4/2018

Landauer's Principle; Thermodynamics & Information.

[What does information theory have to say about thermodynamics ?]

Motivation.

* Understand the thermodynamics of computation
* Resolution of the paradox of Maxwell's demon
* Role of the observer in thermodynamics
* To what extent is thermodynamics and the second law universal ?
  (Thermodynamics is usually presented as a theory of gases, how come we can apply it to solid state physics, chemistry, electromagnetic radiation ("gas of photons"), even black holes.. ?)
* Robust tools to study quantum, small-scale thermodynamics ("finer-grained thermodynamics") — resource theory of thermodynamics.

References.

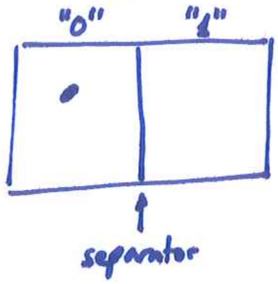
- Feynman lectures on computation, Chap. 5
- C. Bennett, Notes on Landauer's principle, reversible computation and Maxwell's demon (2003)
- C. Bennett, The thermodynamics of computation — a review (1982)

I. Thermodynamics of computation.

Question: Do computers require energy to operate, even in principle?

1. The Szilárd engine. (Szilárd, 1929)

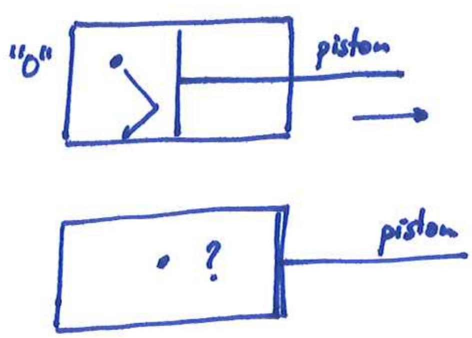
Consider a single-particle gas enclosed in a box:



The particle can be on the left ("0") or on the right ("1") side, representing one bit of information.

(It is OK to consider the single particle as a gas here, because we will be considering very slow operations, and will be averaging over long periods of time.)

* Extract work from knowledge. Say we know that the particle is on the left:



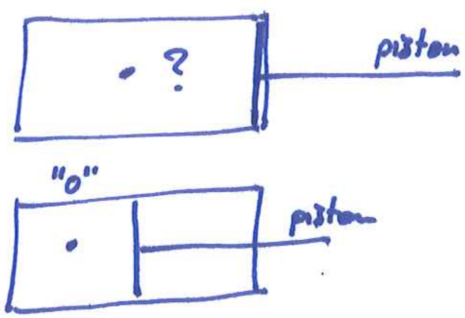
1. Attach piston to separator
2. Let the 1-particle gas expand isothermally, extracting work
   - keep system in contact with environment at temperature T

We can calculate the amount of work extracted using the corresponding formula for the isothermal expansion of an ideal gas:

$$\underline{W_{extr.}} = \underset{\substack{\uparrow \\ \text{Boltzmann's} \\ \text{constant}}}{k}T \cdot \ln\left(\frac{V_{final}}{V_{init}}\right) = \underline{kT \cdot \ln(2)}$$

But the particle can now be anywhere: We lost the knowledge of the bit value.

* Operation RESET TO ZERO. If we don't know where the particle is, we can reset it to the left side ("0") by compressing the gas:



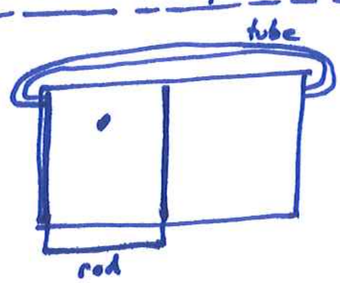
We need to perform work:

$$\underline{W_{RESET}} = kT \cdot \ln\left(\frac{V_{final}}{V_{init}}\right) \underline{= -kT \ln(2)}$$

(reverse of the work extraction operation)

→ We can trade the knowledge of the bit's value for $kT\ln(2)$ work.

* The NOT operation. We can interchange the "0" and "1" states:



1. Insert 2 separators, in the middle and on the left edge. Connect them with a rigid rod.

2. Give a nudge to the right. The 2 separators will set in motion and arrive to the other side, carrying the particle if it was in the "0" state.

We can modify this setup so that it also sends a particle in the "1" state to the "0" state: Attach a tube of negligible volume to both ends of the box. If the particle is initially in the "1" state, it will pass through the tube back into the "0" state, as the separators move over to the right side.

→ The NOT operation costs no work!

* Logically reversible operations. These can be carried out at no work cost. (Logically reversible = there is an unambiguous inverse)

Example: C-NOT (using 2 boxes)

00 → 00
01 → 01
10 → 11
11 → 10

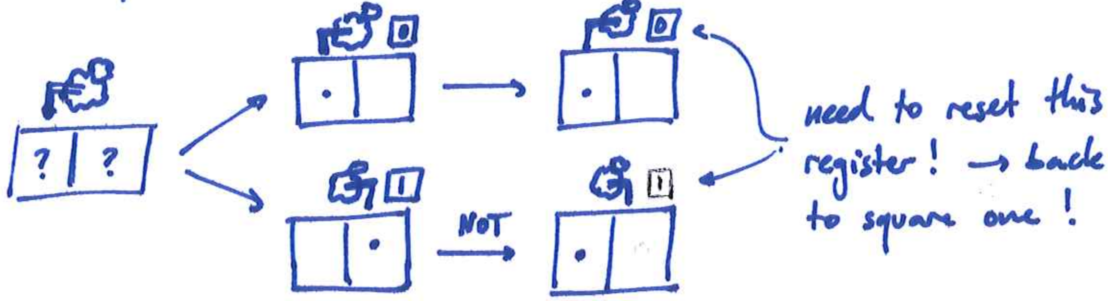
Logically reversible operations cause no entropy change, because the number of possible configurations does not change. (Explicit setups become ugly and cumbersome...)

* What about measurements?

Candidate procedure for RESET: measure the location of the particle, and perform a NOT operation if it is in the "1" state.

In order to account for work fairly, we need to design an autonomous machine which is restored to its initial state at the end of the operation. (otherwise, it could "extract work" by depleting an internal battery.) The machine has to work correctly for both input states.

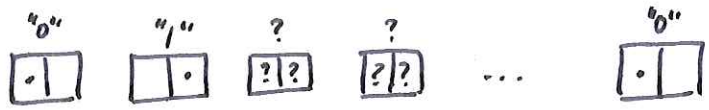
If the machine makes a measurement, then it carries a record of the outcome.



The measurement itself can be carried out at no work cost in principle. For instance: do a C-NOT operation with a second box initialized in the "0" state.

2. The work value of information.

Consider an array of n boxes, each in either an unknown state or a known "0" or "1" state.



How much work do we need to invest to reset the full array to zero?

known "0" boxes: ✓

"1" boxes: perform NOT ✓

unknown boxes: pay $kT \cdot \ln(2)$ per box

total work required $= m \cdot kT \ln(2)$

m ← # of unknown boxes

What is the information content of this array of boxes?
(Information content = how much we learn by looking at the bit values, "ability to surprise", "unknown information")

known boxes: information content $= 0$
unknown boxes: information content $= 1$ bit

total information content $= m$ bits

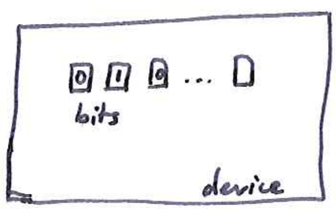
INFORMATION CONTENT $= m$ bits $\xleftrightarrow{\times kT \ln(2)}$ WORK NEEDED TO RESET $= m \cdot kT \ln(2)$

Even better: If there are correlations between boxes (e.g. two boxes are unknown, but are known to be in the same state: 00 or 11, ~~01~~ ~~10~~), these correlations can be exploited to reduce the work cost of resetting. Correspondingly, the information content is lower! (→ exercise)

Given an array of boxes, we can also ask how much work we can extract from the array. Can extract $kT\ln(2)$ work for each known box
total $= (n-m)\cdot kT\ln(2)$. (Lack of) information has a "fuel value"!

3. Landauer's Principle. (Landauer, 1961)

Consider a macroscopic device which stores information.



For instance, each bit is realized by a ferromagnet

$\boxed{0} = \boxed{\begin{matrix}\uparrow\uparrow\uparrow\uparrow\ldots \\ \ldots\uparrow\uparrow\uparrow\end{matrix}}$ $\qquad$ $\boxed{1} = \boxed{\begin{matrix}\downarrow\downarrow\downarrow\ldots \\ \ldots\downarrow\downarrow\downarrow\end{matrix}}$

As macroscopic objects, the device (and its bits) is a thermodynamic system (eg. it has a temperature). There are many microscopic configurations which are irrelevant macroscopically → these form the device's thermodynamic entropy $S = k\cdot\ln(\#\text{ available microscopic configurations})$.

Suppose we would like to reset an unknown bit to zero. Forget that we are processing information, and count the available microstates:

$$\text{before: } \underbrace{2}_{\text{possible bit values}} \times \underbrace{N_{micro}}_{\#\text{of microscopic microstates}} \longrightarrow \text{after: } \underbrace{1}_{\text{only one possible bit value}} \times \underbrace{N'_{micro}}_{\text{(might have changed)}}$$

But the laws of physics are reversible. (Liouville's theorem: the phase space volume remains constant.) $\rightarrow$ the available # of microscopic configurations cannot have decreased.

$\rightarrow$ N_{micro} must have increased: $N'_{micro} = 2 \cdot N_{micro}$.

Causes entropy difference: $\Delta S = k \ln(N'_{micro}) - k \ln(N_{micro}) = k \ln(2)$

$\rightarrow$ heat dissipated $\Delta Q \geq T \Delta S = \underline{kT \cdot \ln(2)}$

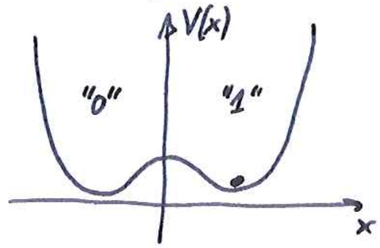
$\rightarrow$ this energy must be provided in the form of work.

The same argument applies to any logically irreversible computation, but not to logically reversible operations.

Landauer's Principle: Logically irreversible computation is necessarily dissipative, i.e., it must be accompanied by an entropy increase in the environment. For example, resetting one bit of information ("erasure of information"), with an environment at temperature T, costs $kT \ln(2)$ work.

Examples.

* Szilárd engine.
* Bistable potential well. The particle sits in the left or right well $\rightarrow$ one bit of information.

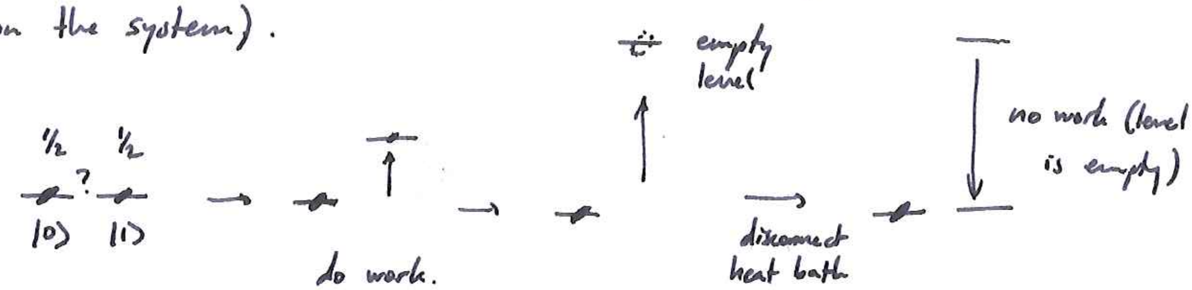


RESET TO ZERO can't be done with reversible dynamics! (We can't merge two trajectories into a single one.) But we can RESET TO ZERO if we turn on dissipation (e.g., friction).

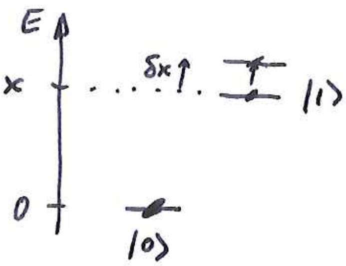
* Hamiltonian with 2 degenerate levels. (our first quantum example!)

How can we RESET TO ZERO an unknown input state? (⚠ "unknown input state" = statistical mixture ≠ superposition $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$!!)

Procedure: lift second level to ∞ energy isothermally (= in contact with a heat bath at temperature T, which imposes a Gibbs distribution on the system).



How much work? During the isothermal process:



$$\delta W = p_1(x) \cdot \delta x$$

$\uparrow$ prob. that $|1\rangle$ is occupied (work only done if $|1\rangle$ is occupied)

$$p_1(x) = \frac{e^{-\beta x}}{1+e^{-\beta x}}$$ imposed by heat bath $\left[p_i = \frac{e^{-\beta E_i}}{Z}\right]$

$\left(\beta = \frac{1}{kT}\right)$

<u>Total work</u> $= \int_{\text{init}}^{\text{final}} \delta W = \int_0^\infty p_1(x)\,dx = \int_0^\infty \frac{e^{-\beta x}}{1+e^{-\beta x}}\,dx$ set $y = 1+e^{-\beta x}$, $dy = -\beta e^{-\beta x}dx$

$$= -\beta^{-1}\int_{x=0}^{\infty}\frac{dy}{y} = -\beta^{-1}\cdot \ln(y)\Big|_{x=0}^{\infty} = -\beta^{-1}(0 - \ln(2))$$

$$= \underline{kT\ln(2)}$$

Concrete example: spin-½ particle in a magnetic field.

Remarks (on Landauer's principle).

* independent of hardware. This is a fundamental limit for irreversible computation.

* any (classical) computation can be made logically reversible, by outputting a copy of the input. So any (classical) computation can be carried out at no work cost, in principle.

* In practice, there is a trade-off between execution speed and energy requirement. (In our examples, the isothermal processes had to be carried out infinitely slowly.)

* $kT \ln(2) \sim 3 \cdot 10^{-21}$ J at room temperature
~ 0.02 eV very small!

Current technology is still several orders of magnitude away.

CMOS $\rightarrow \sim 10^7 - 10^9 \cdot kT$

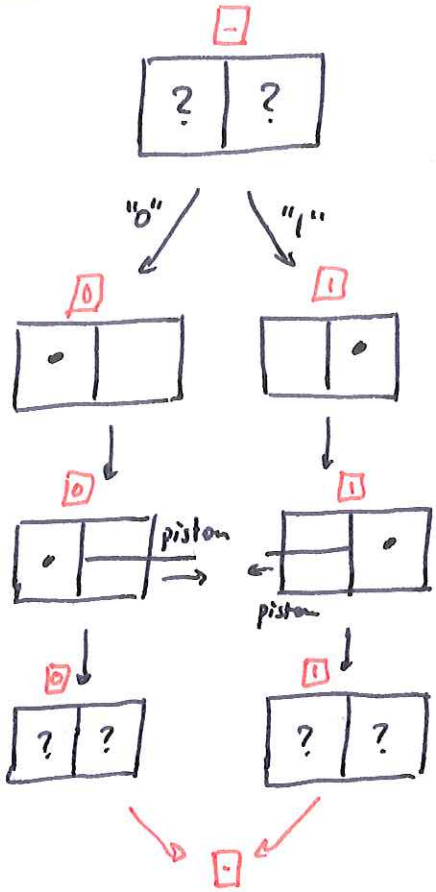
neuron discharge $\rightarrow \sim 10^{11}$ kT

DNA transcription $\rightarrow \sim 20-100$ kT /nucleotide

(biological processes can be very energy efficient!)

II. The role of information in thermodynamics.

1. Apparent paradox with a Szilárd engine. (Bennett '82)



Szilárd engine, in unknown state

measurement

know particle location

attach piston, extract $kT\ln(2)$ work in either case

remove piston, insert separator in the middle of the box

→ back to initial state!

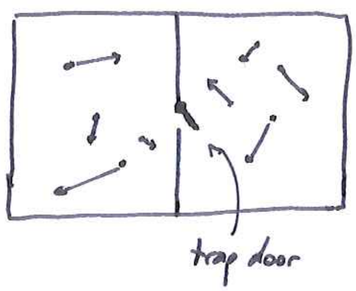
extract arbitrary work for free ??!

No: We need to account for the information about the measurement outcome, which we must have stored somewhere.

To reset this register back to its initial state, we pay back the $kT\ln(2)$ work that we extracted. (Landauer's principle)

2. Maxwell's demon. (Maxwell, 1871; solved: Bennett, early 80's)

* Maxwell's idea: a small, intelligent being can sort out hot from cold particles at no energy cost, simply by operating a trap door:

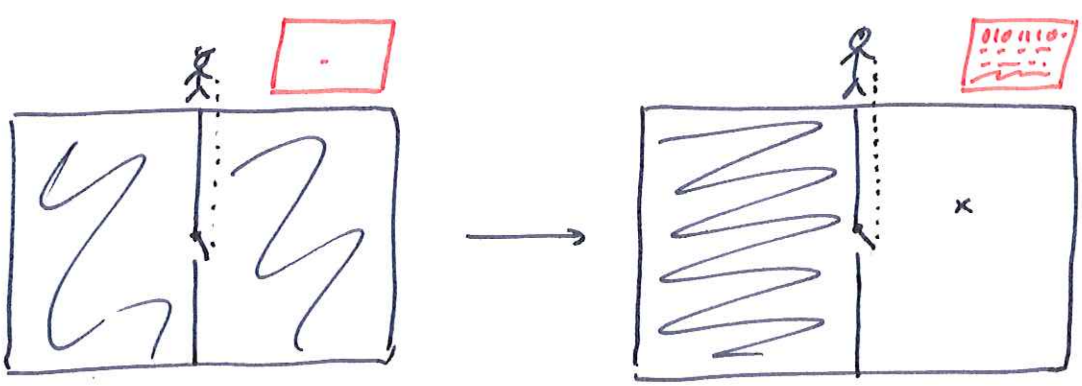


The demon lets
- slow particles go only to the left
- fast particles go ——— right

This creates a temperature difference from a gas at equilibrium → violation of the 2nd law !!

* generated huge debate, over decades
  - several models, examples worked out (e.g., Feynman's ratchet and pawl)
  - early belief: measurement costs energy
* resolution by Bennett using Landauer's principle.

Simpler case: the demon lets <u>all</u> particles go to the left, compressing the gas at no work cost



The demon must observe the particles (make measurements) to know whether to open the trap door or not → we need to account for the ~~records~~ demon's records of these measurements.

By Landauer's Principle, the demon needs to pay work to reset its memory device to its initial state.

We can understand Maxwell's demon as simply transferring entropy from the gas into its memory device.

3. Knowledge and side information

Knowledge about the input state helps to carry out an operation using less work.

$\boxed{?} \longrightarrow \boxed{0}$ cost: $kT\ln(2)$ but $\boxed{0} \longrightarrow \boxed{0}$, $\boxed{1} \longrightarrow \boxed{0}$ requires no work.

We can model an agent's knowledge explicitly with a <u>memory system</u> which is correlated with the system of interest (models <u>side information</u> explicitly). The same situation is described by either:

(A) $\boxed{0}, \boxed{1}$ known (implicit memory) $\longleftrightarrow$ (B) $\boxed{?}$ ⋮ $\boxed{?}$ ← memory register ($\boxed{?}$ is unknown, but the memory is correlated to it.)

Here: (A) knows the bit value; (B) doesn't know it a priori, but knows that the value is also stored in his memory register. We can get observer (A)'s point of view by <u>conditioning</u> (B)'s point of view on his side information, treating the memory implicitly.

Remember: the design of an autonomous machine which performs a given transformation is allowed to depend only on what we know, and not on what we don't know.

Example: Erasure of a known bit

Ⓐ's viewpoint:

$\boxed{0} \longrightarrow \boxed{0}$

$\boxed{1} \xrightarrow{\text{NOT}} \boxed{0}$

we may use different machines because input is known

work cost $= 0$

Ⓑ's viewpoint:

$\boxed{?} \xrightarrow{\text{C-NOT}} \boxed{0}$

memory $\boxed{?} \qquad\quad \boxed{?}$

single machine does the job, exploiting the side information

work cost $= 0$

But if Ⓒ doesn't know the bit value and doesn't have side information,

$\boxed{?} \longrightarrow \boxed{0}$ need $kT\ln(2)$ work by Landauer's principle.

Note: A measurement corresponds to a change of observers.

$\boxed{?} \xrightarrow{\text{meas.}} \boxed{0}$

$\boxed{?} \longrightarrow \boxed{1}$

Instead, we may stick with the global observer with a memory:

$\boxed{?} \xrightarrow{\text{"meas."}} \boxed{?}$

memory $\boxed{-} \qquad\qquad \boxed{?}$

measurement seen as acquiring side information

This is how we explained Maxwell's demon earlier.

Quantifying knowledge, information content

The Shannon entropy $H(X)$ of a random variable X measures the amount of uncertainty about X = information content of X:

$$H(X) = -\sum_x p_X(x) \log_2 p_X(x) \qquad \text{(in bits)}$$

If all values of X are equiprobable $\to$ $H(X) = \log_2(\#\text{ possible values})$

Erasure of data. Landauer's principle: $kT\ln(2)$ work paid per bit erased
$\to$ to erase a system X, we need an amount of work

$$W_{RESET}(X) = H(X) \cdot kT\ln(2)$$

[Subtleties: Use Shannon information theory to show this. Also this is an average work cost.]

Information content with side information.

The conditional Shannon entropy $H(X|Y)$ of a random variable X, conditioned on a random variable Y which may be correlated to X is defined as

$$H(X|Y) = H(XY) - H(Y) = \sum_y p_Y(y) \cdot H(X_{|Y=y})$$

rand. var. X conditioned on $Y=y$

$$H(X_{|Y=y}) = -\sum_x p_X(x|Y=y) \log_2 p_X(x|Y=y)$$

Examples.

$H(\boxed{0}) = H(\boxed{1}) = 0$ bits $\qquad H(\boxed{?}) = 1$ bit

$H(\boxed{?}\boxed{?}\boxed{0}\boxed{?}) = 3$ bits $\qquad$ [note: $\boxed{?}$ means $\boxed{0}$ or $\boxed{1}$ with probability ½ each.]

For $\begin{array}{l} \boxed{?} \leftarrow X \\ \vdots \\ \boxed{?} \leftarrow Y \end{array}$ we have $\begin{array}{l} H(X|Y) = 0 \text{ bits} \\ H(X) = 1 \text{ bit} \end{array}$

Erasure with side information.

Task: erase system X with side information Y.

We may design a machine which depending on the value of Y applies a given "sub-machine" to X (operation on X controlled by Y, like for a C-NOT gate). Strategy: if $Y=y$, then apply to X the machine that resets $X_{|Y=y}$. Average work cost:

$$W_{RESET}(X|Y) = \sum_y p_Y(y) \cdot H(X_{|Y=y}) \cdot kT\ln(2)$$

$$= H(X|Y) \cdot kT\ln(2) .$$

Important observation. Entropy depends on the observer. Different observers might have different knowledge or different side information.

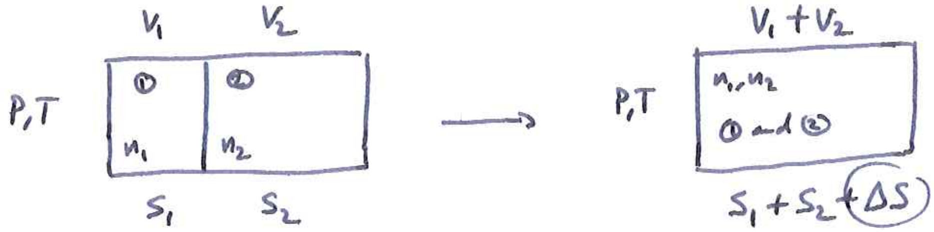
In thermodynamics, it is crucial to analyze a situation consistently from the point of view of a fixed observer.

(ex: Maxwell's demon.)

4. Observers and the Gibbs paradox

Reference: E.T. Jaynes, The Gibbs Paradox (1992).

If we mix two different kinds of gases together, the resulting entropy acquires a mixing entropy term:



$$\Delta S = S_{mix} = -nk\left[f \ln(f) + (1-f)\ln(1-f)\right] \qquad \left(f = \frac{n_1}{n},\ n = n_1 + n_2\right)$$

But if ① and ② are the same kind of gas, then $\Delta S = 0$.

Why does ΔS not depend on "how different" ① and ② are? Why this discontinuity? (Imagine tuning all the properties, such as particle mass, of gas ② continuously until ② is the same kind as ①.)

Recall that the mixing term is due to the fact that work needs to be expended to return back to the initial state, i.e. to re-separate the gases.

On the other hand, if ① = ②, we can just re-insert the separator to go back to the initial state.

→ the discontinuity is in the meaning of "get back to the initial state".

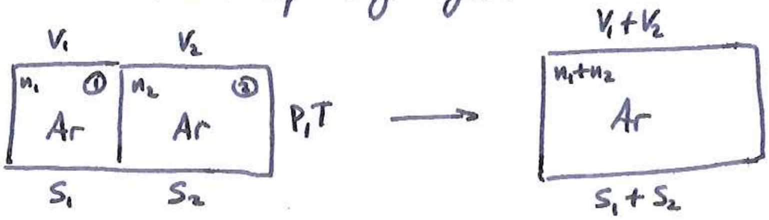
① ≠ ②: all particles originally in V_1 must be returned to V_1

① = ②: we don't care about which particles were originally in V_1

In any case, "go back to initial state" = go back to an equivalent microstate corresponding to the initial thermodynamic state.

Illustration: mixing revisited. (following Jaynes)

Mix 2 volumes of Argon gas.

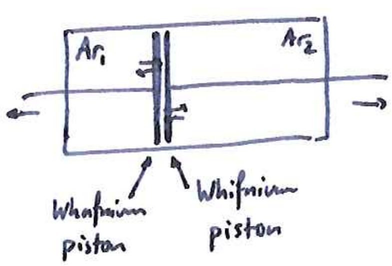


Suppose that, unbeknownst to us today, there are in fact 2 types of Argon, Ar_1 and Ar_2, that are identical in all aspects observable today.

We have no way of preparing pure Ar_1 or Ar_2, or even if we had a source of pure Ar_1 or Ar_2, we would have no way to know that.

Fast-forward 100 years in the future $\rightarrow$ we discover elements Whifnium and Whafnium; Ar_2 is soluble in Whifnium but not in Whafnium while Ar_1 is soluble in Whafnium but not Whifnium. We can distinguish Ar_1 from Ar_2 and prepare pure Ar_1 or Ar_2.

With this technology we can design a more clever mixing experiment:



Let Ar_1 expand in the Ar_2 and the Ar_2 expand in the Ar_1 $\rightarrow$ we extract work $\Delta W = n_1 kT \ln\left(\frac{V}{V_1}\right) + n_2 kT \ln\left(\frac{V}{V_2}\right)$

The free energy must have decreased because we extracted work (at constant temperature). The process is reversible, so

$\Delta F = -\Delta W$, also, $\Delta U = 0$, so

$$\Delta S = \frac{1}{T}(\Delta U - \Delta F) = -n_1 k \ln\left(\frac{n_1}{n}\right) - n_2 k \ln\left(\frac{n_2}{n}\right) = S_{mix}.$$

Our 100-years-in-the-future technology (the Whifnium/Whafnium pistons) gives us increased knowledge about the microscopic state of the gas.
→ We can extract more work with this technology.

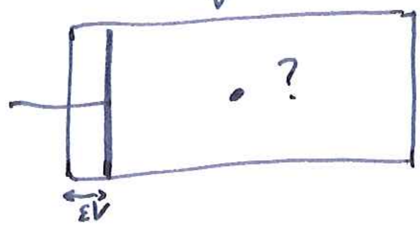
The observer-dependence of entropy is physical, as it reflects the different amounts of work extractable by the different observers.

Even in presence of the future technology, we can still elect to ignore the two different types of Argon and stick to the "old" description. This will correctly describe all thermodynamic properties of the gas as long as we don't use Whifnium and Whafnium pistons.

On the other hand, a more informed observer can use his knowledge to trick an ignorant observer into witnessing a violation of the second law.

5. Betting and failure probability

Consider again a Szilárd engine, with the particle in an unknown location.



Idea: if we place a separator close to the edge, then with high probability the particle is on the right side of the separator.

→ we can extract a little bit of work.

$$P_{success} = 1-\varepsilon \qquad W^{\varepsilon}_{extr.} = kT \cdot \ln\left(\frac{1}{1-\varepsilon}\right) \underset{\text{if } \varepsilon \approx 0}{\approx} \varepsilon \cdot kT$$

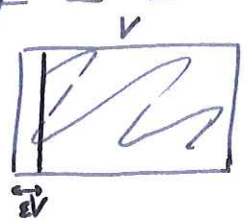
if we are more daring:

$$\varepsilon = 1/2 \quad \rightarrow \quad W^{\varepsilon}_{\text{extr}} = kT \ln(2)$$

$$\varepsilon \rightarrow 1 \quad \rightarrow \quad W^{\varepsilon}_{\text{extr}} = kT \ln\left(\frac{1}{1-\varepsilon}\right)$$ diverges, but only logarithmically

One can always <u>bet</u> on the state, and this allows to extract (or save) some work (but not that much) if the bet is successful. If the bet fails, anything can happen and the situation is unaccounted for.

<u>Example</u> <u>with</u> <u>macroscopic gas</u>. Compressing by betting



bet that all particles are on the right.

$p_{\text{success}} = (1-\varepsilon)^n \longrightarrow 0$ exponentially in n.

(especially minuscule if $n \sim 10^{23}$!!)

in the meager event of success, extract $W^{\varepsilon}_{\text{extr.}} = nkT \ln\left(\frac{1}{1-\varepsilon}\right)$

$\rightarrow$ to extract a <u>linear</u> amount of work, pay an <u>exponential</u> price in the success probability.

This <u>betting</u> is often expressed in terms of <u>fluctuation theorems</u>.

<u>Note</u>: the bet corresponds to a change of observer:

$$\boxed{?\ {\textstyle{\varepsilon \atop 1-\varepsilon}}} \xrightarrow{\text{bet}} \boxed{1}$$

succeeds only with prob. $1-\varepsilon$.

III. The Resource Theory of Thermodynamics.

Goal: A formulation of thermodynamics applicable to small-scale, quantum systems, in the "single instance" regime.

1. Language of quantum information.

We consider only finite-dimensional Hilbert spaces (for simplicity).

* States. An ensemble $\{|\psi_k\rangle\}$ with probabilities $\{p_k\}$ is equivalently described using the density operator

$$\rho = \sum p_k |\psi_k\rangle\langle\psi_k|$$

Properties: ρ is positive semidefinite $(\rho \geq 0)$; $\mathrm{tr}(\rho) = 1$

In quantum information, the state of a system S (with Hilbert space $\mathcal{H}_S$) is any operator $\rho \geq 0$ with $\mathrm{tr}(\rho) = 1$, ie, any density operator.

Measurement of an observable A with eigendecomposition $A = \sum \underset{\text{eigenvalues}}{a}\, \underset{\text{projectors onto eigenspaces}}{P_a}$ gives the outcome a with probability $\mathrm{tr}(\rho P_a)$.

Density operators generalize the concept of classical probability distributions.

* Bipartite states. If we bring two independent systems A and B in states ρ_A and ρ_B, the joint state is given by the tensor product $\rho_A \otimes \rho_B$ on $\mathcal{H}_A \otimes \mathcal{H}_B$. States of this form are product states.

In general, the joint state ρ_{AB} of A and B may be correlated, i.e. measurements on A and B may have correlated statistics.

Given a joint state ρ_{AB}, the <u>reduced state</u> ρ_A on A is given by the <u>partial trace</u>

$$\rho_A = \mathrm{tr}_B(\rho_{AB}) = \sum \langle e_k|_B \, \rho_{AB} \, |e_k\rangle_B$$

any choice of basis of B

* <u>Closed system evolution</u>. A closed system evolves with a unitary transformation: $\rho' = \mathcal{U}\rho\,\mathcal{U}^\dagger \qquad (\mathcal{U}\mathcal{U}^\dagger = \mathcal{U}^\dagger\mathcal{U} = \mathbb{1})$

(Time evolution with Hamiltonian H: $\mathcal{U} = e^{-iHt/\hbar}$)

The unitary $\mathcal{U}$ may act over several systems (e.g. for interacting H)

* <u>Open system evolution</u>. In general, the system evolves according to a <u>superoperator</u> or <u>quantum channel</u> $\mathcal{E}: \rho \to \mathcal{E}(\rho) = \rho'$.
$\mathcal{E}$ must be linear, trace-preserving, and completely positive (i.e. $(\mathcal{E}_S \otimes \mathrm{id}_R)(\rho_{SR}) \geq 0$ for any reference system R and for any state ρ_{SR}.)

* <u>Entropy</u>. The entropy of a system S in the state ρ_S is

$$H(S)_\rho = -\mathrm{tr}(\rho_S \log_2 \rho_S) \qquad \text{von } \underline{\text{Neumann entropy}}$$

matrix log, acts on eigenvalues

As before, the conditional entropy of system S with side information M, in the global state ρ_{SM}, is given as

$$H(S|M)_\rho = H(SM)_\rho - H(M)_\rho$$

2. The resource theory.

Idea: we don't try to describe what actually happens in nature directly, rather, we describe what could possibly happen under a set of simple rules (that nature follows, e.g., energy conservation).

Here, we fix a temperature T (and $\beta = \frac{1}{kT}$). The corresponding thermal state on any system S with Hamiltonian H_S is

$$\gamma_S = \frac{e^{-\beta H_S}}{Z}, \qquad Z = \operatorname{tr}(e^{-\beta H_S}) .$$

The rules:

(a) Are allowed any unitary transformation $\mathcal{U}$ which conserves energy, ie., $[\mathcal{U}, H_{tot}] = 0$

total Hamiltonian of the systems considered

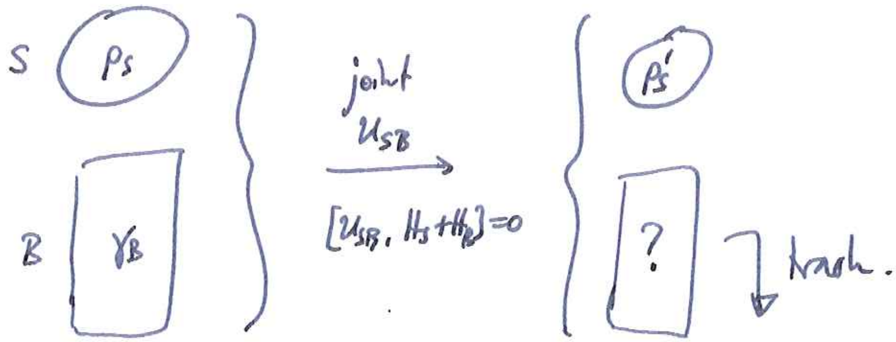
(b) We are allowed to bring in any system B (with any Hamiltonian) in the thermal state γ_B (at the fixed temperature T)

(c) We may discard any system.

Main question: Which transformations $\rho \to \rho'$ are possible?

Observation: Given any sequence of (a), (b), (c) processes, we can merge the similar type processes together to a single (b)-(a)-(c) chain.

→ The most general process we can carry out in this resource theory is a thermal operation:



$$\mathcal{E}(\rho_S) = \mathrm{tr}_B\left(U_{SB}(\rho_S\otimes\gamma_B)\,U_{SB}^\dagger\right)$$

Observation: if $[U_{SB}, H_S+H_B]=0$, then $U_{SB}(\gamma_S\otimes\gamma_B)U_{SB}^\dagger = \gamma_S\otimes\gamma_B$. So any thermal operation preserves the thermal state on S (at the given fixed temperature T): $\mathcal{E}(\gamma_S)=\gamma_S$.

→ A thermal operation can only get you closer to the thermal state.

Examples.

* $|1\rangle_S$  γ_S (swap with thermal state)

* for any ρ, $\rho \xrightarrow{T.O.} \gamma$

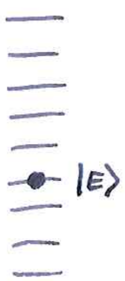
* γ_S may only go to γ_S

*  (unitary within energy eigenspaces)

*  (output is thermal state)

What is "work"?

Define work via an explicit battery system



W

if $\rho_S \otimes |E\rangle\langle E|_W \xrightarrow{T.O.} \rho_S' \otimes |E'\rangle\langle E'|_W$

$\Leftrightarrow$ extracted $E'-E$ work while performing the transition $\rho_S \rightsquigarrow \rho_S'$

Remarks about the resource theory approach.

* The rules look artificial, but they capture the relevant features of thermodynamics in the regimes we are interested in. (Analogy: Turing machine in computer science.)

* The statements are inherently single-shot; extracted work is deterministic ($\neq$ stat. mech., average work is often considered)

* Full mathematical characterization of which transformations $\rho \to \rho'$ are possible with thermal operations [if ρ, ρ' are block-diagonal in the energy eigenbasis; otherwise $\to$ open question.]

* Similar results are obtained by imposing a single rule instead of (a)-(c), that any process applied must preserve the thermal state (but not all such operations are necessarily physical)

* We recover the macroscopic laws of thermodynamics in the macroscopic limit

* These approaches are still a subject of active research (last ~10 yrs)

Recap: Resource Theory of Thermodynamics

* Goal: Understand the laws of thermodynamics at the nano scale, in the "single-shot" regime

* Formulate ruleset, and identify possible state transformations

* Rules: (a) allowed any unitary $\mathcal{U}$: $[\mathcal{U}, H_{tot}] = 0$ ← total Hamiltonian
  (energy conservation)

  (b) allowed any additional system B in state $\gamma_B = \frac{e^{-\beta H_B}}{Z}$, $Z = \mathrm{tr}(e^{-\beta H_B})$
  (heat baths)

  (c) allowed to discard any system.

* Work is invested/extracted by including an explicit work storage system ("battery")

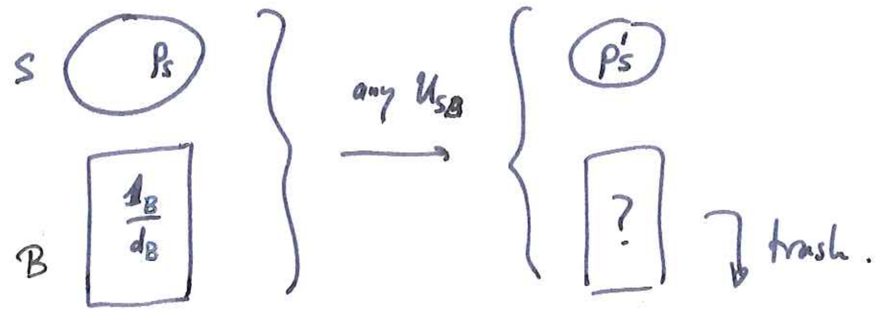
Here: We will

* characterize mathematically which $\rho \to \rho'$ are possible (→ majorization)
* find resource monotones

* calculate the optimal extractable work from ρ, and cost of formation of ρ

3. Noisy Operations.

We first consider the case $H_S = H_B = 0$:



These operations are called noisy operations, because we can only introduce noise into the system S.

It turns out these operations are related to the mathematical notion of majorization.

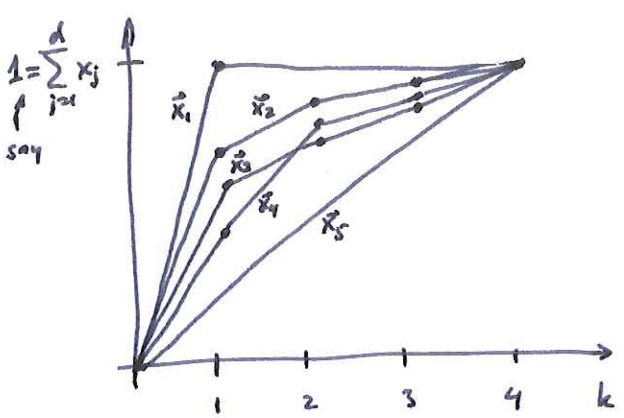
Def: If $\vec{x}, \vec{y}$ are vectors in $\mathbb{R}^d$, denote by $\vec{x}^\downarrow, \vec{y}^\downarrow$ the corresponding vectors with entries ordered in decreasing order, with multiplicities ($x_1^\downarrow \geq x_2^\downarrow \geq \dots$). We say that $\vec{x}$ majorizes $\vec{y}$ (denoted $\vec{x} \succ \vec{y}$) if

* $\sum_{j=1}^{k} x_j^\downarrow \geq \sum_{j=1}^{k} y_j^\downarrow$ for all $k = 1, 2, \dots, d$ and
* $\sum_{j=1}^{d} x_j^\downarrow = \sum_{j=1}^{d} y_j^\downarrow$.

For Hermitian matrices A, B on $\mathcal{H}$, we say $A \succ B$ if $\vec{\lambda}(A) \succ \vec{\lambda}(B)$, where $\vec{\lambda}(X)$ is the vector of eigenvalues of X (with multiplicities).

Note that equivalently, $\vec{x} \succ \vec{y}$ if and only if $\sum_{j=1}^{k} x_j^{\uparrow} \leq \sum_{j=1}^{k} y_j^{\uparrow} \ \forall\, k = 1, \dots, d$ and $\sum_{j=1}^{d} x_j^{\uparrow} = \sum_{j=1}^{d} y_j^{\uparrow}$, where $\vec{x}^{\uparrow}$ are the entries of $\vec{x}$ in increasing order.

Lorenz curves: These are a useful graphical representation to determine whether $\vec{x} \succ \vec{y}$ or not. The Lorenz curve of $\vec{x}$ is the curve connecting the points $\left(k, \sum_{j=1}^{k} x_j^{\downarrow}\right)$:



$\vec{x}_1 =$ single non-zero entry $=$ e.g. $\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

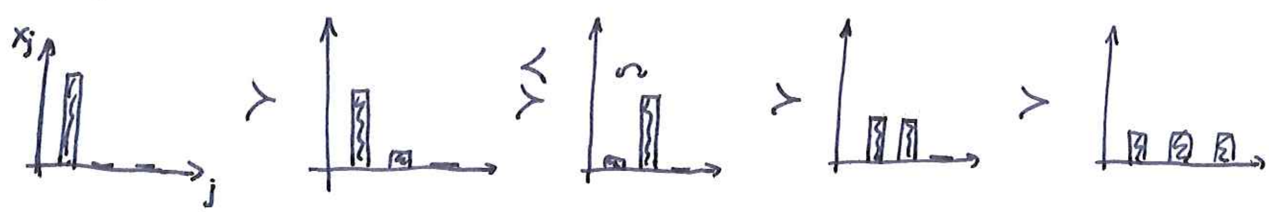
$\vec{x}_5 = \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix}$ uniform vector

$\vec{x}_2 \succ \vec{x}_3$, $\vec{x}_2 \succ \vec{x}_4$, $\vec{x}_1 \succ$ everybody

$\vec{x}_3 \nsucc \vec{x}_4$, $\vec{x}_4 \nsucc \vec{x}_3$, $\vec{x}_5 \prec$ everybody

We have $\vec{x} \succ \vec{y} \iff$ the Lorenz curve of $\vec{x}$ lies above the Lorenz curve of $\vec{y}$ (by definition of majorization). (and $\sum_{j=1}^{d} x_j = \sum_{j=1}^{d} y_j$)

Examples:



Under majorization, at fixed vector normalization, there is a unique least element which is the uniform vector.

A vector with a single non-zero entry majorizes any other vector with the same normalization.

We would like a simple, convenient characterization of majorization. $\to$ doubly stochastic matrices.

<u>Def</u>: A matrix A is <u>stochastic</u> if

* $A_{ij} \geq 0 \quad \forall\, i,j$
* $\sum_{i=1}^{d} A_{ij} = 1 \quad \forall\, j \quad (\Leftrightarrow A^T \vec{e} = \vec{e} \;,\; \vec{e} = (1,1,\dots,1))$

A matrix is stochastic if and only if its columns are probability vectors.

<u>Def.</u>: A is <u>doubly stochastic</u> if

* A is stochastic
* $\sum_{j=1}^{d} A_{ij} = 1 \quad \forall\, i \quad (\Leftrightarrow A\vec{e} = \vec{e})$

<u>Theorem</u>: Are equivalent:

(i) A is doubly stochastic

(ii) $\vec{x} \succ A\vec{x}$ for all probability vectors $\vec{x}$

<u>Proof of (ii)$\Rightarrow$(i)</u>: $\frac{\vec{e}}{d} \succ A\frac{\vec{e}}{d} \Rightarrow A \cdot \frac{\vec{e}}{d} = \frac{\vec{e}}{d}$ (unique least element). $\Rightarrow A\vec{e} = \vec{e}$

If $\vec{e}_j = (0,\dots,\underset{\uparrow_j}{1},0\dots) \to \vec{e}_j \succ A\vec{e}_j = (A_{ij})_i \Rightarrow \sum_i A_{ij} = 1 \quad \forall j$

also $(A_{ij})^{\uparrow}_{i=1} = \min_i A_{ij} \overset{!}{\geq} 0 = (\vec{e}_j^{\,\uparrow})_{i=1} \Rightarrow A_{ij} \geq 0 \quad \forall\, i,j$

(i)$\Rightarrow$(ii) is more tedious, but no surprises.

Observations:

(i) if $\{A_\ell\}$ are doubly stochastic matrices, and if $\{\alpha_\ell\}$ is a probability distribution, then $\sum \alpha_\ell A_\ell$ is doubly stochastic.

$\Rightarrow$ The set of doubly stochastic matrices is convex.

(ii) A permutation matrix (that permutes basis elements) is doubly stochastic.

Example: random permutation. $A = \underset{\substack{\text{prob.}\\ \text{dist.}}}{\sum \alpha_\ell} \underset{\text{perm. matrices}}{P_\ell}$

for $d=2$: $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to A\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \alpha\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + (1-\alpha)\begin{pmatrix} x_2 \\ x_1 \end{pmatrix} = \begin{pmatrix} \alpha x_1 + (1-\alpha)x_2 \\ (1-\alpha)x_1 + \alpha x_2 \end{pmatrix}$

$A = \begin{pmatrix} \alpha & 1-\alpha \\ 1-\alpha & \alpha \end{pmatrix}$ is doubly stochastic.

In fact, this example is generic:

Theorem (Birkhoff): Any doubly stochastic matrix A is a convex combination of permutation matrices: $A = \sum \alpha_\ell P_\ell$ $\quad (\alpha_\ell \geq 0, \sum \alpha_\ell = 1)$.

(Proof: see math books, e.g. Bhatia, Matrix Analysis.)

Doubly stochastic matrices fully characterize majorization:

Theorem: $\vec{x} \succ \vec{y}$ if and only if there exists a doubly stochastic matrix A such that $\vec{y} = A\vec{x}$.

Back to noisy operations.

<u>Theorem (Horodecki², Oppenheim)</u>: The transition $\rho \to \rho'$ is possible with a noisy operation if and only if $\rho \succ \rho'$.

Intuitively, ρ' has to be "more mixed" than ρ.

<u>Proof</u>: <u>Suppose $\rho \succ \rho'$</u>. Then there exists a probability distribution $\{\alpha_\ell\}$ and permutation matrices $\{P_\ell\}$ such that $\vec{\lambda}(\rho') = \sum \alpha_\ell P_\ell \vec{\lambda}(\rho)$.

Notation: let $\vec{p} = \vec{\lambda}(\rho)$ and $\vec{q} = \vec{\lambda}(\rho')$.

Without loss of generality $\to$ $\rho = \mathrm{diag}(\vec{p})$ and $\rho' = \mathrm{diag}(\vec{q})$, because we can always do unitaries for free.

Idea: use the noisy ancillary system to apply the permutation P_ℓ of the quantum basis states, with probability α_ℓ. (Exploit the randomness in B.)

B has d_B states: $\underbrace{|0\rangle, |1\rangle, |2\rangle, \ldots}_{n_1} \underbrace{\ldots}_{n_2} \ldots, |d_B\rangle$

divide into blocks:

such that $\frac{n_\ell}{d_B} \approx \alpha_\ell$ for all ℓ.

Protocol idea: If B is in the state $|b\rangle$, then we apply the permutation P_ℓ on S, where $\ell = \ell(b)$ is the block in which $|b\rangle$ lies:

$$\mathcal{U}_{SB} = \sum_b |b\rangle\langle b|_B \otimes \mathcal{U}_S^{(\ell(b))}$$

$$\mathcal{U}_S^{(\ell)} = \sum_{k=1}^{d_S} |\sigma_\ell(k)\rangle\langle k|_S$$

permutes basis vectors according to P_ℓ. Here $\sigma_\ell \in S(d_S)$ is the permutation corresponding to P_ℓ.

$\mathcal{U}_{SB}$ is unitary (it is a basis transformation).

Then: $$\mathrm{tr}_B\left(\mathcal{U}_{SB}\cdot\left(\rho_S\otimes\frac{\mathbb{1}_B}{d_B}\right)\cdot\mathcal{U}_{SB}^\dagger\right) = \frac{1}{d_B}\sum_b \mathcal{U}_S^{(\ell(b))}\rho_S\,\mathcal{U}_S^{(\ell(b))\dagger}$$

$$= \sum_\ell \frac{n_\ell}{d_B}\underbrace{\mathcal{U}_S^{(\ell)}\rho_S\,\mathcal{U}_S^{(\ell)\dagger}}_{\substack{\text{diagonal matrix, with}\\ \text{entries } \mathrm{diag}(P_\ell\vec{p})}} \approx \sum_\ell \alpha_\ell\cdot\mathrm{diag}(P_\ell\vec{p}) = \rho'$$

The approximation becomes arbitrarily good for $d\to\infty$.

Converse: assume $\rho\to\rho'$ by noisy operation.

Idea: show that $\vec{q}=\vec{\lambda}(\rho')$ can be obtained from $\vec{p}=\vec{\lambda}(\rho)$ by applying a doubly stochastic matrix.

We know: $$\rho' = \mathrm{tr}_B\left\{\mathcal{U}_{SB}\left(\rho_S\otimes\frac{\mathbb{1}_B}{d_B}\right)\mathcal{U}_{SB}^\dagger\right\} = \frac{1}{d_B}\sum_{b,b'}\underbrace{\langle b'|\mathcal{U}_{SA}|b\rangle_A}\,\rho_S\,\underbrace{\langle b|\mathcal{U}_{SA}^\dagger|b'\rangle_A}$$

Def. $C_{b,b'} = \frac{1}{\sqrt{d_B}}\langle b'|\mathcal{U}_{SB}|b\rangle_B$ (acts on S)

As before, suppose $\rho=\sum p_k|k\rangle\langle k|$ and $\rho'=\sum q_k|k\rangle\langle k|$. Then

$$\rho' = \dots = \sum_{b,b'} C_{b,b'}\,\rho\,C_{b,b'}^\dagger \,. \qquad \text{Def } A_{k'k} = \sum_{b,b'}|\langle k'|C_{b,b'}|k\rangle|^2 \geq 0$$

Then $$q_{k'} = \langle k'|\rho'|k'\rangle = \sum_{b,b',k}\langle k'|C_{b,b'}|k\rangle\,p_k\,\langle k|C_{b,b'}^\dagger|k'\rangle = \sum_k A_{k'k}\,p_k \,.$$

$$\sum_k A_{k'k} = \sum_{b,b',k}\langle k'|C_{b,b'}\underbrace{|k\rangle\langle k|}C_{b,b'}^\dagger|k'\rangle = \frac{1}{d_B}\sum_{b'}\left((\langle k'|\otimes\langle b'|)\cdot\underbrace{\mathcal{U}_{SB}\,(\mathbb{1}_S\otimes\mathbb{1}_B)\,\mathcal{U}_{SB}^\dagger}\,(|k'\rangle\otimes|b'\rangle)\right) = 1$$

and

$$\sum_{k'} A_{k'k} = \sum_{b,b',k'}\langle k|C_{b,b'}^\dagger|k'\rangle\langle k'|C_{b,b'}|k\rangle = \frac{1}{d_B}\sum_b\left((\langle k|\otimes\langle b|)\,\mathcal{U}_{SB}^\dagger\,(\mathbb{1}_S\otimes\mathbb{1}_B)\,\mathcal{U}_{SB}\,(|k\rangle\otimes|b\rangle)\right) = 1$$

$\Rightarrow \rho \succ \rho'$. $\square$

We can prove a slightly more detailed theorem:

Theorem: Are equivalent

(i) $\rho \succ \rho'$

(ii) $\exists$ noisy operation $\rho \to \rho'$

(iii) $\exists$ unitaries $\{\mathcal{U}_\ell\}$ and prob. distribution $\{\alpha_\ell\}$ such that

$$\rho' = \sum \alpha_\ell \, \mathcal{U}_\ell \, \rho \, \mathcal{U}_\ell^\dagger \qquad \text{(random unitary)}$$

(iv) $\exists$ quantum channel $\mathcal{E}$ (ie, a completely positive, trace-preserving linear map) such that $\mathcal{E}(\rho) = \rho'$ and $\mathcal{E}(\mathbb{1}) = \mathbb{1}$

Proof: (i) $\Leftrightarrow$ (ii) above.

(i) $\Rightarrow$ (iii) cf. above: in our previous proof, we had $\rho \succ \rho' \Rightarrow$ construction of $\rho' = \sum_\ell \alpha_\ell \, \mathcal{U}_S^{(\ell)} \rho \, \mathcal{U}_S^{(\ell)\dagger}$ which is a random unitary process.

(iii) $\Rightarrow$ (iv) immediate from $\mathcal{E}(\cdot) = \sum \alpha_\ell \, \mathcal{U}_\ell (\cdot) \mathcal{U}_\ell^\dagger$: $\mathcal{E}(\rho) = \rho'$ & $\mathcal{E}(\mathbb{1}) = \mathbb{1}$.

(iv) $\Rightarrow$ (i) similar to previous proof. Set $A_{k'k} = \langle k' | \mathcal{E}(|k\rangle\langle k|) | k' \rangle$ with $\rho = \sum p_k |k\rangle\langle k|$ & $\rho' = \sum q_{k'} |k'\rangle\langle k'|$. Then $A_{k'k} \geq 0$.

$\sum_k A_{k'k} = \langle k' | \mathcal{E}(\mathbb{1}) | k' \rangle = \langle k' | k' \rangle = 1$ and

$\sum_{k'} A_{k'k} = \mathrm{tr}(\mathcal{E}(|k\rangle\langle k|)) = 1$ because $\mathcal{E}$ is trace-preserving.

Also $q_{k'} = \langle k' | \rho' | k' \rangle = \langle k' | \mathcal{E}(\rho) | k' \rangle = \sum_k p_k A_{k'k}$.

$\Rightarrow$ A is doubly stochastic and $\vec{q} = A\vec{p}$ $\Rightarrow$ $\rho \succ \rho'$. $\square$

In a resource theory one is often interested in <u>resource monotones</u>. These are functions which can only increase/decrease under the resource theory's rules.

→ A resource monotone provides necessary conditions for possible transformations.

The <u>entropy</u> is a resource monotone for noisy operations:

$$\rho \succ \rho' \quad \Rightarrow \quad H(\rho') \geq H(\rho)$$

Reason: $H(\rho)$ is concave → if $\rho \succ \rho'$, we can write $\rho' = \sum \alpha_\ell U_\ell \rho U_\ell^\dagger$ and

$$H(\rho') = H\left(\sum \alpha_\ell U_\ell \rho U_\ell^\dagger\right) \underset{\substack{\uparrow \\ \text{concavity of } H}}{\geq} \sum \alpha_\ell \underbrace{H(U_\ell \rho U_\ell^\dagger)}_{= H(\rho)} \underset{\substack{\uparrow \\ H \text{ unitarily invariant} \\ \sum \alpha_\ell = 1}}{=} H(\rho) .$$

Note, however, that $H(\rho) \leq H(\rho') \not\Rightarrow \rho \succ \rho'$. A counter-example:

$H(\rho) = 1$ bit $\qquad$ $H(\rho')$ large

$\rho \not\succ \rho'$ because the first partial sum: $\sum_{j=1}^{1} \lambda_j^\downarrow(\rho) = \lambda_1^\downarrow(\rho) = \frac{1}{2} \not\geq \lambda_1^\downarrow(\rho') = \frac{1}{2} + \varepsilon$.

(→ there is no noisy operation $\rho \to \rho'$.)

4. Thermal Operations and Thermomajorization.

We consider again the general case $H_S, H_B \neq 0$.

Assume: the states we consider are block-diagonal with respect to the energy eigenspaces.

→ As before, without loss of generality, we can write

$$\rho = \sum p_k |k\rangle\langle k| , \quad \rho' = \sum q_k |k\rangle\langle k| ,$$

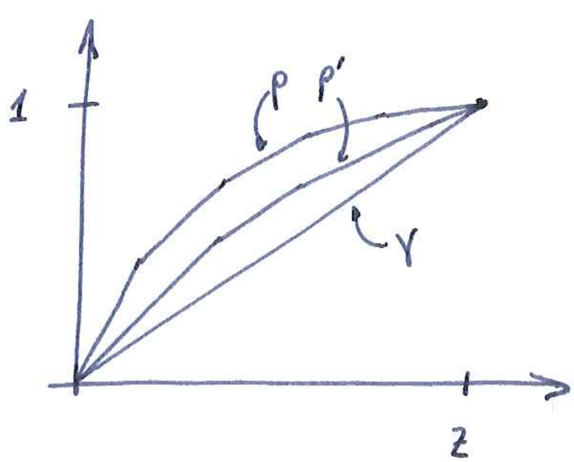
$$\gamma = \sum \frac{e^{-\beta E_k}}{Z} |k\rangle\langle k| , \quad Z = \sum e^{-\beta E_k}$$

for a suitable basis $\{|k\rangle\}$

Thermomajorization: (also d-majorization, relative majorization, ...)

Choose ordering $p_1 e^{\beta E_1} \geq p_2 e^{\beta E_2} \geq \dots$ (β-ordering)

The rescaled Lorenz curve of ρ is obtained by connecting the points $\left(\sum_{j=1}^{k} e^{-\beta E_j} , \sum_{j=1}^{k} p_j\right)$:



ρ thermomajorizes ρ' if its Lorenz curve lies above the Lorenz curve of ρ'.

<u>Theorem</u>: (Horodecki, Oppenheim). Are equivalent, for block-diagonal ρ, ρ':

(i) ρ thermomajorizes ρ'

(ii) there exists a thermal operation $\rho \to \rho'$

(iii) there exists a stochastic matrix A such that

$$\underset{\vec{p}=\vec{\lambda}(\rho)}{A\vec{p}} = \underset{\vec{q}=\vec{\lambda}(\rho')}{\vec{q}} \quad \text{and} \quad A\vec{g} = \vec{g} \qquad \vec{g} = \vec{\lambda}(\gamma),\ g_k = \frac{e^{-\beta E_k}}{Z}$$

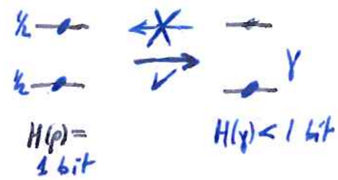
← suitable generalization of doubly stochastic matrices

(iv) there exists a quantum channel $\mathcal{E}$ such that

$$\mathcal{E}(\rho) = \rho' \quad \text{and} \quad \mathcal{E}(\gamma) = \gamma$$

Can we find a monotone for thermal operations?

The entropy is no longer suitable, eg:



Use the <u>relative entropy</u> instead:

$$D(\rho \| \gamma) = \mathrm{tr}\left(\rho\left(\log_2(\rho) - \log_2(\gamma)\right)\right) = -H(\rho) - \mathrm{tr}(\rho \log_2(\gamma))$$

The relative entropy obeys the data processing inequality:

$$D(\rho\|\gamma) \geq D(\mathcal{E}(\rho)\,\|\,\mathcal{E}(\gamma)) \quad \forall \text{ quantum channel } \mathcal{E}$$

The relative entropy is a resource monotone for thermal operations.

If $\rho \xrightarrow{T.O.} \rho'$, then $\rho' = \mathcal{E}(\rho)$ for some channel $\mathcal{E}$ with $\mathcal{E}(\gamma) = \gamma$ and

$$D(\rho'\|\gamma) = D(\mathcal{E}(\rho)\,\|\,\mathcal{E}(\gamma)) \leq D(\rho\|\gamma).$$

What does this quantity represent? Calculate:

$$D(\rho\|\gamma) = D\left(\rho \,\Big\|\, \frac{e^{-\beta H}}{Z}\right) = -H(\rho) - \mathrm{tr}\left(\rho \log_2\left(\frac{e^{-\beta H}}{Z}\right)\right)$$

$$= -H(\rho) + \frac{\beta}{\ln(2)}\mathrm{tr}(\rho H) + \log_2(Z)$$

$$= \frac{\beta}{\ln(2)} \cdot F(\rho) + \frac{\ln(Z)}{\ln(2)} = \frac{\beta}{\ln(2)}\left(F(\rho) - F(\gamma)\right)$$

def $F(\rho) = \langle H \rangle_\rho - kT\ln(2) \cdot H(\rho)$ <u>free energy</u>.

<u>Note</u>: again, $D(\rho\|\gamma) \geq D(\rho'\|\gamma) \not\Rightarrow \rho \xrightarrow{T.O.} \rho'$.

5. Work and Thermal Operations.

Account for work using an explicit energy storage system:

$$\rho \otimes |E\rangle \xrightarrow{T.O.} \rho' \otimes |E'\rangle$$

"transition of $\rho \to \rho'$ while extracting work $E' - E$"

We need to study the effect of the energy storage system onto the thermomajorization curves.

Suppose $\rho_S = \sum p_k |k\rangle\langle k|_S$, $\quad H_S = \sum E_k |k\rangle\langle k|_S$.

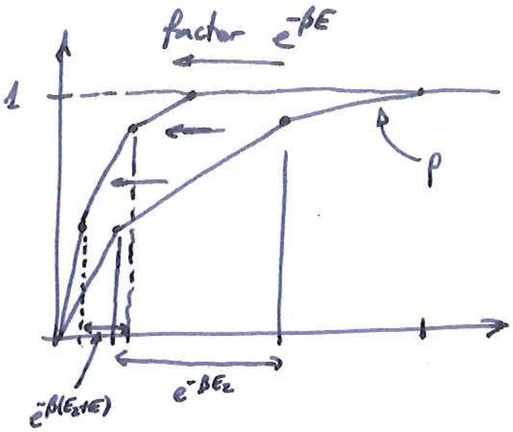
We order for thermomajorization the k's according to

$$p_1 e^{\beta E_1} \geq p_2 e^{\beta E_2} \geq \dots$$

Then $\rho \otimes |E\rangle\langle E| = \sum p_k |k\rangle\langle k| \otimes |E\rangle\langle E|$ has the same β-ordering

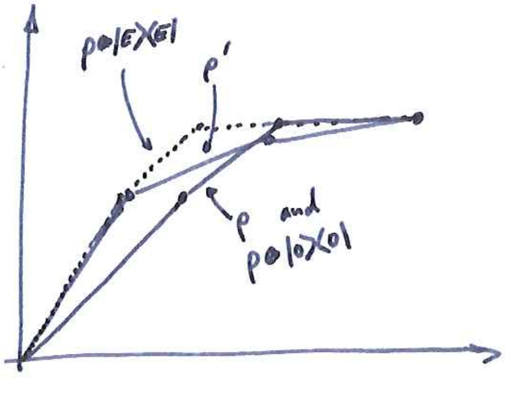
$$p_1 e^{\beta(E_1+E)} \geq p_2 e^{\beta(E_2+E)} \geq \dots$$

$\rightarrow$ effect on Lorenz curve is a compression along the x-axis:



Lorenz curve of $\rho \otimes |E\rangle\langle E|$ is compressed "$\longleftarrow$" by a factor of $e^{-\beta E}$.

We can exploit this to enable previously forbidden transformations.

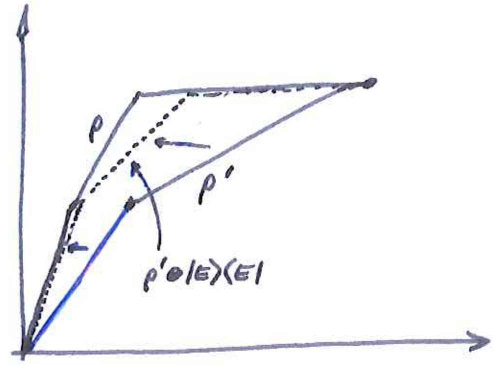


clearly $\rho \overset{T.O.}{\not\to} \rho'$.

but $\rho \otimes |E\rangle\langle E| \xrightarrow{T.O.} \rho' \otimes |0\rangle\langle 0|$

(invested work E).

We can also extract work in a similar way:



$\rho \xrightarrow{T.O} \rho'$ ok but not optimal.

We can in fact do

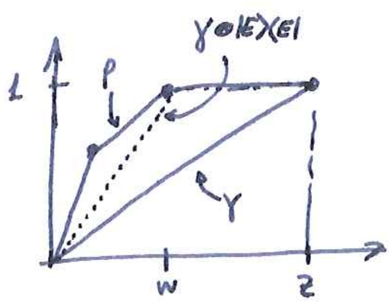
$\rho \otimes |0\rangle\langle 0| \to \rho' \otimes |E\rangle\langle E|$

and extract work E.

Distillation of work and formation of states.

What is the maximal amount of work that one can extract from ρ with a thermal operation and an energy storage system?

$$\rho \otimes |0\rangle\langle 0| \longrightarrow \underbrace{\text{any}}_{\text{w.l.o.g.} \to \gamma} \otimes |E\rangle\langle E| \quad \leftarrow \max E\,?$$



We can compress γ's Lorentz curve until it reaches the last inflection point of ρ's Lorentz curve.

The point w is given by $w = \sum_{p_k > 0} e^{-\beta E_k} = \mathrm{tr}(\underbrace{\Pi^\rho}_{\text{projector onto the support of } \rho} e^{-\beta H}) = Z \cdot \mathrm{tr}(\Pi^\rho \gamma)$

So, the max E is given by $e^{-\beta E} = \text{compression factor} = \frac{w}{Z} = \mathrm{tr}(\Pi^\rho \gamma)$

$$\longrightarrow E = -\beta^{-1} \ln(\mathrm{tr}(\Pi^\rho \gamma))$$

This is the <u>min-relative entropy</u> $D_{min}(\rho\|\gamma) = -\log_2(tr(\Pi^\rho \gamma))$

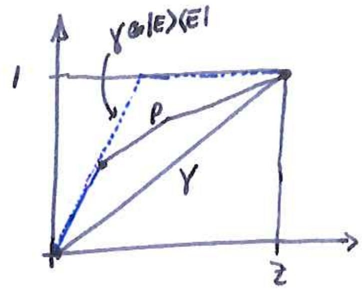
So, the max. extractable work from ρ is

$$= kT \cdot \ln(2) \cdot D_{min}(\rho\|\gamma)$$

On the other hand, how much work do we need to prepare ("to form") ρ from γ ?

$$\gamma \otimes |E\rangle\langle E| \longrightarrow \rho \otimes |0\rangle\langle 0|$$

$\uparrow$ min E ?



We need to compress γ's Lorenz curve until it covers the first kink in ρ's Lorenz curve.

The first kink of ρ's curve is at $(e^{-\beta E_1}, p_1)$ in β-ordering

ie. initial slope of ρ's curve is

$$\text{slope} = \frac{p_1}{e^{-\beta E_1}} = p_1 e^{\beta E_1} = \max_k p_k e^{\beta E_k} = \frac{1}{Z} \| \underbrace{\gamma^{-1/2} \rho \gamma^{-1/2}}_{} \|_\infty$$

(diagonal matrix, all of these commute)

$$\gamma\text{'s curve's slope} = \frac{1}{Z} .$$

$\rightarrow$ we need to compress such that $\dfrac{1}{e^{-\beta E} \cdot Z} \overset{!}{=} \dfrac{1}{Z} \|\gamma^{-1/2} \rho \gamma^{-1/2}\|_\infty$

$$\rightarrow E = \beta^{-1} \ln \|\gamma^{-1/2} \rho \gamma^{-1/2}\|_\infty$$

This is the <u>max-relative entropy</u> $D_{max}(\rho\|\gamma) = \log_2 \|\gamma^{-1/2} \rho \gamma^{-1/2}\|_\infty$

So, the work required to form ρ is $= kT \ln(2) \cdot D_{max}(\rho\|\gamma)$.

Remarks.

* Being valid in the one-shot regime, thermal operations account for fluctuations in e.g. work by considering the worst case

* It is possible to repeat the statements above with a tolerance ε on the accuracy of the process

  → "smooth" unphysically discontinuous statements

* The fully quantum regime is still not fully understood. There are "weird" effects: For instance, there might exist $\mathcal{E}$ with $\rho' = \mathcal{E}(\rho)$ and $\gamma = \mathcal{E}(\gamma)$ but $\rho \not\to \rho'$ by a thermal operation.

* Macroscopic statements can be recovered in two regimes

  → states with "straight" Lorenz curves (eg., microcanonical states)

  → the limit of many copies of ρ: $\rho^{\otimes n}$

In these cases, only the free energy matters for state transformations. (→ recover macroscopic 2nd law)