Critical phenomena are especially common in Condensed Matter Physics. These notes are meant to provide additional context for session 11.1 where we looked for the first time at the Ising model in light of Monte Carlo simulations.

Heisenberg Hamiltonian

To study critical phenomena in Solid State Physics requires some basic notions on Quantum Physics. Let's start with the concept of spin. Contrary to what the name suggests, this is not related to orbital momentum. Rather, it's an intrinsic degree of freedom which, under quantum mechanics, is quantised: for bosons, spin can take integer values, whereas for fermions spins are semi-integers. Despite not being associated with orbital momentum, spins are regularly represented as a vector, which is alligned with a preferential direction, say z in the cartesian coordinate system. For example, an electron is a fermion with spin $1/2$, and has 2 possible states: spin up ($s_z = +1/2$) and spin down ($s_z = -1/2$). These are manifestly quantum states as they have no interpretation in classical mechanics.

Consider a magnetic lattice where in each lattice site there is an atom with a given spin. There are a number of important interaction effects to consider:

- interactions dictated by the dipolar coupling, ie, the interaction caused by the magnetic field of one atom where another atom is. This interaction is quite weak and decays with the cube of the distance between atoms. Sometimes this interaction is referred to as shape anisotropy.

- magneto-crystalline anisotropies which are due to impurities in the lattice.

- surface anisotropy which causes the formation of Bloch's domain walls.

- exchange interactions which are rooted in Pauli's exclusion principle, and which are the dominant interaction term between the two neighbouring spins (this is a very short-ranged interaction).

The last interaction was the focus of our class. Heisenberg described the coulomb interaction between two localised spins with the following Hamiltonian, sometimes referred to as the spin Hamiltonian:[1]

$$H = -2J\vec{S_1} \cdot \vec{S_2} \ . \tag{1}$$

The coupling constant J is positive for ferromagnetics, describing that spins preferentially align to achieve a low-energy state. Don't be deceived by the classical look of Eq. (1)—it's purely quantum.

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[1]The Hamiltonian is a mathematical constructor that describes a physical system's degrees of freedom. In a Quantum Mechanics setup, the Hamiltonian is an operator whose eigenvalues correspond to the energy of a given state it acts upon. So you can think of it broadly as the energy of the system.

To analytically study this Hamiltonian physicists need to perform a number of approximations. Using a Cartesian coordinate system and placing the atoms in X site with neighbours at X', we get

$$H = - \sum_{XX'} J(X - X')\vec{S}(X) \cdot \vec{S}(X') \ , \tag{2}$$

where the factor of 1 has been introduced to avoid over-counting by the two sums above. Introducing spin-raising and spin-lowering operations given by

$$S_{\pm} = S_x \pm iS_y \ , \tag{3}$$

this simplifies to

$$H = - \sum_{XX'} J(X - X')\vec{S}_z(X) \cdot \vec{S}_z(X') - \sum_{XX'} J(X - X')\vec{S_-}(X') \cdot \vec{S_+}(X') \ . \tag{4}$$

The Ising model corresponds to neglecting the last term. Since interactions are negligible except for neighbouring spins, this Hamiltonian is sometimes further simplified as

$$H_I = -J_{ij} \sum_{<ij>} \sigma_i \sigma_j \ , \tag{5}$$

with $<ij>$ denoting two nearest neighbours i and j, and $\sigma_i = \pm 1$.

Ferromagnetic materials exhibit spontaneous magnetisation at low temperatures and in the absence of an externally applied magnetic field as spins tend to align amongst themselves. Notice that their absolute value is irrelevant, it's their relative orientation that contributes to the energy of the system. There is, however, a critical temperature above which the magnetic ordering vanishes—this is known as the Curie temperature, T_C.

Anti-ferromagnetic materials on the other hand do not exhibit any net magnetisation at low temperatures and at zero external magnetic field applied. Magnetic ordering is completely lost above the critical temperature though, which in this case is known as the Néel temperature—the material becomes paramagnetic.

Bloch's law

Ferromagnetic materials exhibit spontaneous magnetisation at low temperatures, and this is mathematically described by

$$M(T) \sim \left(1 - \frac{T}{T_C}\right)^{\beta} \ , \tag{6}$$

with $\beta \approx 0.3$ for iron. At low temperatures, $T \to 0$, there is maximum magnetisation (notice this is the absolute value, so even if all the spins are pointing down, the overall absolute magnetisation is the largest). As the temperature approaches the Curie temperature, the magnetisation falls off and vanishes at the critical temperature.
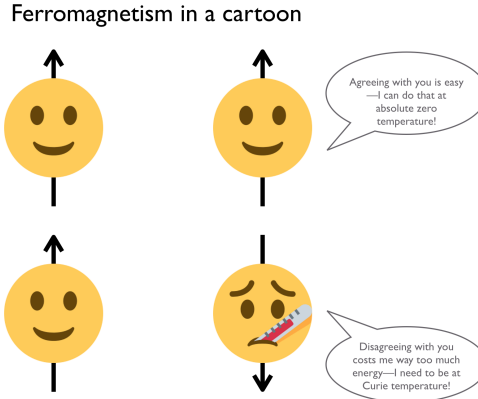
Ferromagnetism in a cartoon

Figure 1: Sketch of the ferromagnetic behaviour.

When implementing the Monte Carlo simulation, we need to compute the probability that a spin will flip given its and their neighbours current configuration. This probability can be computed directly from the Boltzmann factor, $e^{\beta E}$, which corresponds to the probability that a particle occupies a state with energy E. When contemplating a transition, in which the variation of the energy will be given by ΔE, the probability of such transition is then

$$P \sim e^{-\beta \Delta E} \ . \tag{7}$$

Consider a spin, say σ_1, transitioning from configuration A to configuration B illustrated in green in figure 2. The energy of the spin depends on the its alignment with its neighbours.
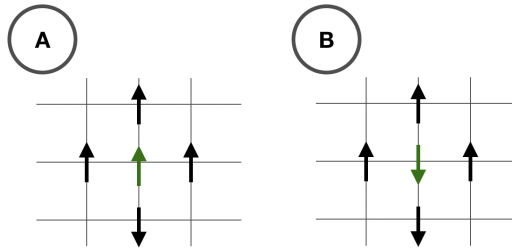

Figure 2: Will the spin flip?

Originally, in the situation described by diagram A, and from Eq. (5), the spin's energy is simply:

$$E_A = -J\sigma_1 \sum_{<1j>} \sigma_j \ , \tag{8}$$

where σ_1 is the spin(-up) value at position i and the sum involves the von Neumann neighbouring spins. On the other hand, in situation B, the energy is

$$E_B = +J\sigma_1 \sum_{<1j>} \sigma_j \ . \tag{9}$$

Notice that the neighbouring spins are static, i.e., their values do not change. Therefore, the variation of the energy from situation A to situation B is

$$\Delta E = E_B - E_A = 2J\sigma_1 \sum_{<1j>} \sigma_j = -2E_A \ . \tag{10}$$

We therefore conclude that the probability of the spin to transition from situation A to situation B is then

$$P \sim e^{2\beta E_A} \ . \tag{11}$$

Let's consider a couple of regimes:

- for fixed temperature, if ΔE is positive, then the probability of transitioning is low. The spin will tend to stay at energy E_A.

- on the other hand, if we were to consider the transition from situation B to situation A, then ΔE would be negative, and the new configuration (A) would be favoured.

- for fixed energy, as $\beta \to 0$, or for large temperature, the probability of the spin flipping sign increases dramatically, which maps to the loss of magnetic orientation.

- in the opposite regime, as $\beta \to \infty$, the temperature is so low that spins naturally align between themselves.

Magnetic domains

Even though the dipolar interaction is insignificant compared to the exchange spin coupling, it so happens that, at the macroscopic level, magnetic domains can form as a means of decreasing the dipolar energy, at the cost of increasing the short-ranged exchange interaction for those spins in the neighbourhood of misaligned magnetic domains. We have encoutered magnetic domains in our class, cf. the following example
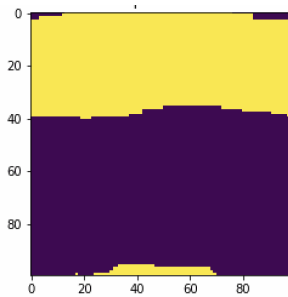

Figure 3: In between the different magnetic regions, domain walls form along which the individual atoms' magnetic moments gradually change from the value in one domain to the value in the other domain.