize subsystems.

(Or any combination of these steps.)
Then every map he can implement can be written in the form

\[ E(S_S) = Tr_E \left[ U (S_S \otimes S_E) U^+ \right] \]

where \[ [U, H_{S,E}] = [U, H_S \otimes H_E + H_S \otimes H_E] = 0 \].

"thermal operation" \( (H_S \otimes H_E = H_S \otimes H_E) \)

For example

\[
\begin{array}{c|c|c}
S_S & H_S & S_E \\
\hline
1 & 2 & 3 \\
\end{array}
\]

\[ H = H_1 + H_2 + H_3 \]
\[ = N_S + N_E \]
\[ = N_S + N_E \]

(total Hamiltonian)

Differences to more standard approaches to thermodynamics:

- All sources and sinks of energy and entropy are explicitly accounted for;
- All interactions are due to the unitary \( U \), and not an interaction term in the total Hamiltonian \( H_{SE} \):

\[
\begin{array}{c}
S \\
\hline
\text{unitary } U \end{array} \quad \begin{array}{c}
S \otimes U \otimes U^+ \\
\hline
\text{external intervention} \end{array} \quad \begin{array}{c}
S_E \\
\hline
E \\
\end{array}
\]

Experimenter's choice/task to implement \( U \) efficiently.

If \([U, H_S + H_E] = 0\) then \( U \) can in principle be done without any work cost.

- No attempt made a priori to restrict the allowed operations to be physically realistic; experimenter assumed to have complete control.
yields ultimate restrictions on thermodynamic operations from quantum mechanics

→ turns out to be equivalent to other "more realistic" formulations

→ reproduces standard thermodynamics in the thermodynamic limit

→ no assumptions whatsoever on the concrete model.

Important observation: "Zeroth law"

If we allowed any other state (rather than the thermal state $\beta$) for free in the definition of the resource theory, then the theory would become trivial:

- arbitrary state transitions would be possible;
- one could draw an infinite amount of work from "nothing".

→ this is related to the fact that the thermal states (or ground states) are the only completely passive states!

If we restrict to fully degenerate Hamiltonians (i.e. all $H_S \equiv H$), we get back the resource theory of non-invariance.

3.3. Warm-up: how heat baths unlock state transitions

Ex: $N_S = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} = 2 \cdot \ket{2s} \bra{2s} + 3 \cdot \ket{3s} \bra{3s}$
Without extra system $E$, which unitaries would be allowed?

$[U, N_S] = 0 \iff U = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{i\theta} \end{pmatrix}, \quad \phi, \theta \in \mathbb{R}$.

This could only change the relative phase between energy levels, but not their populations:

$$U \left[ \alpha |2_s> + \beta |3_s> \right] = \alpha e^{i\phi} |2_s> + \beta e^{i\theta} |3_s>$$

$$= \alpha |2_s> + \beta e^{i(\theta - \phi)} |3_s>$$

Now introduce extra system $E$ with $H_E = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

Gibbs state $\rho_E = \begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta} \end{pmatrix} / (1 + e^{-\beta})$.

$$\implies N_S + N_E = \begin{pmatrix} 2 + 0 & 2 + 1 & 3 + 0 & 3 + 1 \\ 2 + 0 & 2 + 1 & 3 + 0 & 3 + 1 \end{pmatrix} = \begin{pmatrix} 2 & 3 & 3 & 4 \end{pmatrix}$$

$$= 2 \sum_1 |2,0 \times 2,0| + 3 \sum_1 |2,1 \times 2,1| + 3 \sum_1 |3,0 \times 3,0| + 4 \sum_1 |3,1 \times 3,1|.$$  

$[U, N_S + N_E] = 0 \iff U = \begin{pmatrix} e^{i\phi} & 0 & 0 & 0 \\ 0 & e^{i\theta} & 0 & 0 \\ 0 & 0 & (V)_{3 \times 3} & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix}$, $V^+V = I$.

This allows new transitions on $S$ (after tracing out $E$) that would be impossible without $E$.

Note that the energies in $N_E$ have to fit the energy gaps in $N_S$ to unlock transitions!