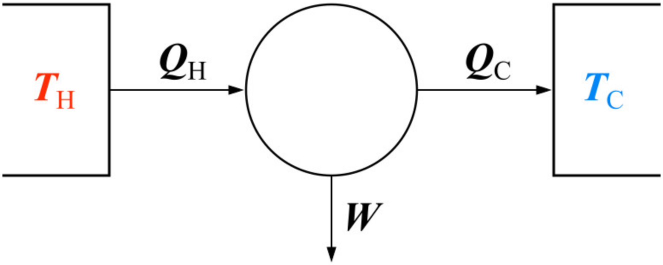
A simple formalism for resource efficiency in thermodynamics

arXiv:1607.01302, arXiv:1504.03661

November 2017

Heat engines



Effect of a heat engine with efficiency η:

$$1\,\mathsf{J}\ \text{heat at}\ T_H \longrightarrow \eta\,\mathsf{J}\ \text{work}\ +\ (1-\eta)\,\mathsf{J}\ \text{heat at}\ T_C$$

Formally, this is analogous to a chemical reaction equation like

$$\mathrm{N_2} + 3\,\mathrm{H_2} + \mathrm{Os} \longrightarrow 2\,\mathrm{NH_3} + \mathrm{Os}.$$

Similar equations appear in many other contexts!

- As a toy example, consider carpentry,

$$2\,\text{planks} + 8\,\text{nail} \longrightarrow \text{table}.$$

- Or the mixing of paint,

$$1\,\text{bucket yellow} + 1\,\text{bucket red} \longrightarrow 2\,\text{bucket orange}.$$

- In information theory, given a noisy channel of capacity C,

$$1\,\text{use of channel} \longrightarrow C\,\text{bits of communication}.$$

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There is a general theory of resource efficiency (under development) of which all of these equations are instances.

Let me explain how this works in the case of thermodynamics—arbitrarily far away from equilibrium!

To keep things simple, let us consider the macroscopic limit of $n \gg 1$ identical systems with single-system Hamiltonian H.

Definition

A **macrostate** is a pair of values (E, S), such that there is a state ρ with entropy $S = S(\rho)$ and expected energy $E = E(\rho) = \mathrm{tr}(\rho H)$.

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This is justified by the following result:

Theorem

Given two states ρ and σ, identical copies $\rho^{\otimes n}$ and $\sigma^{\otimes n}$ are interconvertible by **energy-preserving unitaries** and a small ancilla system as $n \to \infty$ if and only if

1. $S(\rho) = S(\sigma)$, and
2. $E(\rho) = E(\sigma)$.

A derivation from physical first principles remains to be found.

The energy-entropy diagram

The set of macrostates (E, S) forms the **energy-entropy diagram**. What does it look like?

For given $E \in [E_{\mathrm{min}}, E_{\mathrm{max}}]$, the possible values for S are all those between:

- 0, on a suitable pure superposition of energy eigenstates,
- The entropy of the **thermal state** τ_β with energy $E(\tau_\beta) \overset{!}{=} E$.

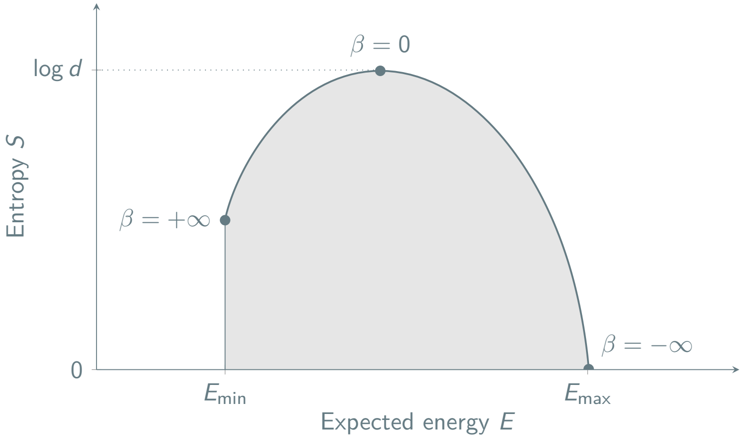
Quick reminder on thermal states:

$$\tau_\beta = Z(\beta)^{-1} e^{-\beta H}, \qquad Z(\beta) = \mathrm{tr}(e^{-\beta H}),$$

$$E(\tau_\beta) = \mathrm{tr}(H\tau_\beta) = -\frac{\partial \log Z(\beta)}{\partial \beta},$$

$$S(\tau_\beta) = -\mathrm{tr}(\tau_\beta \log \tau_\beta) = \beta E(\tau_\beta) + \log Z(\beta).$$

Here's a generic energy-entropy diagram:

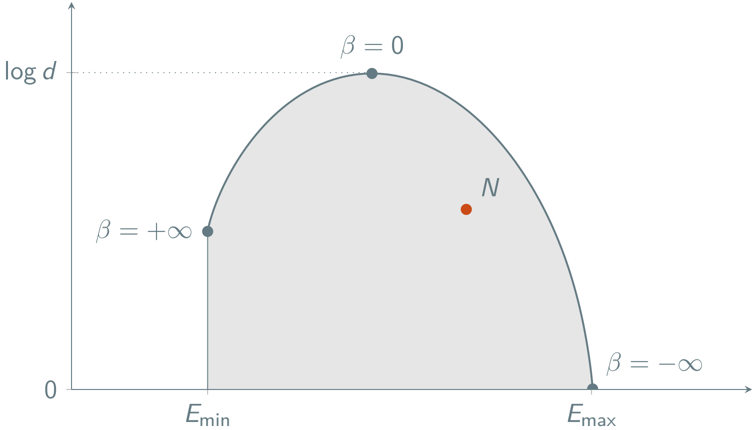


It is the set of all points (E, S) that satisfy $S \geq 0$ and the inequality

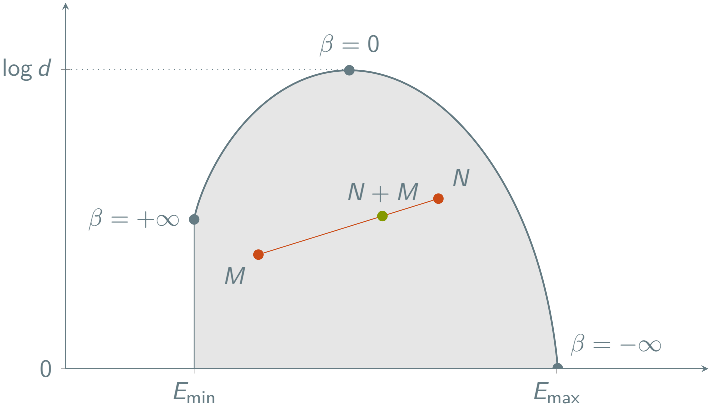
$$\beta E - S + \log Z(\beta) \geq 0$$

for every β.

It is useful to consider a third dimension, which measures **amount of substance** N, by which we mean number of copies of the system. Instead of drawing this in $\mathbb{R}^3$, we can also use normalized energy and entropy and label the macrostate by N,



Energy and entropy are additive under combining systems. So given a system of size N and one of size M, the total system is described by a **convex combination** of normalized macrostates:



In this sense, thermodynamics is a **general probabilistic theory**!

Let's see how to use this to answer questions like:

Problem

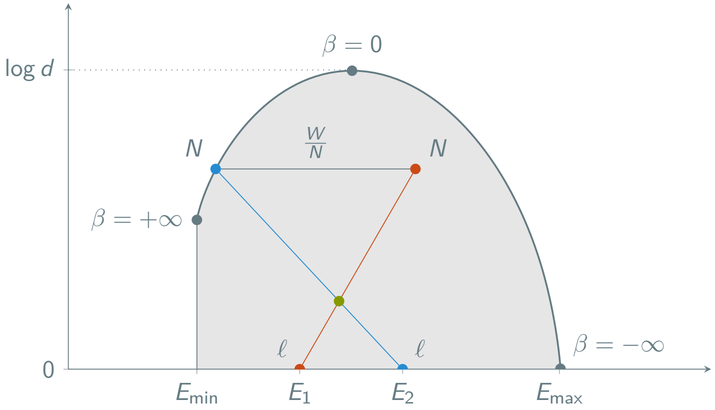
How much work can maximally be extracted from (many copies of) a given state?

Setup:

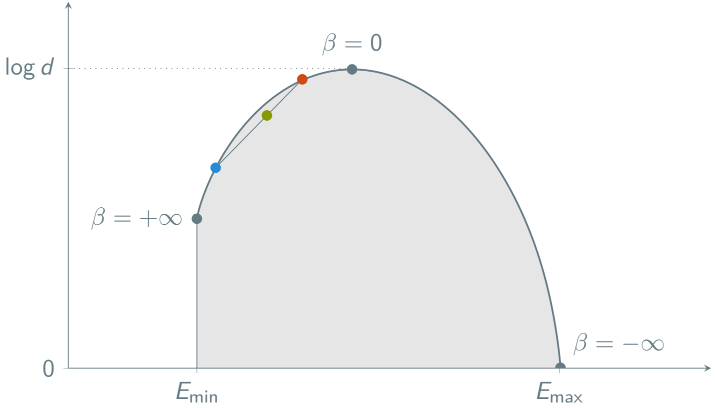
- Couple the system of size N to a **battery** system of size ℓ, which is initially in a pure state $|E_1\rangle$.
- Apply some energy-preserving unitary to the total system, such that the battery ends up in a pure state $|E_2\rangle$ with $E_2 > E_1$.

The extracted work is then $\ell(E_2 - E_2)$.

The maximal extractable work W is N times the horizontal distance to the boundary:



For example, the initial state may itself be a combination of two thermal baths which are finite (but large),



$\Rightarrow$ We can compute the maximal efficiency of a heat engine with **finite** baths. This picture is very abstract: it applies regardless of the protocol used to implement the transformation, using a “working body” or any other mechanism.

- It is possible to extend this picture to include other thermodynamic quantities, like volume, angular momentum, etc, as long as they commute.
- The energy-entropy diagram then becomes a higher-dimensional convex set, again bounded above by the equilibrium states.
- The noncommuting case is technically more challenging, but it could be that the results stay the same.
- Which quantities need to be considered depends on the physical context in a way that I don't understand.

- There are many other analogous situations like channel coding, quantum entanglement under LOCC, etc.
- All of these cases should be instance of a general toolbox for resource efficiency, involving convex cones to describe resource efficiency asymptotically.
- Generally applicable definitions and methods are still under development.
- In some cases, the convex cones will be one-dimensional (e.g. in classical channel coding).
- In other cases, they will be infinite-dimensional (e.g. for pure bipartite entanglement under LOCC without approximations).