

UBC Physics Circle



Session 2: Problems

October 17, 2019

This week, we will be delving into the mysteries of matter. Our first problem shows how the competition between energy and disorder controls the structure of crystals. We then move on to magnets, and deduce (for a simple model) that there are magnetic materials in 2D, but no magnets in 1D. We end with a scheme for simulating the 2D Ising model with a biased coin, and relate the bias to the temperature.

1. The cost of free energy

How do energy and entropy dictate the structure of a crystal?

Place a glass of ice cold water in a hot room at temperature T . Over time, the glass will heat up until it stabilises to the ambient temperature; this is called *thermal equilibrium*. In equilibrium, we can predict the energy of the glass, using the basic principle that nature is lazy. But perhaps it is more apt to say that *nature is cheap*: it wants to choose a state which "costs" as little as possible, and energy is expensive. But just like Costco, there is a discount if you buy in bulk!

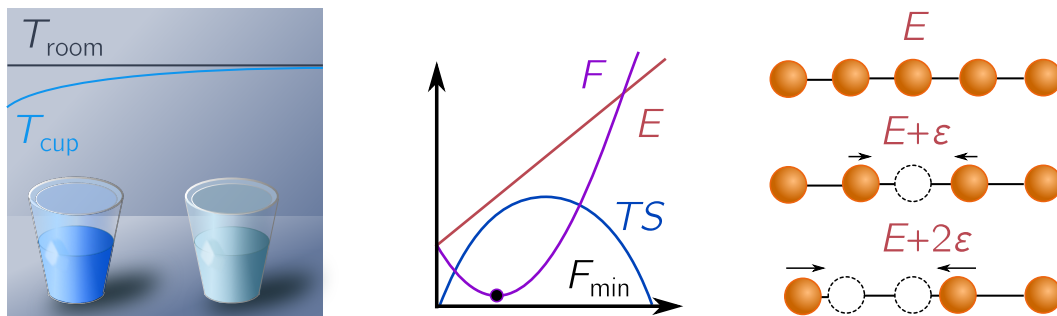


Figure 1: *Left.* A cool glass in a hot room soon reaches thermal equilibrium. *Middle.* The free energy is the energy cost with an entropy discount. *Right.* A crystal of N iron atoms. Removing atoms causes a strain on nearby sites, with an associated energy cost ϵ per vacancy.

Let's make this precise. Systems in equilibrium like to minimize the *free energy*:

$$F = E - TS.$$

Here, E is the energy of the state, while T is the system temperature (usually measured in Kelvin). The last term, S , is the *entropy*. You may not have seen this before, but we will

now define it! If there are W states with the same energy as the one we are considering, the associated entropy is

$$S = k_B \log W,$$

where $k_B = 1.4 \times 10^{-23}$ J/K is *Boltzmann's constant*. When comparing states A and B of a system at temperature T , state A will be favoured over state B when the free energy cost of A is smaller than B :¹

$$0 > \Delta F = \Delta E - T\Delta S,$$

where $\Delta E = E_A - E_B$ and $\Delta S = S_A - S_B$.

Consider a crystal² made of N iron atoms. Crystals can form with gaps in the lattice where an atom is missing. The more gaps or “defects” that are present, the weaker the crystal, so if the crystal is grown in the lab, we might hope for a way to reduce the number of defects. Removing an atom from the crystal lattice places a strain on the remaining atoms, with an energy cost of ε per vacancy, so the total energy is $E = N_d \varepsilon$ for N_d atoms removed. Let's use the free energy principle to find how many defects a lab-grown iron crystal is likely to have.

1. (a) How many defects are present in the lowest energy state? What is the entropy?
- (b) What is the energy for a single defect? Compute the number of single-defect configurations and the associated entropy.
- (c) There are $N = 8.5 \times 10^{22}$ iron atoms in a cubic centimetre of iron. How low must the temperature be for the zero defect state to be favoured over the one defect state? Take $\varepsilon = 1.4 \times 10^{-19}$ J.
2. For this problem, you will need the *binomial coefficients*

$${}_n C_k = \binom{n}{k} = \frac{n!}{(n-k)!k!}.$$

- (a) What is the free energy for a system with N_d defects out of N possible sites? No need to simplify your answer.
- (b) What is the change in free energy when going from N_d to $N_d + 1$ defects? You may assume that there are many defects, $N_d \gg 1$. Express your answer in terms of the *concentration of defects*, $n = N_d/N$.
- (c) Recall that the configuration which minimises free energy $F = E - TS$ (at some fixed temperature T) is the one that is actually realised. We can keep adding defects while $\Delta F < 0$, but when we reach the minimum, we find that $\Delta F = 0$. Use this to show that the thermodynamically favoured number of defects n_{eq} at temperature T is

$$n_{\text{eq}}(T, \varepsilon) = \frac{1}{1 + e^{\varepsilon/(k_B T)}}.$$

- (d) Use the previous question to estimate the number of vacancies in 1 cubic centimetre of iron at room temperature, using the parameters from Question 1(c).

—Daniel Korchinski

¹We will see why in today's last problem.

²A crystal is any structure which repeats periodically in space, including a metallic lattice.

2. Ising into phase transitions

Why are there magnetic materials in 2D, but not in 1D?

The simplest model of magnetic material is the *Ising model* (pronounced "easing"), a lattice of tiny bar magnets that can point up or down. These little magnets, or *spins*, feel their immediate neighbours and want to align with them. For a one dimensional chain, we label spins 1 through N , and they take values $s_i = \pm 1$, with $+1$ called "up" and -1 "down".

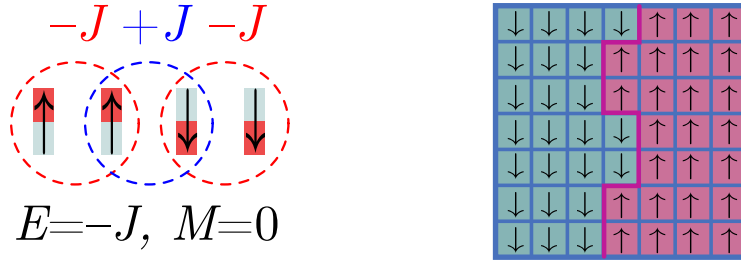


Figure 2: *Left.* Aligned Ising spins have an energy $-J$, while anti-aligned spins have energy $+J$. *Right.* Two spins domains, separated by a boundary of length $L = 10$, in a 7×7 grid.

Whenever two neighbouring spins are the same, they have energy $-J$ and whenever they are different, they have energy $+J$. The energy is therefore

$$E = -J(s_1s_2 + s_2s_3 + s_3s_4 + \cdots + s_{N-1}s_N).$$

The sum of spins

$$M = s_1 + s_2 + \cdots + s_N$$

is called the *magnetization*.

1. (a) What is the energy of the configuration: $\{-1, -1, -1, 1, 1, -1, -1, -1, +1, -1\}$?
- (b) For N spins, find the configurations with smallest and largest energy. What is the magnetization M in each case?

Our next goal is to check whether a hot, one-dimensional chain can be *magnetically ordered*. A material is magnetically ordered if most of its spins point in the same direction.

2. (a) What is the energy when all N spins are aligned up, i.e. $\uparrow \cdots \uparrow$. What is the entropy?
- (b) Imagine we flip N_1 spins to -1 , all in a row. The spins now look like

$$\uparrow \cdots \uparrow \overbrace{\downarrow \cdots \downarrow}^{N_1 \text{ times}} \uparrow \cdots \uparrow.$$

What is the energy of the system now? Count the possible configurations and find the associated entropy.

- (c) Using the previous two questions, calculate the change in energy from aligned to N_1 disaligned spins. Show that when $N_1 = N/2$, the free energy change is

$$\Delta F = 4J - k_B T \log(N/2).$$

Conclude that if the chain is long ($N \gg 1$) the blob of disaligned spins are favoured at *any* temperature. We cannot have one-dimensional magnets!

Our final goal will be to show that, for a *two-dimensional* Ising model, a net magnetization is possible, but only if the magnet is cold enough. The critical temperature below which magnetization is possible is called the *Curie temperature*. We will compare two states: one with all spins aligned, and one with the system partitioned by a wall into a region of up spins and a region of down spins. The technical term for these regions is *spin domains*.

The state with a single domain of aligned spins is called the *magnetically ordered phase*. It is a phase of matter like solid, liquid, and gas. Thus, at the Curie temperature there is a *phase transition* from magnetic order to magnetic *disorder* where spins are allowed to point in different directions.

3. (a) Argue that $\Delta E \approx 2JL$, where L is the length of the wall. (You may assume the boundary is mainly straight lines.) Assuming the boundary crosses from one side of an $N \times N$ grid to the other, give a lower bound on L in terms of N .
- (b) For an $N \times N$ grid, estimate the number of boundary configurations N_L of length L . *Hint.* A very loose estimate is

$$N_L \sim CA^L$$

for some numbers C and A . What are reasonable guesses for C and A ?

- (c) Calculate the difference in free energy, ΔF , between a single spin domain (all aligned) and two domains separated by a vertical wall of length L . You should find

$$\Delta F \approx (2J - k_B T \log A)L - k_B T \log C.$$

- (d) Plug in your values for C , A and the lower bound on L from the previous questions. What happens when N is large? Use these results to estimate the critical temperature T_c at which $\Delta F = 0$. *Hint.* $N \gg \log N$ for large N .

—Daniel Korchinski

3. Mean field theory

Can we simulate 2D magnets with a biased coin?

Imagine that we have cooled down our two-dimensional Ising system enough that it is solidly magnetized in one direction or another. Most spins are pointing up, let's say. However, for $T > 0$, there will still be *thermal fluctuations*. A few spins will be pointing down, even if all of those around them are pointing up.

To see why this happens, think back to the problem about crystal defects. A single spin pointing down out of thousands pointing up is like a single crystal defect in a large crystal: it adds a lot of entropy at the cost of increasing the energy by only a little. This is what we mean by thermal fluctuations: unless $T = 0$, some fraction of the spins will be pointing against the magnetization. If T is small, this is a small fraction, if it is large, the fraction is larger, and if $T > T_c$, the magnetization goes away entirely: 50% of spins are pointing in each direction.

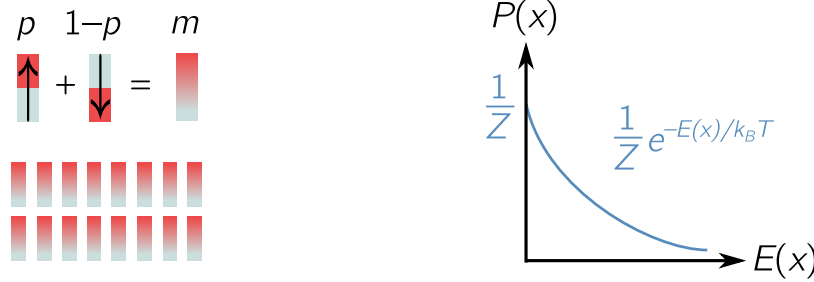


Figure 3: *Left.* The average value of spin, m , is determined by the probability the spin will point up or down. In the mean field approximation, the whole lattice is made of these averaged spins. *Right.* The Boltzmann probability distribution suppresses high energy states.

At finite temperature, the interaction of nearby spins makes the Ising model extremely difficult to analyse. We can simplify the calculation by ignoring this dependence, and instead modelling each spin as having some probability p of pointing up. This is called the *mean field theory* approximation. At a fixed temperature T , the probability of a configuration x is given by the *Boltzmann factor*:

$$P(x) = \frac{1}{Z} e^{-E(x)/k_B T},$$

where k_B is Boltzmann's constant, and Z is a normalization factor to ensure the probabilities add up to 1. This captures the intuition that low energy configurations are more likely. But by carefully distinguishing between the state, x , and its energy $E(x)$, we can finally see why free energy is minimised.

1. (a) If $W(E)$ is the number of states with energy E , show that the Boltzmannian probability distribution for energy is

$$P(E) = \frac{1}{Z} W(E) e^{-E/k_B T}.$$

- (b) Recall that the entropy for states at energy E is $S(E) = k_B \log W(E)$. Use this to rewrite the probability distribution for energy as

$$P(E) = \frac{1}{Z} e^{-F(E)/k_B T},$$

where $F = E - TS$ is the free energy as before. Conclude that states minimising the free energy are the most probable.

Let's return to the 2D Ising model.

2. (a) If each spin has probability p of pointing up, what is the average value m of the spin?
 (b) Consider two spin states, s_1 and s_2 , with respective probabilities

$$P(s_1) = \frac{e^{-E_1/kT}}{e^{-E_1/kT} + e^{-E_2/kT}}, \quad P(s_2) = \frac{e^{-E_2/kT}}{e^{-E_1/kT} + e^{-E_2/kT}}$$

Show that these formulas really only depend on the energy difference, $\Delta E = E_1 - E_2$.

3. (a) Imagine a spin s whose four neighbors all have an average spin of m . It has two possible states: up and down. What is the average energy difference ΔE_{av} between these states? *Hint.* Recall that a neighbouring spin s' contributes energy $-2Jss'$.
 (b) In the mean field approximation, we treat average energy differences as exact, $\Delta E_{\text{av}} = \Delta E$. Plug the result of the previous problem into the Boltzmann distribution from Problem 1(b), and calculate the probability $s = +1(\uparrow)$.
 (c) In Problem 1(a), you related the probability p that a spin points up to its average value m . But in the previous problem, you found an expression for $p = P(\uparrow)$ which involves m ! By equating these expressions for m , derive the *mean field self-consistency equation*,

$$m = \tanh\left(\frac{4Jm}{k_B T}\right) = \frac{e^{8Jm/k_B T} - 1}{e^{8Jm/k_B T} + 1}.$$

This tells us something remarkable. We can simulate the spins on a 2D Ising model, consistently taking interactions into account, by flipping a coin with bias m ! This is the magic of mean field physics.

- (d) The self-consistency equation cannot in general be solved exactly. Instead, consider the limits (i) $T \rightarrow 0$ and (ii) $T \rightarrow \infty$. Do these limits make sense, given a phase transition at the Curie temperature T_c ?

—Phillip Bement

Brainteaser: rainbows

What are the necessary conditions for a rainbow to form? Where would you look for one? Could you make your own?