Single-shot thermo, lecture 9

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

From now on, every quantum system S has a state ρ_S and a Hamiltonian H_S.

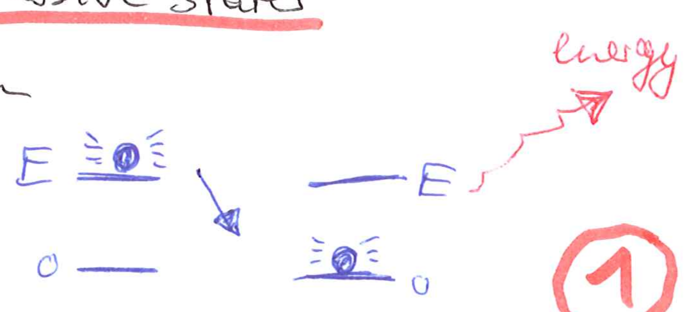
There are several well-known characterizations of Gibbs states (thermal states), $\gamma_\beta = \exp(-\beta H_S)/Z$, $\beta = 1/(k_B T)$, Z such that $\mathrm{tr}\, \gamma_\beta = 1$:

- Text-book 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: γ_β maximizes von Neumann entropy $S(\rho)$ among all ρ with fixed inner energy $U = \mathrm{tr}(\rho H)$
- Pusz 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:

$|E\rangle \mapsto |0\rangle = U|E\rangle$



Def.: A state ρ_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.

$$\mathrm{tr}(\rho_S H_S) \leq \mathrm{tr}(U \rho_S U^\dagger H_S) \text{ for all } U \text{ unitary.}$$

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

Def.: ρ_S is completely passive if $\rho_S^{\otimes n}$ is passive for every $n \in \mathbb{N}$ (with respect to the Hamiltonian $H = \underbrace{H_S + \ldots + H_S}_{n \text{ addends}}$).

Theorem: ρ_S is passive if and only if $[\rho_S, H_S] = 0$, i.e. $\rho_S = \begin{pmatrix} p_1 & & \\ & \ddots & \\ & & p_m \end{pmatrix}$ in the Hamiltonian's eigenbasis (some eigenbasis of H_S), and

$$E_i > E_j \Rightarrow p_i \leq p_j .$$

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

$$E_1 \leq E_2 \leq \ldots \leq E_m . \quad H_S = \begin{pmatrix} E_1 & & & \\ & E_2 & & \\ & & \ddots & \\ & & & E_m \end{pmatrix}$$

Consider $\sigma := U S_S U^\dagger$. We have to show that the energy $\mathrm{tr}(\sigma H_S)$ is minimal if and only if

$$[redacted]\ \sigma = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_m \end{pmatrix},$$

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

For any $\sigma = U S_S U^\dagger$, we can consider the diagonal elements $\sigma_{ii} = \langle i | \sigma | i \rangle$. The
SCHUR-HORN
Schur-Horn Theorem tells us that

$$(\lambda_1, \ldots, \lambda_m) \succ (\sigma_{11}, \ldots, \sigma_{mm})$$

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

Suppose $a_1 \geq a_2 \geq \ldots a_m \geq 0$ is a set of numbers, and we compare $\sum_i \lambda_i a_i$ and $\sum_i \sigma_{ii} a_i$. Since

$$\sum_{i=1}^{m} \lambda_i a_i = a_m + \sum_{k=1}^{m-1} \underbrace{\left(\sum_{i=1}^{k} \lambda_i \right)}_{\text{partial sums!}} \underbrace{(a_k - a_{k+1})}_{\geq 0},$$

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

$$\sum_{i=1}^{m} \sigma_{ii} a_i \leq \sum_{i=1}^{m} \lambda_i a_i$$

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

$$A := E_m \mathbb{1} - H_S = \mathrm{diag}(a_1, \ldots, a_m).$$

$$\Rightarrow \operatorname{tr}(U \rho_S U^\dagger) = \operatorname{tr}(\sigma H_S) = \operatorname{tr}(\sigma E_m \mathbb{1}) - \operatorname{tr}(\sigma A)$$

$$= E_m - \sum_{i=1}^{m} \sigma_{ii} a_i \geq E_m - \sum_{i=1}^{m} \lambda_i a_i$$

$$= \operatorname{tr}\left[\operatorname{diag}(\lambda_1, \ldots, \lambda_m) H_S \right].$$

One can show that equality holds <u>only if</u> $[\sigma, H_S] = 0$.

$\square$

<u>Theorem</u> (Proof not here):
ρ_S is completely passive if and only if
- either there is some $\beta \geq 0$ such that $\rho_S = \exp(-\beta H_S)/Z$,
- or ρ_S is a ground state, i.e.

$$\operatorname{tr}(\rho_S H_S) \leq \operatorname{tr}(\rho_S' H_S) \quad \forall \rho_S'.$$

3.2. Definition of the resource theory of athermality

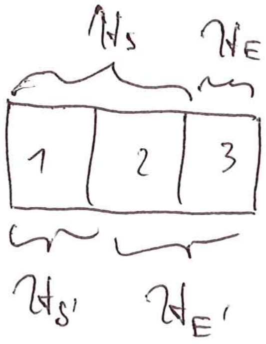
Fix some inverse temperature $\beta = 1/(k_B T) \geq 0$.
The agent is given some quantum state ρ_S on a finite-dimensional Hilbert space $\mathcal{H}_S$ with Hamiltonian H_S.
Then he may
- introduce any extra system $\mathcal{H}_E$ with any Hamiltonian H_E in the thermal state $\gamma_E := \exp(-\beta H_E)/Z$;
- apply any energy-preserving unitary on any subsystem X, i.e. unitaries U with $[U, H_X] = 0$,
- disregard [redacted] subsystems, i.e. trace over / marginalize subsystems.

(Or <u>any combination</u> of these steps.)

Then every map he can implement can be written in the form

$$\boxed{\begin{array}{c}\mathcal{E}(\rho_S) = \mathrm{Tr}_{E'}\left[U(\rho_S \otimes \gamma_E)U^\dagger\right] \\ \text{where } [U, H_{S,E}] = [U, H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E] = 0. \\ \text{"thermal operation"} \quad (\mathcal{H}_S \otimes \mathcal{H}_E = \mathcal{H}_{S'} \otimes \mathcal{H}_{E'})\end{array}}$$

For example

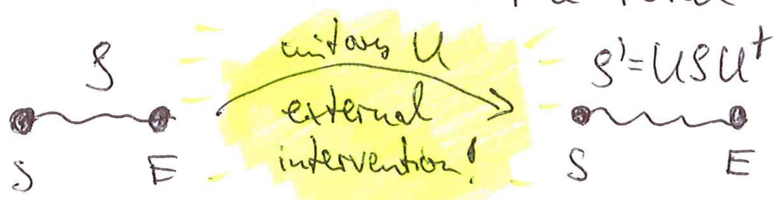


$$\begin{aligned} H &= H_1 + H_2 + H_3 \\ &= H_S + H_E \\ &= H_{S'} + H_{E'} \end{aligned}$$

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 <u>not</u> an interaction term in the total Hamiltonian H_{SE}:



Experimenter's choice / task to implement U efficiently.
If $[U, H_S + H_E] = 0$ then U can <u>in principle</u> be done without any work cost.

- No attempt made <u>apriori</u> 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: "zeroeth law"

If we allowed any othe state (rather than the thermal state γ) 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 [redacted] only completely passive states!

If we restrict to fully degenerate Hamiltonians (i.e. all $H_S \simeq \mathbb{1}$), we get back the resource theory of nonuniformity.

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

Ex.: $H_S = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} = 2 \cdot |2_S\rangle\langle 2_S| + 3 \cdot |3_S\rangle\langle 3_S|$

Without extra system E, which unitaries would be allowed?

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

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

$$U[\alpha |2_S\rangle + \beta |3_S\rangle] = \alpha e^{i\varphi} |2_S\rangle + \beta e^{i\theta} |3_S\rangle$$
$$\simeq \alpha |2_S\rangle + \beta e^{i(\theta-\varphi)} |3_S\rangle$$

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

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

$$\Rightarrow H_S + H_E = \begin{pmatrix} 2+0 & & & \\ & 2+1 & & \\ & & 3+0 & \\ & & & 3+1 \end{pmatrix} = \begin{pmatrix} 2 & & & \\ & 3 & & \\ & & 3 & \\ & & & 4 \end{pmatrix}$$

$$= 2|2,0\rangle\langle 2,0| + 3|2,1\rangle\langle 2,1| + 3|3,0\rangle\langle 3,0| + 4|3,1\rangle\langle 3,1|.$$

$$[U, H_S + H_E] = 0 \iff U = \begin{bmatrix} e^{i\varphi} & 0 & 0 & 0 \\ 0 & \multicolumn{2}{c}{\multirow{2}{*}{(V)}} & 0 \\ 0 & & & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{bmatrix}, \quad V^\dagger V = \mathbb{1}.$$

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

Note that the energies in H_E have to fit the energy gaps in H_S to unlock transitions!