The energy-entropy diagram as a fundamental tool of thermodynamics

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We consider a system with finite-dimensional Hilbert space $\mathbb{C}^d$ and Hamiltonian H. A state ρ has energy $E(\rho) = \mathrm{tr}(\rho H)$ and entropy $S(\rho) = -\mathrm{tr}(\rho \log \rho)$.

Theorem

For states ρ and σ, the following are equivalent:

1. There exists an ancilla system of size $O(\sqrt{n \log n})$ with state η and Hamiltonian H_{anc} satisfying $\|H_{\mathrm{anc}}\| \leq O(n^{2/3})$ as well as an energy-preserving unitary U such that

$$\left\| \mathrm{Tr}_{\mathrm{anc}}\left[U(\rho^{\otimes n} \otimes \eta) U^\dagger \right] - \sigma^{\otimes n} \right\|_1 \overset{n\to\infty}{\longrightarrow} 0.$$

2. There exists an ancilla system of size $o(n)$ with states η and ν and Hamiltonian H_{anc} satisfying $\|H_{\mathrm{anc}}\| \leq o(n)$ as well as energy-preserving unitaries U and V such that

$$\left\| \mathrm{Tr}_{\mathrm{anc}}\left[U(\rho^{\otimes n} \otimes \eta) U^\dagger \right] - \mathrm{Tr}_{\mathrm{anc}}\left[V(\sigma^{\otimes n} \otimes \eta) V^\dagger \right] \right\|_1 \overset{n\to\infty}{\longrightarrow} 0.$$

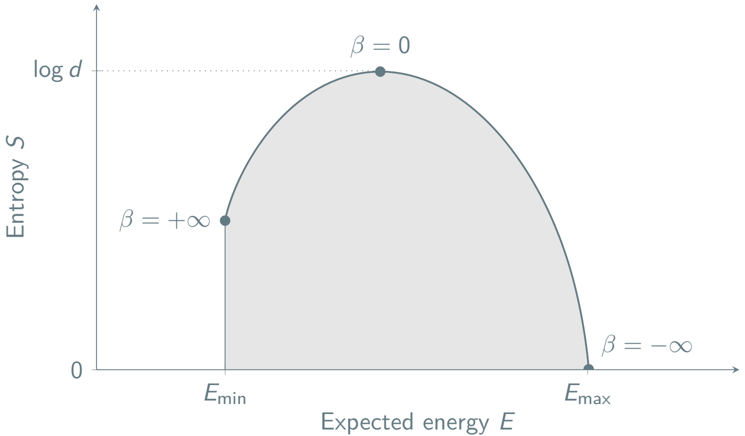
3. The states have equal energy and entropy,

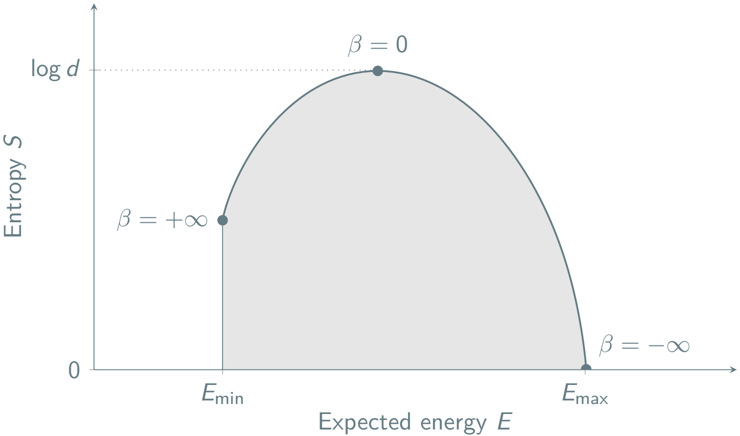
$$E(\rho) = E(\sigma), \qquad S(\rho) = S(\sigma).$$

Definition

A **macrostate** is an equivalence class of states with respect to asymptotic interconvertibility as in the theorem.

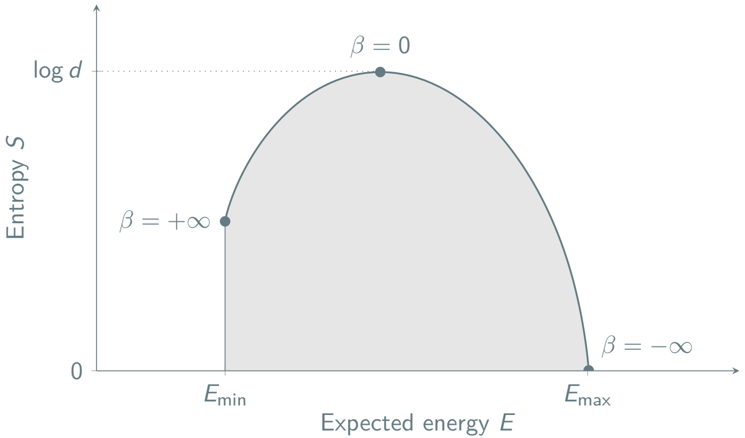
$\Rightarrow$ Macrostates correspond to pairs (E, S) that can be jointly achieved. The set of macrostates makes up the **energy-entropy diagram**:





The thermal states $\tau_\beta = Z_\beta^{-1} e^{-\beta H}$ form the upper boundary.

But the diagram also describes thermodynamics arbitrarily far away from equilibrium!



The energy-entropy diagram is the set of all points (E, S) that satisfy $S \geq 0$ and the inequality

$$A_\beta := \beta E - S + \log Z(\beta) \geq 0$$

for every β. The **athermality** A_β is essentially the free energy $E - \beta^{-1} S$.

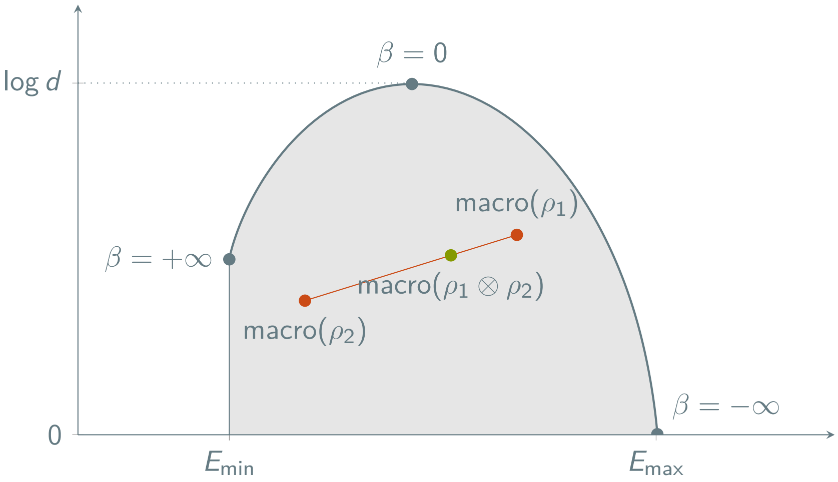
Given a state ρ on N copies of the system $(\mathbb{C}^d)^{\otimes N}$, we renormalize energy and entropy for convenience,

$$\text{macro}(\rho) := \left(\frac{E(\rho)}{N}, \frac{S(\rho)}{N}\right).$$

Like this, we can represent systems of any amount of substance in the energy-entropy diagram.

Now forming a total system out of ρ_1 on $(\mathbb{C}^d)^{\otimes N_1}$ and ρ_2 on $(\mathbb{C}^d)^{\otimes N_2}$ results in a **convex combination** of normalized macrostates,

$$\text{macro}(\rho_1 \otimes \rho_2) = \frac{N_1}{N_1 + N_2}\text{macro}(\rho_1) + \frac{N_2}{N_1 + N_2}\text{macro}(\rho_2).$$



$\log d$
$\beta = 0$
$\beta = +\infty$
$\mathrm{macro}(\rho_1)$
$\mathrm{macro}(\rho_1 \otimes \rho_2)$
$\mathrm{macro}(\rho_2)$
$\beta = -\infty$
0
E_{min}
E_{max}

So *what is it all good for*? For example, let's determine how much work can be extracted out of many copies $\rho^{\otimes n}$ of a given state ρ.

Definition

Extraction of work is coupling the system to an **empty battery**,

$$\rho^{\otimes n} \otimes |E_1\rangle\langle E_1|^{\otimes \ell}, \tag{1}$$

performing a thermodynamic transformation, and obtaining a final state of the form

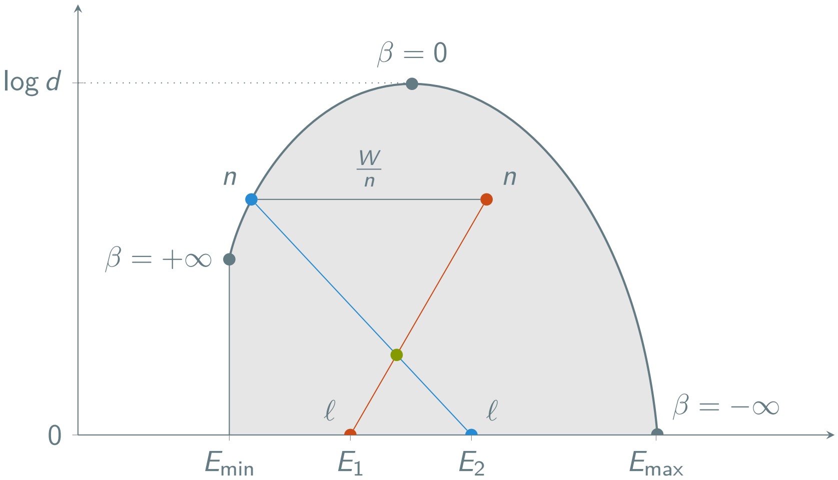
$$\sigma^{\otimes n} \otimes |E_2\rangle\langle E_2|^{\otimes \ell} \tag{2}$$

with $E_2 > E_1$. The amount of work extracted is then

$$\ell \cdot (E_2 - E_1).$$

The maximal amount of work that can be extracted can now be easily read off geometrically from the energy-entropy diagram!

The maximal extracted work per copy is $\frac{W}{n}$, given by the horizontal distance to the boundary:



A similar analysis applies to the case of a heat engine. Let's take the initial state to be

$$\tau_{\beta_{\text{cold}}}^{\otimes n} \otimes \tau_{\beta_{\text{hot}}}^{\otimes m} \otimes |E_1\rangle\langle E_1|^{\otimes \ell},$$

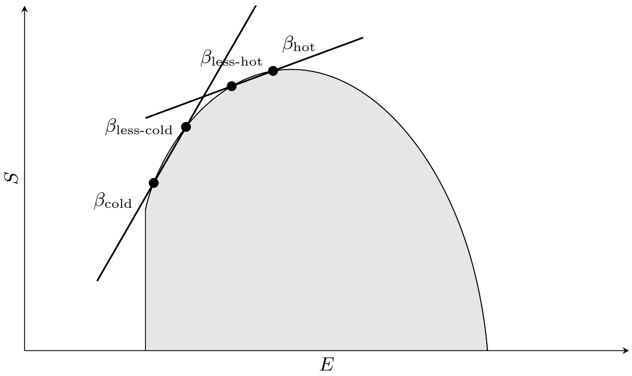
and by symmetry the final state

$$\tau_{\beta_{\text{less-cold}}}^{\otimes n} \otimes \tau_{\beta_{\text{less-hot}}}^{\otimes m} \otimes |E_2\rangle\langle E_2|^{\otimes \ell},$$

$\Rightarrow$ Determine $\beta_{\text{less-cold}}$ and $\beta_{\text{less-hot}}$ such that the final macrostate coincides with the initial macrostate.

- This model of a heat engine *abstracts away* from concepts of "working body" or "cycle".
- Instead, we only need to consider the initial and final states!
- There exists **some** protocol transforming one into the other if and only if these states define the same macrostate.

Let $\beta_{\text{eff-cold}}$ and $\beta_{\text{eff-hot}}$ correspond to the slopes in



Then a straightforward computation determines the efficiency to be

$$\eta = 1 - \frac{\beta_{\text{eff-hot}}}{\beta_{\text{eff-cold}}}.$$

For very small battery $\ell \ll n, m$, this approaches the Carnot efficiency!