

Lesson 8 : Entropy, reversibility, and magnetism

*Notes from Prof. Susskind video lectures publicly available
on YouTube*

Poincaré recurrences

Let's go back to the second law and talk about Poincaré recurrences – which might also have been named Boltzmann recurrences because Boltzmann (1844-1906) studied them too, somewhat before Poincaré (1854-1912).

Here is a question we might ask. Let's suppose we start out with the air all on one side of the room. This is not an impossible thing to do. We put up a dividing wall in the middle. We evacuate the air out of one side of the room, stick it in the other side, and start with initial conditions where all the air is on, say, the right side of the room. And now we let it go.

What happens? It fills the room pretty much uniformly. It comes to thermal equilibrium. Entropy increases. But what if we sit there and wait, and wait, and wait?

Sooner or later the unlikely will happen. By accident or by just waiting long enough in time, all of the air will reappear on the right side of the room, or the top half of the room, or wherever. But let's say the right half of the room.

That is called a *Poincaré recurrence*. And that is really no different than saying that, if we flip a coin enough times, we will eventually get a million heads in a row. It is very unlikely if we flip a coin, say, a couple million times. But, if we do it long enough, such fluctuation will happen.

So the question is : How long do we have to wait for the air to all appear on one side of the room again? Is it a year? Is it ten years? Is it a hundred years? Is it the age of the

universe? So let's see if we can get a handle on that.

We start out with the idea of phase space, figure 1.

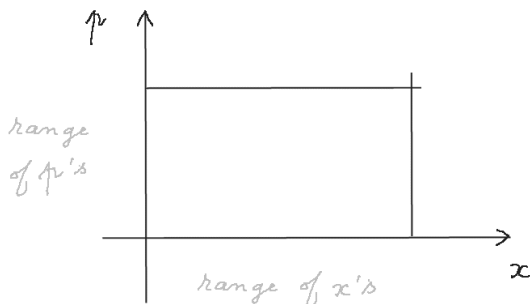


Figure 1 : Phase space of the air in the room.

The phase space is the space of the spatial coordinates of the molecules and the momenta of the molecules. Of course it is a very high dimensional space. It has $6N$ dimensions, because each particle spatial coordinate has 3 components, and its momentum also has 3 components. And there are N particles. So the x -axis in figure 1 is a schematic representation of $3N$ dimensions, and so is the p -axis.

As far as the momentum space goes, it is bounded because if any particle has an enormous momentum, it will also have an enormous energy, and we put only a certain amount of energy in the box and no more. So the momentum, on the p -axis, is definitely within some bounded range.

It doesn't matter how many particles we have. It doesn't matter how big the system is. It does matter what the tem-

perature is. The higher the temperature, the larger the momentum range. But if the temperature stays reasonable, then the momentum direction in figure 1 is bounded.

And as far as the x -axis is concerned, it runs from the left part of the room to the right part of the room. So to say that we started out in one half of the room meant that the phase point was in the region shown in figure 2.

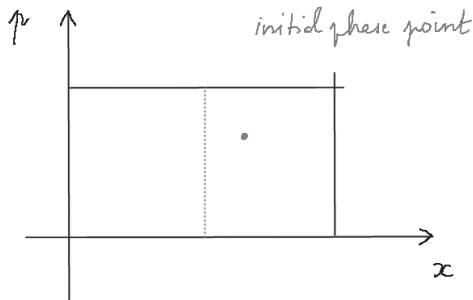


Figure 2 : Initial phase point.

In fact, let's not be detailed about where it is. It is somewhere in the region corresponding to all the particles on the right side of the room. The probability distribution is spread out over that region.

Remember also that the entire possible region in phase space, for the point representing the air in the room, is not a rectangle as in figure 2 but a high dimensional parallelepiped. So imagine splitting the parallelepiped in two parts. The first part corresponds to all the particles in one half of the room, and the second part is the complement. And the

initial point is in the first part. That is what figure 2 wants to suggest. But pay attention to the fact that in reality the two volumes are not equal at all!

Now we wait for a while. What happens? The phase point starts to move. It moves chaotically. From last chapter, we know precisely what chaotically means, But for our purposes here it simply means pretty unpredictably.

It is unpredictable not because the laws of physics are unpredictable in principle, but because, in trajectories like for example that of a billiard ball, errors or slight differences in initial detection tend to magnify themselves after a while. And so, even if we started out along two very similar trajectories, they would quickly depart.

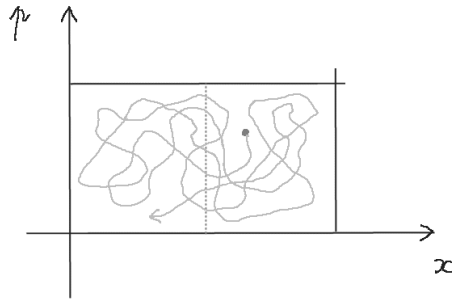


Figure 3 : The trajectory of the phase point covers pretty much uniformly the entire phase space.

Thus we can imagine that the phase point moves around in the entire range in very complicated ways, and covers pretty much uniformly the phase space, figure 3.

We say it covers pretty much uniformly the phase space in the sense that if we coarse grain it, if we blur our sight a little bit, wearing somebody else's glasses, it will look like it has pretty much filled up uniformly the phase space, figure 4.

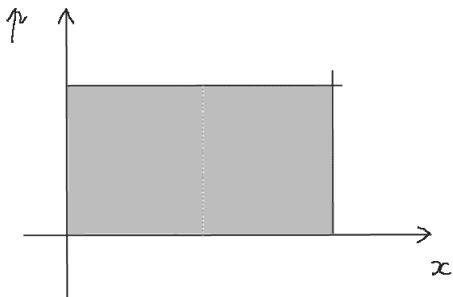


Figure 4 : Coarse graining the trajectory after a while.

Then what percentage of the time would you expect the phase point to reside in the region corresponding to all the particles in one half of the room ?

It looks like half the time. But that is crazy. We don't expect half the time the molecules to be in the left half of the room or the right half of the room.

The mistake we are making, as said, is we are drawing a picture in just two dimensions, one of position and one of momentum. If there were indeed only one spatial dimension, then it would be correct to split the area in two equal halves as shown in figure 4.

But what if we have N particles ? We are talking about the

region where, for each particle, say its first spatial coordinate is on the right half of its range.

Let's reason on two particles, i.e. $N = 2$. And let's forget about their momenta. Suppose the first particle has spatial coordinates (x_1, x_2, x_3) and the second has (y_1, y_2, y_3) . To say that the first particle is in one half of the room is to say that x_1 is in one half of its range. Same for the second particle and y_1 . So the volume of phase space where both particles are in the same half of the room is $1/4$ of the total volume of phase space.

Consequently, the percentage of the time when the air – made of two particles – is all in one half of the room is $1/4$.

What if there are three particles? Then the volume of the region in phase space where all three particles are in one half of the room is $1/2^3$. And if there are N particles, it is

$$\frac{1}{2^N} \tag{1}$$

There is another way to think about it. Let's take the phase space and identify a subregion of it. We first consider the room. The volume of the room is V , and the volume of a small region of interest in the room is v . Then the spatial volume of the entire phase space is V^N , and the volume of the subregion in phase space corresponding to all the particles in the small region of interest is v^N , figure 5.

So the percentage of the time when all the particles are in v is

$$\left(\frac{v}{V}\right)^N \tag{2}$$

If $v = V/2$ we get back formula (1).

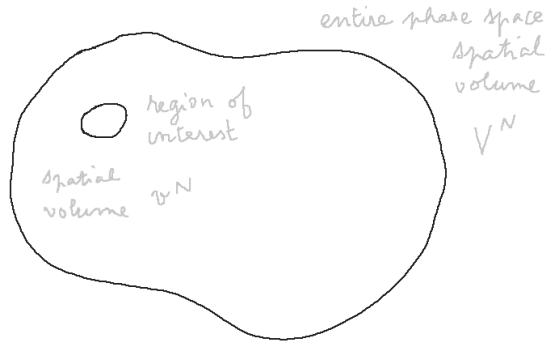


Figure 5 : Entire phase space and small region of interest.

Observe is that V^N is the exponential of the entropy of the whole system¹.

Indeed, remember that the entropy of a region of phase space is the logarithm of the volume of that region. Or, said another way, if all we know is that the system is in some region of phase space with uniform probability, then the logarithm of the volume of that region is the entropy of the system. We saw that in chapter 1 and used it in chapter 7.

What is the entropy of the molecules in thermal equilibrium in the whole room? It is $\log V$ times the number N of molecules. The order of magnitude of N is between 10^{27} and

1. To be rigorous, we should multiply by a constant factor coming from an integral over the momenta axes, but it is irrelevant in the subsequent reasonings.

10^{30} depending on the size of the room. But anyway it is a huge number. And when we take any number less than 1 to that power, we get essentially 0.

Therefore, at any time the probability for the molecules to be all in one part of the room is essentially 0, even if the part of the room is 99.999999% of it ².

What may make the above reasoning dizzying is that we alternate between considerations of volumes in the room and in the phase space. As soon as we consider a volume v in the room that is smaller than the entire volume V of the room, the corresponding volume v^N in the phase space is absolutely tiny compared to V^N , which is the exponential of the entropy of the system in thermal equilibrium.

So the probability, in a random draw of points in the phase space, that we find ourselves in the tiny volume v^N in figure 5, in case we look at half of the room, is

$$\left(\frac{1}{2}\right)^{10^{30}} \tag{3}$$

It is a pretty small number.

If globally, over an immense length of time, the fraction of time that we spend in that odd little region v^N is 1/2 to the 10th to the 30th, starting from that point, or from any point in the phase space, how long do we have to wait till we find ourselves back in that region ?

2. 99.999999% to the power 10^8 is approximately 0.4. So that number to the power 10^{20} is absolutely negligible.

It is the question of return time in probability theory, and more precisely in the theory of random walks or the theory of Markov³ processes. It is intuitively natural that the mean return time is of the same order of magnitude as the inverse of the probability at any one time to be in that region. So it is 2 to the 10th to the 30th. In what units, years, seconds? We could make it more precise, taking into account the speed of molecules and things like that, but it doesn't matter to conclude that we will never see it.

Why did we do this exercise? We did it to develop our intuition about how gases of molecules behave, and more precisely to understand in what sense systems are reversible.

We see that, if we wait long enough, they will reverse themselves. If we consider a sealed room, and we let the gas evolve, let's say starting from the odd state where all the molecules are in one corner of the room, or in one half of the room, it will quickly fill the room and come to thermal equilibrium or what looks like thermal equilibrium. It will spend a long long time there. But every so often, every once in two to the 10th to the 30th years or whatever, we will find the molecules in half of the room.

Then it will again fill the whole room, equilibrate, look conventional. And we wait another eon and all of a sudden we find the molecules in the other half of the room or in another corner of the room.

The huge number of molecules in a gas give a peculiar

3. Andrei Andreievich Markov (1856 - 1922), Russian mathematician.

meaning to the probabilistic reasonings about its behavior. Thermodynamics was developed in the XIXth century at first without any considerations of probabilities. Entropy was identified as a useful quantity in the equation $dS = dE/T$, see equations (17) or (18) of chapter 2. But when Carnot⁴ wrote that equation, in his investigation of the workings of steam engines, he did not relate it to any probability that would represent our imperfect knowledge of the state of the system.

Highly improbable events like all the molecules going back to one half of the room are to be compared with picking the black ball in the urn in figure 1 of chapter 1. And the states of thermal equilibrium are to be compared with the series like H, H, T, H, T, T, H, H where the counts of heads and tails are about equal. In most of the 2^N series of N tosses, they are about equal. That is the meaning of the *law of large numbers* : when the number of trials is large enough, the experimental frequency of heads is close to $1/2$.

One could say that thermodynamics is about the *law of very large numbers*. So probabilities are always equal to experimental frequencies. In some sense, values observed are always mean values or typical values, states are always typical states, etc.

Thermodynamics was developed at a time when the atomic hypothesis, that is the idea that matter was composed of very small particles, was only a vague supputation made by chemists like Dalton⁵ to try and explain the neat ratios of

4. Nicolas Sadi Carnot (1796 – 1832), French military engineer and physicist.

5. John Dalton (1766 – 1844), English chemist,

reactants that one always observed in chemical reactions. Therefore thermodynamics did not relate to molecules, let alone to random behavior. In fact it is the development of statistical thermodynamics by Maxwell and Boltzmann, but chiefly Boltzmann, and its great successes in explaining so clearly the classical results of thermodynamics, which reinforced the atomic hypothesis. But the reader should be aware that it was still disputed by many eminent physicists and chemists as late as 1900.

So we understand how systems like gases of molecules in a box evolve toward maximum entropy. It is an instance of the law of large numbers. Yet they are still reversible. And once in an eon they go back to an atypical state corresponding to the black ball in the urn.

In other words, if you integrate the system or study it over sufficiently long times, you will discover that the entropy sometimes goes down. Or, if you prefer, the oddness goes up and down, up and down, in a completely time symmetric way.

What is not time symmetric is what happens if you knowingly start in a very odd configuration. If you start in a tiny volume of phase space, most likely the next thing is to find yourself out of that volume. If you start in an odd situation with all the molecules in the corner of the room, you expect the next thing to find is the molecule spread out.

Perhaps the following simple example will make it even clearer. You start from H, H, T, H, T, T, H, H and you randomly change or leave unchanged each of the trials, the next series will most likely also be typical, in the sense

that it will also have roughly half heads and half tails. That is also true if we start from an unlikely series, like all heads.

We naturally go from the atypical to the typical. We also naturally go from the atypical to the typical. But we rarely go from the typical to the atypical⁶. That is the sense of irreversibility in thermodynamics. The systems however remain perfectly deterministic and reversible.

So, starting from an odd state and going to a typical one, then to another typical one, and to another typical one, and so forth, sounds like it violates the reversibility of the physical laws.

But in fact, if you waited long enough, you would find the system reversing itself and doing everything imaginable for a closed system.

That is more than an interesting point. It is a deep conceptual point that enabled Boltzmann to resolve the puzzle of time being apparently only one-way toward more disorder and more entropy, and the laws of motion being two-way.

6. These considerations do not exhaust the fascinating topics of information theory and complexity theory. What is a typical state? Is it having half heads and half tails? What about H, H, H, H, T, T, T, T ? Is it having that approximate equirepartition also in any subsequence? What about H, T, H, T, H, T, H, T ? Are the decimals of π random? What is a meaningful message, as opposed to a garbled one? Those questions in which Gödel made great progress didn't drive him to suicide, but did drive him to what is generally described as insanity. In the later part of his life, when he lived at Princeton near Einstein, Gödel was convinced that he had a mathematical proof of God. Would that be the (probable) explanation for their similar names?

Of course we will then have to understand why the universe started in a little corner of phase space. That is a separate issue. Boltzmann knew that, and he pointed out the problem.

Questions / answers session

Q. : Does this have application in cosmology ?

A. : Absolutely. And there is still this open question : Why did the universe start in a small corner of phase space? Cosmologists and physicists work on it.

Q. : So the universe is globally going toward more entropy, and will eventually reach a state of thermal equilibrium⁷. But, after it has spread out, if we waited long enough, we could see it come back once in a while close to its initial state?

A. : Yes, under the assumptions of the above reasoning, the universe is globally evolving toward thermal equilibrium.

7. Notice that "the state of thermal equilibrium" for a thermodynamical system is not one state, it is the collection of states $\Omega = \{\omega_1, \omega_2, \dots\}$, calculated from the maximization of entropy under constraints that we did in chapter 3, and over which it then roams in a random process. And, in classical physics, the randomness doesn't come from nature but from our incomplete knowledge of the exact state of the system.

Then it will "once in a while" go to an odd state, like for instance its initial one. In other words, if the universe is a closed system, it will just recur and recur and recur.

To avoid this somewhat strange conclusion, and its strange implications (see below), I think the answer is the universe must not be a closed system. A closed system doesn't make for a good statistical explanation of the world.

Q. : You said that the laws of motion are symmetric toward the future and toward the past. Then you said that time appears to be only one-way, only toward more entropy, and that was the puzzle that troubled physicists. But you added that in fact time is symmetric too. What do you mean by time is symmetric ?

A. : Consider a closed system. And you have some measure of the localization of the particles. Suppose the system starts in a corner of phase space. That is the particles start concentrated around some location, and therefore their localization measure begins with a high value.

If you sit and follow your measure of localization as the system evolves, you will see that the particles become quickly less localized. And then they will be pretty delocalized for a long time.

Suddenly at some unexpected time they will localized again. So, over a very long period, you will see the localization measure go down and up, down and up...

However the timescale to discover this reversibility – and therefore this symmetry of time –, that what goes up must come down so to speak, or the other way around if you prefer, is a time length of 2 to the 10th to the 30th.

Q. : Would the process of going back to some order be symmetric with that of going into disarray ?

A. : Yes, they would look the same, except with time reversed.

Every now and then you would find the molecules in exactly the right configuration to swoosh into the corner, pretty much the same way they swooshed out of the corner.

In fact you will see everything happen, every possible states and every possible evolutions. And they will happen in both directions of time.

Q. : So this has nothing to do with the fact that we started in a small region of phase space ?

A. : Yes, that is correct. The evolution to an odd state doesn't require that we started from an odd state.

But precisely, if we are trying to understand why the world looks the way it does, we must explain why it seems to have started not from any state, but from a very orderly one.

The problem can be formulated as follows – and Boltzmann already knew it, but it has known a renewal in recent years with the discovery of exoplanets. Suppose the universe really were a closed box and you asked : What is the most likely configuration to find a planet with people on it ? What is the most likely possibility ?

You would discover that the most likely possibility is to have uniform gas everywhere, except the smallest possible amount of gas, necessary to make up a planet, having condensed into the planet.

The chances that you see one planet are very small, say ϵ . And the chances that you see two planets are vastly more negligible. In a simple model it is ϵ^2 . But we won't even have to resort to that latter probability to explain why what we see doesn't really make sense in a closed universe.

If you are asking the question : What should astronomers expect to see out there – conditional on the fact that there is already a planet in the universe with astronomers on it doing astronomical observations ? What is the most likely thing they will see ?

The most likely thing is they would look out and see nothing, because, even conditionally on the existence of their planet, the chances that they see a second planet are very small. They are again ϵ . May be they will see some gas out there. But they will not see it condensed into another planet. So by far the most likely thing we should see is our own planet and no others.

What is the probability to see the universe filled with stars ?

Absolutely negligible, unless you knew that in a fairly recent past you started from some very exceptional and unusual starting point. And then the flow out from that starting point is likely to have certain kinds of structure that a random fluctuation would not have.

It is called the problem of Boltzmann brains. It bears that name because people are a little bit excessive on it. They say the most probable astronomer would be a single astronomer's head, looking like Boltzmann's, disconnected from anything else.

The crux of the matter is trying to use statistics and random fluctuations to understand why our world is the way it is. We consider an unlikely event X – us in the world, with probability ϵ – and then another unlikely event Y – anybody else out there? We ask what is the conditional probability of Y given X , or things like that. We may even use ϵ^2 if we don't want to take ourselves for granted.

Anyway we try to make it work, it is not a good theory to think that we are just the result of a random fluctuation.

Observe, by the way, that if we were the result of a random fluctuation where things just assemble themselves sort of accidentally, or what is apparently accidentally, into a planet with people on it, we would have no good explanation for the coherence of history. Why would there be a consistency to the sequence of historical facts if the universe had materialized then by random fluctuation? Why would all history books describe history the same way?

Let's not worry about it. It is not a good theory of nature.

Q. : Can't we just say that we live in world that takes a very long time to reach equilibrium?

A. : Yes, you could say that. But you would nevertheless run into the problem of having to explain how we got where we are from a random fluctuation, to explain what we see, to explain the coherence of history, etc.

Serious theoretical cosmologists do worry about it. But I am not going to try to sell you anything.

It is something that is of concern, that if we want to use statistics and ask what is the most probable thing we should see, given that we are here, we have to take into account all the ways we could have gotten here.

Most of the ways we could have gotten here would be by random fluctuation. History would not be coherent, etc.

Ok, that is it for the problem of Boltzmann brains.

Q. : Isn't the problem solved by the fact that life creates order and decreases entropy?

A. : No, no, not at all. Life doesn't decrease entropy.

You may see order brought about by life, and see something decreasing its entropy, but it is always at the cost of some-

thing else increasing its entropy.

The second law does not say that some subsystem of the world can't decrease its entropy. But it will always be at the cost of some other subsystem increasing its entropy even more.

Q. : A living process, however, seems to last for a very long time. It is not something that comes together then goes away, like, in phase space, the random passage of the system through an odd state. The fact that life is auto-maintained is a little strange.

A. : Life on Earth is caused by the flow of energy from the Sun. The Earth is not in equilibrium. It is in a stationary configuration. Stationary means that it stays the same, but there is a flow.

If you have a system which has a flow moving through it, it can create interesting structures. For example a flow of water through a pipe can create vortices. Those vortices have a structure, little eddy currents and so forth.

You could imagine that the little eddy currents have enough structure to display interesting properties. But if you stop the flow by turning off a tap or sealing off the ends of the pipe, then what happens? The eddy currents disappear. The system just returns to a quiescent, dull, boring equilibrium.

Let's also stress that, even in that steady flow situation, of

course the total entropy of the whole system is increasing. Even though you are making a pump and a sink, water coming in one end, going out the other end, interesting eddy currents in the middle, etc., the water comes out warmer than it came in. So altogether the second law is not being violated.

The same thing is true on Earth. What is the flow, in the case of life, that allows this kind of apparent violation of the second principle? It is the flow of energy from the Sun.

If we sealed up the Earth, didn't let sunlight in, didn't let sunlight out, everything would eventually come to thermal equilibrium. It would be dull. There would be no life. And there would just be a featureless thermal equilibrium.

Life is a kind of eddy currents or little vortices that appear in a moving fluid, the fluid being energy from the Sun.

That is it for this questions / answers session where we discussed vast questions. Now we can get back to some more mundane things : magnets.

Magnets

When we talk about magnets in statistical mechanics, we are usually not talking about pieces of iron. We are talking about mathematical models for a class of systems that have certain features which resemble magnetism.

So, first of all, what is a magnet? Whatever an ordinary magnet is, it is made up of lots of little magnets. The little magnets could even be as small as single atoms. Or they could be little crystal grains. But, whatever, a magnet is made up of a large number of little magnets.

Typically, at ordinary room temperature – such temperature being considered rather high in this context –, and certainly at very high temperature of a thousand degrees or more, those little magnets are randomly oriented in such a way that the whole sample doesn't have a net orientation.

The orientation is random. And not only is the orientation of the whole thing random, but the relative orientation of the parts of it are random. And so there is no net magnetization. We don't see a macroscopic magnetic field from it.

Now we cool it down. If the energy which is stored in pairs of these little magnets is such that the magnets like to line up in the same direction, then, as we start to cool it down, we find out that groups or lumps of little magnets tend to be an alignment. Other lumps of magnets will also tend to be in alignment but in other directions.

So we will find sort of domains which are magnetized, meaning they tend to point in the same direction. But these domains are still fairly small.

These are experimental facts. And they are not too hard to understand. In the energy considerations, when we say that things like to be in the same direction, "like" means that the energy is lower if the little magnets are parallel and pointing in the same directions.

So as we cool the sample down more and more, if the energy is lower when the magnets are parallel, then as we suck energy out of the system more and more of them will want to come into alignment. And these domains will start to grow.

Eventually, at some low temperature, but not zero temperature, we may or may not hit a point at which all of a sudden these domains become infinitely big, so that the magnets tend to be somewhat lined up everywhere in the same direction.

That is called a ferromagnetic transition. It is a *phase transition*. And it is basically the simplest kind of phase transition.

Certainly at zero temperature we expect the elementary magnets to be all lined up. Why is that? Because, at zero temperature, the only state of importance in the Boltzmann distribution is the lowest energy state. When the temperature is zero the system is with probability 100% in the lowest energy state. And in the lowest energy state all the microscopic magnets line up.

This tendency to alignment of the microscopic magnets when we lower their energy is counterintuitive. Actually it depends on the details of the material. In a piece of iron they like to align. This runs contrary to the macroscopic observation that the North Pole wants to grab the South Pole.

It is just a little more complicated. And that is partly why there aren't that many magnetic materials. It is right that

in a microscopic pair there is also a tendency for them to want to anti-align. But there are competing phenomena going on.

Question : Don't we need an external magnetic field for them to line up? Answer : No. When their temperature is lowered they will line up spontaneously. But, without external field, which direction they line up in maybe random.

The lining-up in itself is called *spontaneous symmetry breaking*. We are going to talk about simple magnetic systems, and their tendency toward order as we cool them – "order" meaning parallelism in this case.

When the microscopic magnets line up, they can line up in this direction, or that direction, or whatever direction. So which way do they wind up lining up? That itself might be determined by the tiniest little stray magnetic field. Just one elementary microscopic magnet of the sample, one molecule, even one atom, being in an external magnetic field, which will tend to orient it, may govern the way the whole system lines up.

There is a symmetry, which is which way each little thing can point. If they wind up all pointing in one direction, that symmetry is broken. That is called breaking the symmetry. There is no more symmetry – or at least it looks like there is no more symmetry –, but it is spontaneous.

It is not the result of a magnetic field pushing everything in one direction. It just had to pick a direction, apparently randomly⁸. The direction picked may be because of a tiny

8. It is like when we flip a coin. We call it random, but the side

little stray magnetic field acting on even a single microscopic element.

These are the things we are going to talk about. We are going to examine what happens at the point where the symmetry is broken, the point where the magnets tend to line themselves up in some direction. That is a phase transition. In the case of magnets, it is called a magnetic phase transition.

First of all, don't think about literal magnets. We use models, which draw their inspiration from magnetism, to apply them to situations in statistical mechanics. But these model systems would often be quite unrealistic as actual theories of ferromagnetic chunks of iron.

What makes these models inspired by magnets interesting is of course that they resemble a lot of other things in nature. Moreover they are mathematically simple enough to be studied, and interesting enough to exhibit features like phase transitions.

Let's start with the very simplest magnet – and, as said, don't think of it as a real magnet. This kind of magnet either points up or it points down, figure 6. It doesn't get to point in all possible 3D directions.

You can think of it as heads and tails if you like. For obvious reasons, I may sometimes myself lapse into calling it a spin.

the coin ends up showing may be the result of the tiny action of some molecules during its motion. It is not like the air forcing all the molecules of the coin to arrange themselves to show heads, or tails.



Figure 6 : Simplest magnet. It has only two possible positions : up or down.

Now let's consider a collection of these elementary magnets. It doesn't matter how they are laid out on the page, but for simplicity let's lay them out in a line, figure 7. Some of them are up, some of them are down.



Figure 7 : Magnet made of a collection of N elementary magnets.

You can think of them as atoms in a crystal. The atoms have electrical currents, or maybe they have spins. Electrical currents make little electromagnets. So each atom is a magnet with a North Pole and a South Pole. The same applies to spins.

But for the simplest model that has ever been studied, and which we are going to begin with, the atoms point up or

point down. They can't point any other way. The purpose of this is to be simple.

We want to make some statistical mechanics of this, and ask such questions as : What is the relative percentage of ups and downs? What is the energy of the magnet? And so forth.

So before we begin, if we are going to be talking about statistical mechanics and the Boltzmann distribution, we must have an *energy function*. If we want to compute things like $Z = \sum e^{-\beta E_i}$ or $P_i = e^{-\beta E_i} / Z$, we need to know what the energy is.

The magnet of figure 7 is made of N elementary magnets, N being a large number. And we are going to start with the following very simple model for the energy :

- Each elementary magnet i has a magnetic moment μ , oriented either up or down.
- The orientation of i is represented by a function $\sigma(i)$ which takes the values either $+1$, for up, or -1 , for down.
- There is no interaction between the elementary magnets at all.
- Moreover, independently of the little magnets, there is a global magnetic field H in which the system is plunged.
- μ and H are positive numbers. But think of the magnetic field H as pointing downward.
- So the potential energy of the little magnet i is $\sigma(i)\mu H$. It is higher if i is pointing upward than if it is pointing downward.

- n little magnets are up, and m little magnets are down. Thus $n + m = N$.

The energy of the whole system, that is of the magnet formed by the N elementary magnets, is

$$E = (n - m)\mu H \quad (4)$$

which could also be written

$$E = \mu H \sum_{i=1}^N \sigma(i) \quad (5)$$

But we won't use the notation with the σ 's for the moment. Moreover since the figures μ and H are given constants entering the model only through their product, sometimes μH is simply called h . It is clearer, however, to spell out how the model is built.

How many configurations are there with n ups and m downs, without imposing which ones are which? There are N choose n , denoted $\binom{N}{n}$. And the formula is

$$\binom{N}{n} = \frac{N!}{n! m!} \quad (6)$$

remembering that $m = N - n$. That is the number of configurations which have the given energy E of equations (4) or (5).

$\binom{N}{n}$ is called a binomial coefficient. To refresh his or her knowledge of the binomial coefficients, the following exercise is proposed to the reader.

Exercise 1 : Prove that

$$\sum_{n=0}^N \binom{N}{n} = 2^N \quad (7)$$

Now what is the Boltzmann weight corresponding to *one* configuration? By definition it is $e^{-\beta E}$, where E is the energy of that configuration.

The partition function is the sum of all the Boltzmann weights. So we have

$$Z = \sum_{n,m} e^{-\beta \mu H(n-m)} \quad (8)$$

where the sum is meant over *all* the configurations, with the appropriate multiple counting.

Now, for each value of $(n-m)$, there is going to be a certain number of configurations. And that number of configurations is the combinatorial coefficient of equation (6).

In order to simplify expressions, and to trigger memories from high school, let's define the two variables

$$\begin{aligned} X &= e^{-\beta \mu H} \\ Y &= e^{+\beta \mu H} \end{aligned} \quad (9)$$

Then equation (8) for the partition function can be rewritten

$$Z = \sum_{n=0}^N \binom{N}{n} X^n Y^{N-n} \quad (10)$$

And lo and behold, that is the binomial expansion of $(X + Y)^N$. So we have figured out that Z is :

$$\begin{aligned} Z &= (X + Y)^N \\ &= \left(e^{-\beta\mu H} + e^{+\beta\mu H} \right)^N \\ &= 2^N \left(\frac{e^{-\beta\mu H} + e^{+\beta\mu H}}{2} \right)^N \\ &= 2^N \left(\cosh(\beta\mu H) \right)^N \end{aligned} \quad (11)$$

The factor 2^N is a multiplicative constant. We know that, in a partition function, it has no importance, because we shall take the log and then differentiate. And when we differentiate a constant we get zero. But let's leave it there for the sake of completeness.

Now, suppose we are interested in the question : What is the relative percentage of up spins and down spins? This quantity has a name. It is called the *magnetization*.

The magnetization is 0 if there are as many up spins as down spins. It is positive if there are more up spins than down spins. And it is negative in the opposite situation.

The number $(n - m)$ is the difference between up spins and down spins. So it is linked to the magnetization. The usual definition of the magnetisation is

$$M = \frac{(n - m)}{N} \quad (12)$$

So it becomes a percentage between -1 and $+1$. We can view it as the magnetization per little magnet if we like. It is the bias for each elementary magnet toward up or toward down.

The magnetization is clearly related to the energy. We will just write a few equations and then we will be able to use the partition function. To start with

$$E = NM\mu H \quad (13)$$

We will use definition (12) and equation (13). Let's keep them in mind. We will come back to them.

We have introduced many definitions, but *magnetization* is an important one. It is roughly speaking the probability of being up minus the probability being down for a given spin.

How can we calculate the magnetization? One easy way is to calculate the energy of the system. If we know the energy of the system, and we know the number of particles⁹, and we know μ and we know H , from equation (13) we can calculate the magnetization.

So the first thing we shall calculate from the partition function is the average energy. From that we can read off the magnetization.

9. We use indifferently the terms particles, little magnets, or spins, to describe the elementary magnets making up the system in figure 7.

Of course in the same way there is an energy per configuration and there is an average energy, there is a magnetization per configuration and there is an average magnetization. Equations (12) and (13) hold for each configuration. And they also hold for the average, or expected, values.

What we are interested in is the *average magnetization* of the system under various circumstances which we shall look at. So it should be denoted, more properly,

$$M = \left\langle \frac{(n - m)}{N} \right\rangle \quad (14)$$

It is the expected value of the magnetization of the configurations when they have the Boltzmann distribution of probability $P_i = e^{-\beta E_i} / Z$.

Remember that generally speaking in statistical mechanics we consider a system which can be in a collection Ω of states, see chapter 1, with a probability distribution, or measure, P over Ω . Each state, or configuration, has various characteristics, like its own energy, or here its own magnetization. But unless otherwise specified, when we talk about the energy, or the magnetisation, or any other characteristics of the system, we mean the average value over the probability distribution P . And, unless otherwise specified too, the probability distribution P is the Boltzmann distribution at equilibrium – which is the one which maximizes the entropy, see chapters 3 and 4¹⁰.

10. Unlike energy, or magnetization, which can be defined for *each state*, the entropy is only defined for the collection Ω of states and the probability measure P on it. P is a measure of our incomplete knowledge of the exact state $\omega \in \Omega$ the system is in. The probability measure which maximizes the entropy under the constraint that the

Now what do we do to calculate the average energy? We take the logarithm of the partition function, differentiate it with respect to β , and change the sign of the result.

Before we do this calculation, let's build our intuition about this system. Remember that it is a very simple model of N little magnets plunged into a magnetic field H as described in the comments to figure 7. The energy of each particle is positive if it is up, negative if it is down. Systems like to have lower energy, meaning to say that the Boltzmann distribution favors lower energy.

Which way will it be at zero temperature? All little magnets down. So, at zero temperature, what do we expect the magnetization to be? If everybody is down, from equation (14) that means the magnetization will be -1 .

What do we expect at infinite temperature? Fifty fifty. At infinite temperature everything is maximally random. All states are equally probable. Therefore, at infinite temperature, we expect the magnetization to be 0.

So M goes from -1 at zero temperature, to 0 at infinite

average energy is a given, is called the Boltzmann distribution.

The *Boltzmann distribution* should not be confused with another fundamental concept of statistical thermodynamics introduced by Boltzmann too, and which we haven't talked about : the *Boltzmann equation*, which governs the time evolution of the probability distribution for a system not in equilibrium. For a book mixing good biographical elements and good science and equations, see for instance, *Ludwig Boltzmann, The Man Who Trusted Atoms*, by Carlo Cercignani, Oxford University Press, 1998.

temperature. This is what we expect. At no point will M be positive. The average magnetization will not be positive because of the bias down. The infinite temperature will defeat the bias. At infinite temperatures it is just so random that a little bit of magnetic energy is unimportant.

As we saw, instead of calculating the average magnetization, we are going to calculate the average energy, using the equation

$$E = -\frac{\partial \log Z}{\partial \beta} \quad (15)$$

There is a little bit of algebra to do here. From equation (11), and dropping the constant coming from 2^N , we get

$$\log Z = N \log (\cosh(\beta\mu H)) \quad (16)$$

Notice first of all that is proportional to N . That is a good thing because typically energies when we differentiate will be proportional to N .

Let's differentiate equation (16) with respect to β . We apply the chain rule for differentiating a function of a function :

$$(f \circ g)' = (f' \circ g) \times g' \quad (17)$$

also written

$$\frac{df(g)}{d\beta} = \frac{df(g)}{dg} \frac{dg}{d\beta} \quad (18)$$

to explain heuristically the rule. It requires, however, a bit

of elementary differential calculus to justify cleanly.

In equation (16), f is the function logarithm, whose derivative is $1/f$. And g the hyperbolic cosine, whose derivative is hyperbolic sine. So we get

$$\frac{\partial \log Z}{\partial \beta} = N \frac{\sinh(\beta\mu H)}{\cosh(\beta\mu H)} \mu H \quad (19)$$

Is that the average energy? Not quite. We must put a minus sign

$$E = -N \tanh(\beta\mu H) \mu H \quad (20)$$

Now, from equation (13), to get the average magnetization, we divide by N and by μH .

$$M = -\tanh(\beta\mu H) \quad (21)$$

Now all we have to do to understand the system is understand what the \tanh function looks like. Incidentally β is one over the temperature. So we just want to plot this function as a function of the temperature. μ times H is only a number. It is not so interesting. We could absorb it into β and plot $\tanh(\beta\mu H)$ as a function of $\beta\mu H$. They come in together.

But first of all, simply, what does the \tanh function look like? The reader can do it by him- or herself. It can be figured out easily from what \cosh and \sinh are. Remember

that

$$\begin{aligned}\cosh x &= \frac{e^x + e^{-x}}{2} \\ \sinh x &= \frac{e^x - e^{-x}}{2}\end{aligned}\tag{22}$$

The functions \sinh and \cosh , for very large values of the argument, become equal to each other, because the term e^{-x} becomes negligible. They are then basically both exponential of x , divided by two.

On the other hand, when the argument becomes very small, the \sinh tends to 0, and \cosh tends to 1. Therefore \tanh tends to 0.

To see what is the slope of \tanh at 0, we can expand \sinh . It is easy to see that $\sinh \approx x$. So the first derivative of \sinh as well as \tanh , at zero, is one.

Here is the graph of \tanh , figure 8.

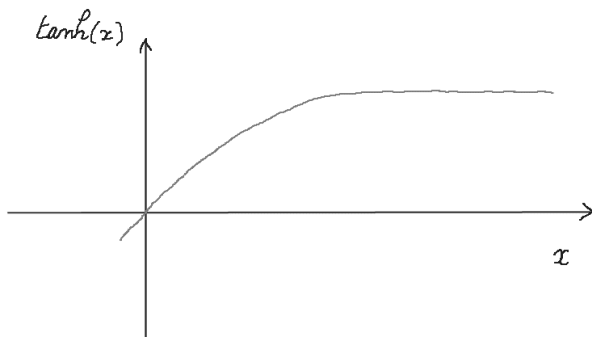


Figure 8 : Graph of hyperbolic tangent.

The function is symmetric about the origin, but we are not concerned with negative values of the argument in our study of M . Indeed we want to study the value of $-\tanh(\beta\mu H)$ as a function of temperature.

Since $\beta = 1/T$, we see that when the temperature becomes very high, $\beta\mu H$ becomes very small, and the average magnetization is zero. Whereas when the temperature becomes very low, β and $\beta\mu H$ become very large, and then $-\tanh(\beta\mu H)$ tends to -1 .

Going back to the physical meaning of these results, when the temperature is very low, all the spins are down, the energy is minimum, and $M = -1$. When the temperature is very high, $\beta = 0$, the entropy is maximum, and the magnetization is 0 as expected.

The graph in figure 8 just fills in the exact details for the problem of how the magnetization goes from -1 at low temperatures to 0 at high temperatures.

Notice that the evolution of the magnetization from 0 to -1 when we go from high to low temperatures is continuous. There is no jump in the magnetization at some temperature. This is an important point we will now take up, and pursue in the next chapter. The simple system we just studied has no *phase transition*. The reason is that it is too simple.

The first interesting system that has a phase transition is the two-dimensional Ising model¹¹. But first of all we are going to do the one-dimensional Ising model, because the

11. named after Ernst Ising (1900 - 1998), German physicist, who, after 1947, lived and worked in the United States.

system we just studied doesn't belong to the class of Ising models. It was even simpler than them.

In the 1920's Ernst Ising was a student of Wilhelm Lenz¹² at the University of Hamburg. Lenz gave Ising, as a subject for his Ph.D. thesis, the study of a model of magnet made of a linear chain of small magnetic moments coupled by interactions between neighbors. What Ising had to determine was whether in that model there was a phase transition.

Ising solved the problem and gave the correct answer that in one dimension there is no phase transition. Then he wrote that he thought in two dimensions there would not be a phase transition either. That was wrong. Actually it was a much harder problem to tackle. Two physicists, Kramers and Wannier, solved it in the 1940's.

Ising models turn out to be very important in statistical mechanics and other branches of physics. And Ising's name is most famous. It might be thought that his fame is somewhat larger than his merits. So it often goes in science.

The interesting thing about Ising models is that they are symmetric between up and down. Therefore, if there is any magnetization, it is because somehow the system has spontaneously broken the symmetry. In the one-dimensional Ising model that does not happen. In the two-dimensional Ising model it does happen.

Let's define all of the Ising models. The energy is not stored particle by particle. And there is no external field. So, if the little magnets didn't interact with each other, there would

12. Wilhelm Lenz (1888 - 1957), German physicist.

be no energy. And, if there's no energy, all configurations are equally likely.

In the simplest Ising model the magnetic field that each spin sees is due to its two neighbors. If both neighbors are up, it feels the magnetic field up. If both neighbors are down, it feels the magnetic field down. And, if one is up and one down, it feels no magnetic field. In other words, the energy is associated with pairs of neighboring spins.

Now we have to make a choice of model. We can choose the energy of a pair to be minimum when the two spins are pointing in the same direction – we call them *aligned*. Or we can choose the energy of a pair of spins to be minimum when they are *antialigned* or *unaligned*. We will come back to the variables σ 's defined above to express that.

Let's decide that the energy of a pair is minimum if they are aligned, and maximum if they are unaligned. Then we express the energy of a pair as follows

$$E = -j \sigma(1) \sigma(2) \tag{23}$$

j is just a number with units of energy. The particles are on a lattice which is just *a line* as in figure 7. And particle 1 and particle 2 are two neighboring particles. Later on, we will allow the lattice to be two-dimensional or more.

1 and 2 are called neighboring *sites on the lattice*. Equation (23) is the energy of the 1-2-pair. If the two spins in the two sites are unaligned, the product of their σ 's is -1 . So their energy is j . Whereas, if they are aligned, the energy of their pair is $-j$. Therefore the energy is lower when they

are aligned.

Now supposing we have a line of them, and each one is interacting with its neighbor, then we can write for the energy of the whole system

$$E = -j \sum \sigma(n) \sigma(n + 1) \quad (24)$$

This is the sum of the energy in neighboring pairs. And each of these neighboring pairs is counted once.

Let's pore over equation (24) for a moment. What do we expect to happen at infinite temperature? The general rule is that infinite temperature is just random chaos¹³. Everything is equally likely. The spins are randomly up or down, and this leads to zero magnetization.

The products $\sigma(n) \sigma(n + 1)$ on the average will be equal to zero. This looks disturbing because $\sigma(i)$ is either -1 or $+1$. So how come the product of $\sigma(n)$ and $\sigma(n + 1)$ can be zero? But we are talking about its *average*. And don't forget that the average of a random variable is not necessarily one of its possible values. The average of a well balanced die is 3.5 for instance.

So high temperature corresponds to zero energy – which is high energy in our model – and to zero magnetization.

What about zero temperature? The spins will be aligned. But which way are they going to be aligned? Are they going

13. Chaos here is used in its general English sense, not in the technical sense used for the behavior of certain equations when we change a bit initial conditions.

to be all up, or all down? Unlike in the first model studied above, where figure 7 was plunged in an external field H , we can't tell offhand.

There are two ground states now. Ground state means state of minimum energy. And the two ground states will come out with equal probability.

Now let's add one more thing. Let's suppose that there is an external magnetic field. But it is only acting on one particle. One out of 10^{23} particles is subject to a little stray magnetic field. And let's say that magnetic field is along one axis, i.e. up or down. Then what is the ground state? Now the ground state has a definite orientation.

Even if that magnetic field is very small, the ground state still has a definite orientation. And at strictly zero temperature, the Boltzmann distribution always favors infinitely strongly the lowest energy state. That means that even with the tiniest little stray magnetic field, the Boltzmann distribution will favor all of the spins pointing along one direction.

If you were to apply that tiny magnetic field, let the system come to equilibrium at zero temperature, and then remove the magnetic field, then the system would remember it. Everybody is holding everybody else in place, and the possibility of them all simultaneously jumping to the opposite state is remote if there is enough of them.

That is what is called *spontaneous symmetry breaking*. In this case it is very simple. And this example, characterized by equation (24), has a symmetry. We can actually say

quantitatively, or mathematically, what that symmetry is.

A symmetry is usually represented by a mathematical operation on the degrees of freedom. What operation would you do on σ to change from up to down? Multiply by -1 .

Let's go back to the earlier case where the energy was proportional to just σ itself, not σ times a neighboring σ . Does this have a symmetry? No. The energy itself changes sign when you change σ . And that is not a symmetry. Symmetries are actions that you can do that don't change the energy.

Now what about the simplest Ising model that we studied next? Furthermore, suppose there is only one pair. In equation (23), you change the sign of one spin, just one of them, for instance $\sigma(1)$ but not $\sigma(2)$. Is that a symmetry? No. The energy changes, figure 9a.

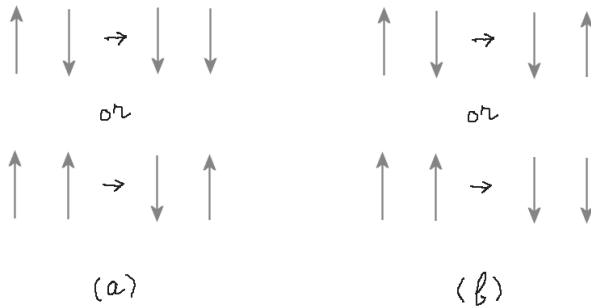


Figure 9 : Ising model, one-dimensional, and with only one pair. On the left part, we change only one spin. On the right part we flip both spins.

But what if you change them both? Then the energy of the pair doesn't change sign, figure 9b. For instance if you take them from two up to two down that is a symmetry, figure 9b lower case.

But now consider the whole vast array of spins, or magnetic moments, figure 10.

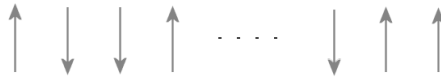


Figure 9 : Ising model, one-dimensional, many elementary magnetic moments.

What if we change all of the sigmas simultaneously? We can write formally the equation of the transformation

$$\text{for all } i, \sigma(i) \rightarrow -\sigma(i) \quad (25)$$

In other words, we replace every σ by minus its value. Then the energy doesn't change. And that is what it means to have a symmetry.

A symmetry is an operation we can do on the coordinates of a system such that, no matter what state we started from, the end state has the same energy.

That ensures that in some sense there is no bias to up or down. If the system is going to flop itself all simultaneously into up at zero temperature, that means it could have also flopped itself into down. There is no way to predict in ad-

vance, unless you know that tiny little stray magnetic field.

There is no way to predict in advance which way it is going to go. But it is going to go one way or the other, because the Boltzmann distribution says we have got to be in the ground state for 0 temperature. As we said, the little tiny stray magnetic field will determine which one it is¹⁴, but it will be one of them.

The next thing we want to do is solve the one-dimensional Ising model. From equation (24), we want to calculate the partition function for the system.

We will do that in chapter 9. We will work it out. And we will see that it does not have a phase transition at a finite temperature. Nothing funny happens at finite temperature in the one-dimensional case as Ising showed in his Ph.D. thesis.

Then it took a few more years for Kramers and Wannier to prove that if the system is a two-dimensional lattice, then, contrary to what Ising believed and wrote, there is a phase transition.

That is a beautiful story, of which we will try to get a whiff.

14. Like the result of flipping a coin will be determined by tiny, hard to measure, atmospheric conditions, but it will end up heads or tails with equal probability.