Statistical Mechanics
E0415

Fall 2021, lecture 7
Entropy

Take home… on snowflakes

"The reason for why no two snowflakes are alike, is that the particular shape is determined by the path the flakes take through the clouds as they are forming. It is unlikely that two would take the same path. In addition, a snowflake consists of 10^9 molecules of water. Having an identical arrangement of such a number of molecules is practically impossible."

”Snowflakes starts of as roughly spherical crystals up in the atmosphere. As the crystal grows an instability develops resulting in the so-called dendrites that forms a six-fold symmetric shape as a result of the six-fold   the molecular crystal structure of ice. The detailed structure of a snowflake however develops during its decent through the atmosphere where it is exposed to a variety of fluctuating conditions,such as changing temperatures, humidity levels,particles in the atmosphere,etc…all of which affect the growth of the snowflake. So the particular structure of a snowflake depends on its path through the atmosphere and the exact conditions it experience on that path and since it is very unlikely any two snowflakes will have the experience the exact same conditions the saying “no two snowflakes are alike” is largely correct.As the site provided demonstrates even snowflakes grown in a lab, exposed to almost exactly identical conditions, grows into very similar, but not precisely the same , looking snowflakes.”

”Firstly, six-fold radial symmetry arises from the crystalline structure of watermolecules in ice. However, different conditions, like pressure and tempera-ture, affect how the crystal will grow. For example, the snowflake can growinto a hexagon or it can grow spikes. Interestingly, these spikes in a snowflaketend to grow faster because they are farther away from the core and the heatfrom sublimation diffuses faster. Hence, the overall shape of a snowflake de-pends on conditions it experiences while it is growing. Thus, snowflakes areusually different, since it is very unlikely that two snowflakes undergoes sameconditions.In conclusion, nothing really says that two snowflakes could not have equalshape but it is very unlikely – indeed, it is very unlikely that two snowflakesgo through exactly same paths of different conditions.”

Why bother?

Says Sethna:

We shall see in this chapter that entropy has three related interpretations.[1] *Entropy measures the disorder in a system;* in Section 5.2 we will see this using the entropy of mixing and the residual entropy of glasses. *Entropy measures our ignorance about a system;* in Section 5.3 we will give examples from non-equilibrium systems and information theory. But we will start in Section 5.1 with the original interpretation, that grew out of the nineteenth century study of engines, refrigerators, and the end of the Universe. *Entropy measures the irreversible changes in a system.*

Irreversibility and the Carnot cycle

Four steps:

(ab): heat flow at T_1

(bc): expansion without heat transfer

(cd): gas compressed, heat flow at T_2

(da): compression, warm the gas back without heat transfer

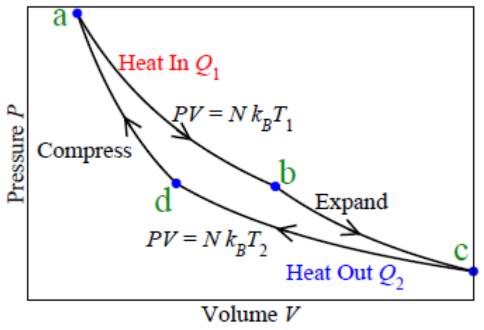
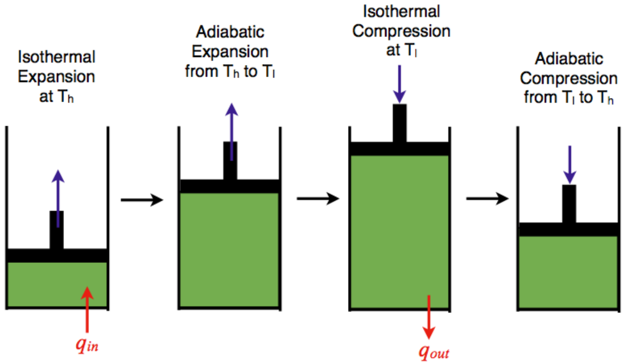


Fig. 5.3 Carnot cycle P–V diagram. The four steps in the Carnot cycle: a→b, heat in Q_1 at constant temperature T_1; b→c, expansion without heat flow; c→d, heat out Q_2 at constant temperature T_2; and d→a, compression without heat flow to the original volume and temperature.

$$\Delta S_{\text{thermo}} = \frac{Q}{T}.$$

Entropy, arrow of time (and irreversible heat machines)

$$\frac{Q_1}{T_1} = \frac{Q_2}{T_2}.$$



Mixing entropy

Information and entropy via mixing: how much information there is in a configuration?

“Counting entropy”

Maxwell’s demon and entropy – and information.

$$S_{\text{unmixed}} = 2\,k_B \log[V^{N/2}/(N/2)!], \qquad S_{\text{mixed}} = 2k_B \log[(2V)^{N/2}/(N/2)!],$$

$$\Delta S_{\text{mixing}} = S_{\text{mixed}} - S_{\text{unmixed}} = k_B \log 2^N = N k_B \log 2.$$

$$S_{\text{counting}} = k_B \log(\text{number of configurations})$$

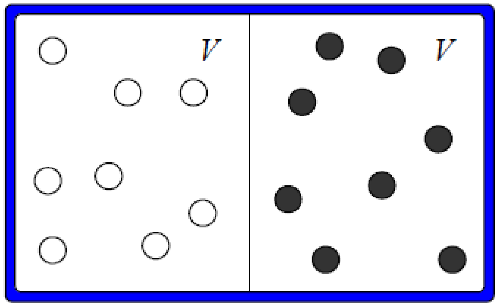


Fig. 5.4 Unmixed atoms. The premixed state: $N/2$ white atoms on one side, $N/2$ black atoms on the other.

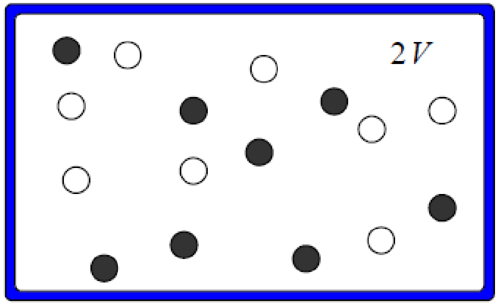


Fig. 5.5 Mixed atoms. The mixed state: $N/2$ white atoms and $N/2$ black atoms scattered through the volume $2V$.

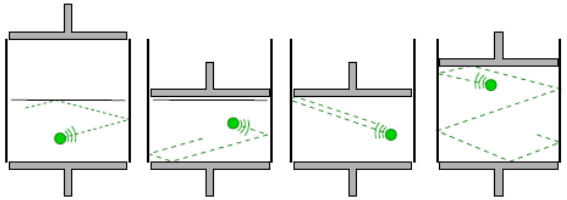
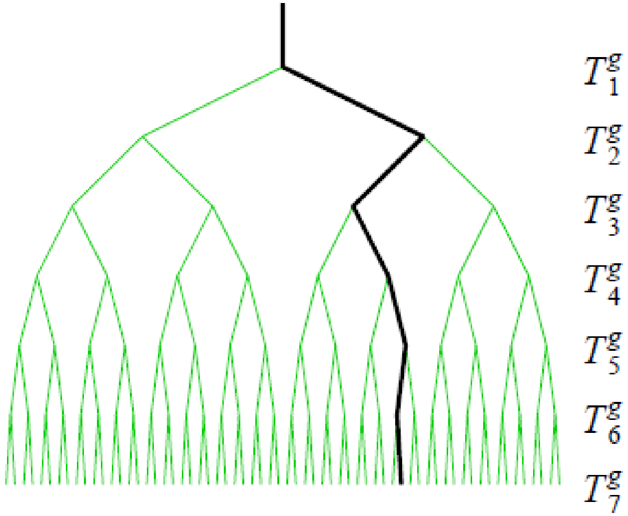


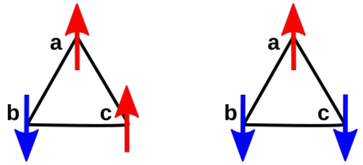
Fig. 5.11 Expanding piston. Extracting energy from a known bit is a three-step process: compress the empty half of the box, remove the partition, and retract the piston and extract $P\,dV$ work out of the ideal gas atom. (One may then restore the partition to return to an equivalent, but more ignorant, state.) In the process, one loses one bit of information (which side of the the partition is occupied).

Residual entropy of glasses

Argument: locally glasses are two-state systems (position of an atom in an amorphous system). Cool a glass from a liquid: freezing will lead to a random configuration, with a lot of frozen, metastable two-state configurations (extensive).

$$S_{\text{residual}} = S_{\text{liquid}}(T_\ell) - \int \frac{1}{T}\frac{\mathrm{d}Q}{\mathrm{d}t}\mathrm{d}t = S_{\text{liquid}}(T_\ell) - \int_0^{T_\ell} \frac{1}{T}\frac{\mathrm{d}Q}{\mathrm{d}T}\mathrm{d}T \quad ($$





Compare: Triangular Ising Antiferromagnet
(Residual T=0 entropy known)

Entropy: information, non-equilibrium

Various ways of considering the question, how random is a probability distribution (discrete, continuous, quantum statistical mechanics [density matrix – based], information theoretic).

$$S_{\text{discrete}} = -k_B \langle \log p_i \rangle = -k_B \sum_i p_i \log p_i.$$

$$S_{\text{nonequil}} = -k_B \langle \log \rho \rangle = -k_B \int \rho \log \rho$$
$$= -k_B \int_{E<\mathcal{H}(\mathbb{P},\mathbb{Q})<E+\delta E} \frac{\mathrm{d}\mathbb{P}\,\mathrm{d}\mathbb{Q}}{h^{3N}} \rho(\mathbb{P},\mathbb{Q}) \log \rho(\mathbb{P},\mathbb{Q}).$$

$$S_{\text{quantum}} = -k_B \mathrm{Tr}(\boldsymbol{\rho} \log \boldsymbol{\rho}).$$

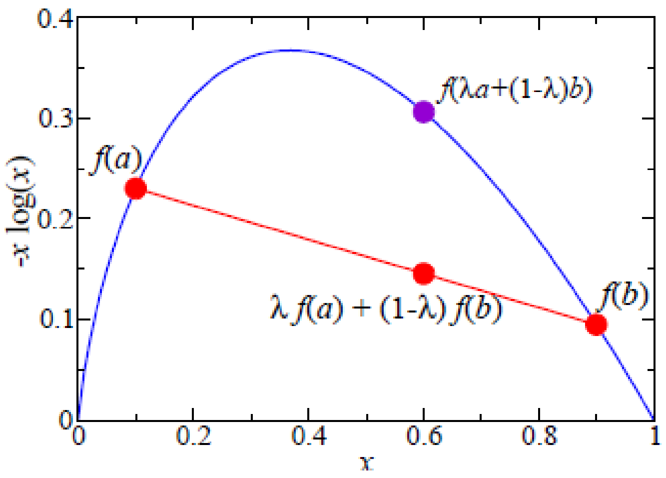
Shannon’s entropy (base 2).

$$S_S = -k_S \sum_i p_i \log p_i = -\sum_i p_i \log_2 p_i,$$

Properties of entropy

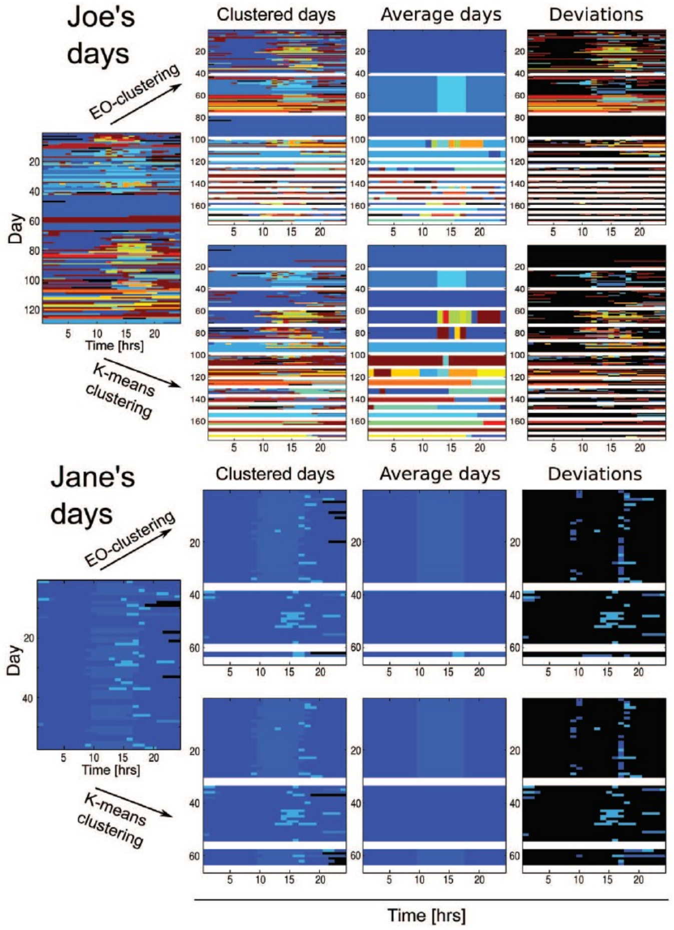
1) Maximum for equal probabilities.
2) Extra states with zero probability not important.
3) Entropy and conditional probabilities – ignorance is additive and entropy is extensive:

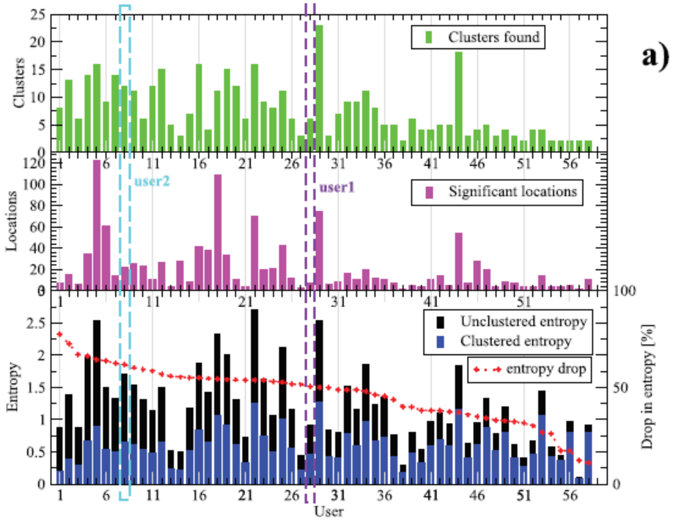
$$\langle S_I(A|B_\ell)\rangle_B = S_I(AB) - S_I(B).$$

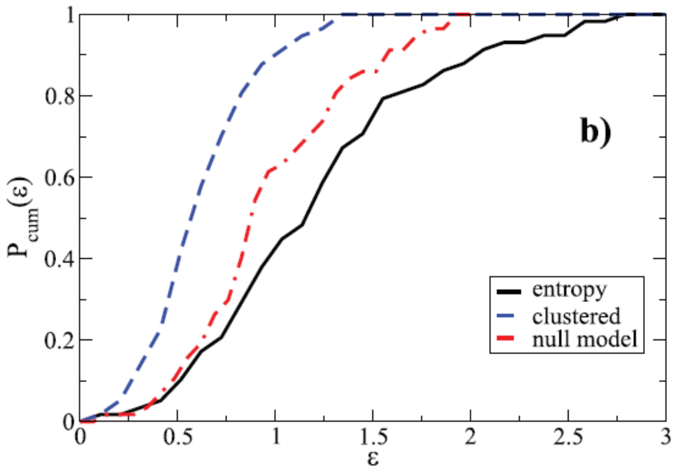


Entropy is concave!

Applications: human life







Patterns, Entropy, and Predictability of Human Mobility and Life

Shao-Meng Qin[1], Hannu Verkasalo[2,3], Mikael Mohtaschemi[1], Tuomo Hartonen[1], Mikko Alava[1]*

Take home…

We now concentrate on Ch. 5 of Sethna (Entropy). The argument splits into three main points: role of entropy in classical thermodynamics, it as a measure of disorder, and finally entropy as a way to quantify information whether the system is in equilibrium or not. Check that you get the Carnot engine argument, and - referring to the last of these - what the (Shannon) entropy must have as its fundamental properties.

The take home quiz splits into two parts. We have two applications, one of which has to do with glasses (and their entropy) and the other one refers to the use of entropy outside of physics - brain science. Your task is now to pick one of these. After that, justify why you wanted that particular one, and read the article in question and summarize it with a few sentences. A target max length for your take home is 2+8 sentences.

And, the choice is between:

https://journals.aps.org/prresearch/abstract/10.1103/PhysRevResearch.2.013202 (glasses)

https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0089948 (brains and NMR)