Unit 4-2: The Ising Model - A Qualitative Discussion

For the Ising model with fixed magnetic field h we had the Hamiltonian

$$\mathcal{H}[s_i; h] = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i \tag{4.2.1}$$

Having defined the Ising model and the constant magnetic field ensemble, we can ask what sort of behavior should we expect? For a given magnetic field h, what do we expect for the resulting magnetization density $m(T, h)$?

For $h > 0$ we expect to have $m > 0$, as it is energetically favorable for the spins to align parallel to h. For $h < 0$, we similarly expect to have $m < 0$.

In general we expect to have $m(T, -h) = -m(T, h)$, since the Hamiltonian has the symmetry, $\mathcal{H}[s_i; h] = \mathcal{H}[-s_i; -h]$.

What do we expect if $h = 0$?

As $T \to \infty$, the thermal energy will greatly exceed the spin coupling energy J, and so we expect each spin to behave randomly, pointing equally likely up as down, and so $m = 0$. But even at finite T we might expect $m = 0$ because of symmetry. We have $\mathcal{H}[s_i; 0] = \mathcal{H}[-s_i; 0]$, so a configuration $\{s_i\}$ in the partition function sum will enter with the same weight as the configuration $\{-s_i\}$. Thus we would expect to find $\langle s_i \rangle = 0$, and so $m = \dfrac{1}{N} \sum_i \langle s_i \rangle = 0$.

But at $T = 0$, the system has two *degenrate* ground state: <u>all up</u> or <u>all down</u> spins, with $m = \pm 1$. The ground state *breaks the symmetry* of the Hamiltonian.

More specifically we can write,

$$\lim_{h \to 0^+} \left[\lim_{T \to 0} m(T, h) \right] = +1 \qquad \text{while} \qquad \lim_{h \to 0^-} \left[\lim_{T \to 0} m(T, h) \right] = -1 \tag{4.2.2}$$

In the above, we first take the limit $T \to 0$ with a finite h applied, and then we take the limit $h \to 0$. The notation $h \to 0^+$ means we take $h \to 0$ from the positive side, while $h \to 0^-$ means we take $h \to 0$ from the negative side.

Can one have such a state of broken symmetry at a finite temperature T? That is, can we have at finite $T > 0$,

$$\lim_{h \to 0^+} m(T, h) = m > 0 \qquad\qquad \lim_{h \to 0^-} m(T, h) = m < 0 \tag{4.2.3}$$

For a *finite size* system, i.e. a system with a finite number of spins N, the answer is ***no!***. For a finite system size, the energy $\mathcal{H}[s_i; h]$ is always finite. The statistical weight of $\{s_i\}$ will always be equal to that of $\{-s_i\}$ as we take $h \to 0$.

However, in the *thermodynamic limit*, $N \to \infty$, the answer can be ***yes!*** Consider a configuration in which $\frac{1}{N} \sum_i s_i$ is finite (i.e. a macroscopic fraction of the spins are aligned). Now consider a vanishingly small but finite h. The energy of such a configuration will grow infinitely large as $N \to \infty$. The statistical weight of such a configuration $\{s_i\}$ can then be infinitely different from that of $\{-s_i\}$, due to the interaction with the vanishingly small but finite h. The weight of the magnetic field term in the Boltzmann factor is $(h) \times (\sum_i s_i)$. If the second terms diverges, while the first term vanishes, the resulting product $(0) \times (\infty)$ becomes ill-defined. In other words,

$$\mathcal{H}[s_i; h] - \mathcal{H}[-s_i; h] \propto hN \qquad \text{does not necessarily vanish as } h \to 0 \text{ if } N \to \infty \textit{ first!} \tag{4.2.4}$$

Therefore, it remains possible that at finite T we could have,

$$\lim_{h \to 0^+} \left[\lim_{N \to \infty} m(T, h) \right] = m > 0 \qquad\qquad \lim_{h \to 0^-} \left[\lim_{N \to \infty} m(T, h) \right] = m < 0 \tag{4.2.5}$$

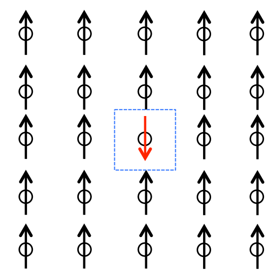
It is crucial to take the limits in the above order, i.e. first take $N \to \infty$, and only then take $h \to 0$. Reversing the limits ($h \to 0$ first, and then $N \to \infty$) must give $m = 0$ by the symmetry of $\mathcal{H}$.

We can now give a more physical reason why we can have $m \neq 0$ when $h \to 0$ *only* when $N \to \infty$ and the system is in the infinite thermodynamic limit.

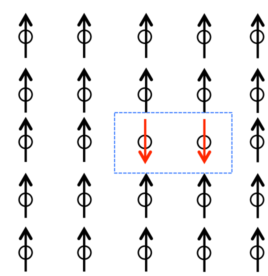
In principle, when $h = 0$, the configuration $\{s_i\}$ has exactly the same statistical weight as the configuration $\{-s_i\}$, and so these would cancel each other out when computing $\langle s_i \rangle$ in a usual ensemble calculation. However, let's consider the physical process by which the system, when originally ordered in the configuration $\{s_i\}$, might later wind up in the configuration $\{-s_i\}$.

Consider $h = 0$ at low T, when the configuration is mostly all spins up. We will assume that the dynamics is *local* – the probability for any given spin to flip depends on the orientations of its neighbors. In particular, we can imagine that the probability to flip is proportional to the Boltzmann factor $\mathrm{e}^{-\beta \Delta E}$, where ΔE is the change in energy if the spin flips.

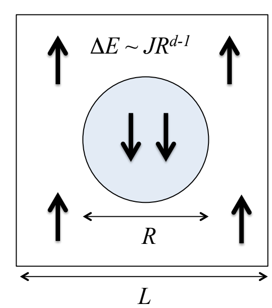
Consider a region in which all the spins are oriented up. As a thermal fluctuation, there is a finite probability that one of these spins will flip down. The probability for it to do so is $\propto \mathrm{e}^{-\beta \Delta E}$, where the energy cost ΔE can be computed as follows. Initially the energy of interaction of the spin with its neighbors is $E_i = -zJ$, where where z is the number of nearest neighbors; z is called the *coordination number of the lattice*. After the spin flips, its energy is $E_f = +zJ$, because it is now antiparallel to its neighbors. The change in energy is therefore $\Delta E = E_f - E_i = 2zJ$.



Most likely, that spin will soon flip back up, since that is the energetically favored position. But there is also a chance that, before that happens, one of the neighbors of this flipped spin will also flip down. The energy cost for that is as follows. Initially, the neighbor has energy $E_i = -(z-1)J + J$, since it is aligned with all but one of its neighbors. After it flips, it has energy $E_f = (z-1)J - J$, since now it is anti-aligned with all but one of its neighbors. The change in energy is $\Delta E = E_f - E_i = 2(z-1)J - 2J = 2zJ - 4J$, which is thus lower than the cost for the first spin to flip.



In such a manner we can imagine that, as a thermal fluctuation, a small domain of length R can appear in which all the spins have flipped down. The energy cost of having this domain would be proportional to the surface area of this domain, since the surface of the domain is where one finds spins that are anti-aligned. The energy cost of such a domain is therefore proportional to $\Delta E \propto JR^{d-1}$, where d is the dimensionality of the model, so the domain surface area goes as R^{d-1}.



Now suppose the size of such a spin flipped domain got large enough to comprise half the size of the system. Consider an up spin at the boundary, just outside this domain. And consider a down spin at the boundary, just inside this domain. The energy cost to flip such an up spin to down would be the same as the energy to flip such a down spin to up. It would therefore be equally likely for this domain to either grow or to shrink. If it grows and becomes larger than half the size of the system, it then becomes energetically more favorable for the domain to continue to grow and fill the entire system, than it is to shrink back down to zero and restore the initial up ordered state. We thus have a mechanism for transitioning the system from an initial state in which all the spins are up to a final state in which all the spins are down.

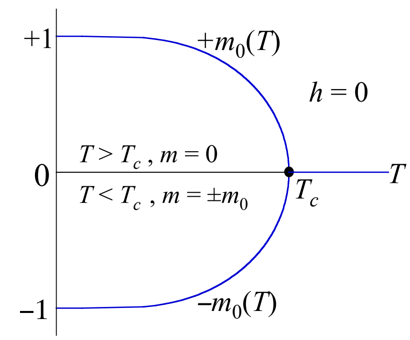
The process, by which an initial configuration with all spins up can flip to a configuration with all spins down, therefore depends on the probability to create such a spin flipped domain that fills half the system. We call this the *critical domain excitation*. Since the size of such a domain is $R \sim L/2$, where L is the length of the system, then the energy cost of such a domain is $\Delta E \sim JL^{d-1}$, and the probability to form such a domain is $\propto \mathrm{e}^{-\beta J L^{d-1}}$. When L is large, this probability is exceedingly small, and it would take a very long time for such a critical domain to appear in the system. However, as long as L is finite, this probability is finite, and if we are prepared to wait long enough, then in principle it will happen and the system will flip all its spins. If we average on such exceedingly long time scales, we then must find that $\langle s_i \rangle = 0$.

But if we are in the thermodynamic limit, then $L \to \infty$, and the probability to form the critical domain $\propto \mathrm{e}^{-\beta J L^{d-1}} \to 0$. A system in the thermodynamic limit, in a configuration with $m > 0$, will therefore not necessarily flip its average magnetization even if we wait forever. So we can then wind up with the situation that $\langle s_i \rangle \neq 0$. The key point is that we must be in the thermodynamic limit of $N \to \infty$, so that $L \to \infty$.

Note one point: If our system were one-dimensional, then $L^{d-1} = 1$ stays finite as $L \to \infty$, and the energy to create the critical domain is always finite. We would thus expect, and we will later confirm, that the one-dimensional Ising model at $h = 0$ will always have $m = \langle s_i \rangle = 0$ at any finite T.

Another point: Our above estimate $\Delta E \propto J L^{d-1}$ was an estimate of the *energy* of a critical domain. However, at finite temperature, the probability to form a critical domain should be proportional the the *free energy* to make the domain, $\Delta F = \Delta E - T\Delta S$, where ΔS is the entropy associated with fluctuations in the surface of the domain. We therefore expect $\Delta F = \sigma(T) L^{d-1}$, where the temperature dependent surface tension $\sigma(T)$ replaces the coupling J.

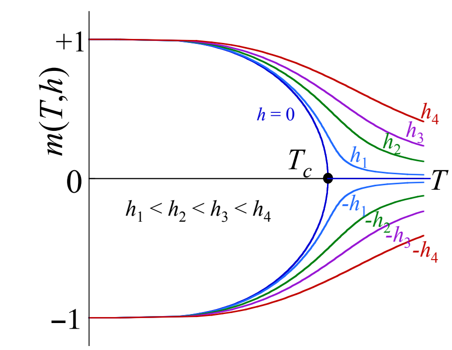
If such broken symmetry states exist at some finite T, do we expect it to exist at all finite T? or do they disappear above a well defined T_c? If the latter, then we have a ferromagnetic phase transition. In terms of the above discussion of the free energy ΔF to create a critical domain, such a transition would be viewed as the temperature at which the surface tension of a large spin flipped domain vanishes. For such a ferromagnetic phase transition we might expect behavior as sketched to the right below.



When $h = 0$, we have two degenerate states, one with $+m_0(T)$ and the other with $-m_0(T)$, where $m_0(T)$ is the magnitude of the spontaneous magnetization in the ordered phase at $T < T_c$. Above T_c we have $m = 0$. It could be that $m_0(T)$ drops discontinuously to zero as T increases to T_c (that situation is referred to as a *first order* transition). But we will see instead that $m_0(T)$ vanishes continuously as $T \to T_c$ from below. This is know as a *continuous* phase transition. In either case, $m_0(T) = m(T, h = 0)$ is singular at $T = T_c$.

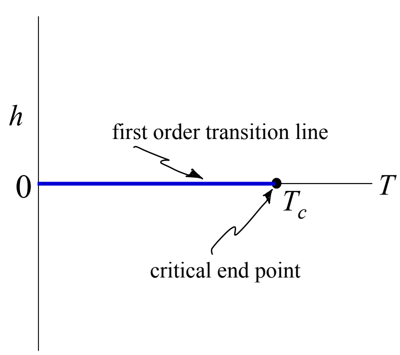
As the system is cooled below T_c at $h = 0$, the system will pick *either* the up state with $+m_0$, *or* the down state with $-m_0$, to order in. We say that the system orders into a state of *spontaneously broken symmetry*, since the choice of either $+m_0$ or $-m_0$ breaks the symmetry of the Hamiltonian.

At *finite* magnetic field h, we expect $m(T, h)$ to behave as in the sketch to the right. Now $m(T, h)$ is a smooth function of T for any fixed $h \neq 0$.



Phase Diagram in the $h - T$ plane

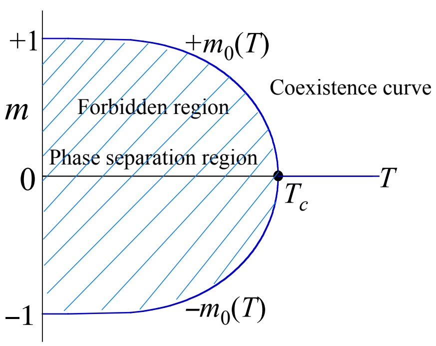
The phase diagram for the ferromagnetic phase transition of the Ising model in the $h - T$ plane is as in the sketch below. At $h = 0$ there is a *first order* phase transition line that extends from $T = 0$ up to $T = T_c$. As one crosses this line in the $h - T$ plane, for example by decreasing h at fixed T, the magnetization has a discontinuous jump from $+m_0(T)$ to $-m_0(T)$. This first order transition line is also called the *coexistence line* because the two phases with $+m_0$ and $-m_0$ can coexist in equilibrium together on this line.



The end point of this first order line at T_c is called the *critical end point*. As $T \to T_c$ from below, the jump in the magnetization upon crossing the first order line, $2m_0(T)$, vanishes continuously. The critical end point is therefore called a *continuous* phase transition. The magnetization $m(T, h)$ is continuous if one crosses the $h = 0$ line anywhere above T_c.

Phase Diagram in the $m-T$ plane

We can also draw the corresponding phase diagram in the $m-T$ plane, as shown in the sketch below.



The coexistence line in the $h-T$ plane now becomes the coexistence curve enclosing the *forbidden region* – so called because there are no *spatially homogeneous* equilibrium states with T and m in this region. The forbidden region is also called the *phase separation region* – if one cools the system at fixed m into this region, the system will phase separate into one domain of up spins with magnetization $+m_0$, and the complementary domain of down spins with magnetization $-m_0$. The size of these domains will be such that the average magnetization is equal to the fixed value m.

There are many similarities between the Ising model phase diagram and the liquid-gas phase diagram if one makes the analogies $h \leftrightarrow p$ (the pressure), and $m \leftrightarrow \rho$ (the density).

Absence of Phase Transitions in Finite Sized Systems

We said that to have a state of spontaneous broken symmetry at finite T it is necessary to be in the thermodynamic limit $N \to \infty$. More generally, a true singular phase transition can only occur in the $N \to \infty$ limit. Previously we gave a physical argument for this in terms of the critical domain excitation. Now we give a mathematical proof of this.

Consider the partition function sum,

$$Z(T,h) = \sum_{\{s_i\}} \mathrm{e}^{-\beta\mathcal{H}[s_i;h]} \tag{4.2.6}$$

For a finite sized system (N finite) the number of configurations to sum over is 2^N is finite. Z is therefore the sum of a finite number of analytic functions. By an analytic function we mean in the sense of complex function theory – the function has a convergent Taylor series expansion at any point, and so is infinitely differentiable and has no singularities; $\mathrm{e}^{-\mathcal{H}/k_BT}$ is analytic in T and h, except at $T=0$.

Since Z is a finite sum of analytic functions, then Z must also analytic in T and h, so Z can have no singularities. Therefore the free energy has no singularities, and no thermodynamic quantities will have any singularities. Thus there can be no phase transitions.

In the thermodynamic limit $N \to \infty$, however, Z is the sum of an *infinite* number of analytic functions. Such an infinite sum need *not* be analytic, so this then allows for the possibility of a phase transition.

Having outlined above the behavior we might expect to see in the Ising model, we would now like to compute properties and see what happens! However an *exact* solution is not in general possible. Exact solutions have only be found so far in $d=1$ and $d=2$ dimensions. For $d=1$ we will do the calculation later, and will find that there is no ferromagnetic phase transition at any finite T. For $d=2$ there is the famous solution found by Onsager in 1944. This solution has a ferromagnetic phase transition. Similarly there is a ferromagnetic phase transition in all $d>2$. For $d=3$ we have no exact solution and must rely on accurate numerical results. For $d>4$ one can show that *mean-field theory* describes the phase transition exactly. In the next section we therefore discuss this mean-field theory solution.