0.1 Disordered Systems

(Lesson ? of 28/11/19)
Compiled: December 2, 2019

A *disordered system* is a set of particles that interact in a non-regular way, leading to a *very complex* "potential landscape", with no clear recognizable shape.
For example, consider a set of interacting fermions, e.g. atoms in a ferromagnetic material. If the *strength* of interactions is the same for every couple of particles, then we have a **ordered system**. In this case, for example, the Hamiltonian will be:

$$H = -J \sum_{i,j} S_i S_j$$

with $J < 0$ for a ferromagnetic material. Here the "setup" is regular, and so the behaviour of the system is relatively easy: one can show that, for sufficiently low temperatures, all spins will *align* in the same direction (spontaneous magnetization).
However, if we choose the *strength* of each coupling J_{ij} *at random*, we get a **disordered system**:

$$H = -\sum_{ij} J_{ij} S_i S_j$$

If J_{ij} are randomly chosen at the *start*, i.e. they are part of the system's "setup" and **do not evolve with time**, the disorder is denoted as **quenched**. Otherwise, if the random J_{ij} depend also on time, we talk about **annealed disorder**.
It is clear that in the *disordered* case the system's behaviour is much more difficult to predict. In fact, there is *no clear behaviour* at small temperatures. This is due to the presence of *many local minima* of the potential, which are very similar to each other. If a system exhibits many equivalent stationary states with equal (minimum) energy, we call it **frustrated**.
If the random parameters contributing to the system's setup are of *very different scale* from each other, we talk about **structural disorder**. From an energy point of view, this leads to local minima separated by *high local maxima*, which are very difficult to surpass. So the system will be effectively *locked* in some configuration, unable to explore the *potential landscape* in a reasonable time. This phenomenon is referred as **ergodicity breaking** - meaning that it is difficult to compute a significant *time average* of the state of the system, as the behaviour of the system on a small timeframe will be highly dependent on the initial state, and not representative of the *average over a sufficient sized set of states in phase-space* (as they are not explored in that timeframe, because of "locking").

Some examples of disordered systems are:

1. A net of *resistors* with random resistance
2. Anderson localization in condensed matter (waves over a lattice with impurities)
3. Protein folding

0.2 Review of Statistical Mechanics

Consider a system in equilibrium at temperature T. Denoting:

$$\beta = \frac{1}{k_B T}$$

the *average value* of some quantity of interest is given by the canonical ensemble's formula:

$$\langle X \rangle = \frac{\sum_S X[S] e^{-\beta H[S]}}{\sum_S e^{-\beta H[S]}}$$

where S represents a specific *configuration* of the system, i.e. a choice of *all* its microscopical parameters (e.g. all the spins S_i in a spin lattice). The quantity X is evaluated for every state S, and the result is weighted by the *Boltzmann weight*:

$$e^{-\beta H[S]}$$

The overall sum is then *normalized* by the **Partition function** Z:

$$Z = \sum_S e^{-\beta H[S]}$$

We note that $\log Z$ plays the role of a generating function, meaning that we can extract from it the *moments* of X. If we define:

$$H' \equiv H + \alpha X$$

then:

$$\langle X \rangle = -\frac{1}{\beta} \frac{\partial}{\partial \alpha} \ln Z \Big|_{\alpha=0} = -\frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial \alpha} Z \Big|_{\alpha=0}$$

And the **free energy** is:

$$F = -\frac{1}{\beta} \ln Z = -k_B T \ln Z$$

so that:

$$\langle X \rangle = \frac{\partial}{\partial \alpha} F \Big|_{\alpha=0}$$

0.3 Mean field Ising Model

Consider now a *lattice* of spin-interacting particles subjected to an external magnetic field h. If we suppose that the the system is ordered, meaning that the

coupling strength for each particle is J/N (where N is the number of particles), the Hamiltonian will be:

$$H = -\frac{J}{N}\sum_{i\neq j} S_i S_j - h\sum_i S_i \qquad S_j = \pm 1$$

In the large system limit ($N \to \infty$), a certain particle j will "see" only the *average magnetization* of the system:

$$m = \frac{1}{N}\sum_i S_i$$

So the energy of j will be:

$$H_j = S_j\left[\frac{2J}{N}\sum_i S_i + h\right] \underset{N\to\infty}{\approx} S_i\left[\frac{2J}{N}\sum_i \langle S_i\rangle + h\right] \approx S_j h_m \qquad h_m \equiv 2Jm + h$$

As $S_j = \pm 1$, we can compute the *probability* of measuring one case or the other:

$$\mathbb{P}(S_j) = \frac{e^{-\beta H_j}}{Z_j} = \frac{e^{\beta h_m S_j}}{e^{\beta h_m S_j} + e^{-\beta h_m S_j}}$$

so that the *most probable* value of S_j is the one *aligned* with all the other spins. The particle j must contribute to the total magnetization with the *same average magnetization*, meaning that:

$$m = \sum_{S_j=\pm 1} \mathbb{P}(S_j) S_j = \frac{e^{\beta h_m} - e^{-\beta h_m}}{e^{\beta h_m} + e^{-\beta h_m}} = \tanh(\beta h_m) = \tanh\left(\beta 2Jm + \beta h\right)$$

Note that m appears on both sides of the equation (*self consistent*), and it is not possible to find an analytical situation.
So, let's simplify the situation and consider, at first, the *case with no external magnetic field*, i.e. with $h = 0$. We have:

$$m = \tanh(2\beta J m)$$

The solution will be the intersection between the diagonal $y = m$ and the curve $y = \tanh(2\beta Jm)$. Depending on β we can find three *interesting cases* to study. The separating one is when the tanh function is tangent to $y = m$ at the origin:

$$\frac{\partial}{\partial m}\tanh(2\beta Jm)\Big|_{m=0} = 1 \Rightarrow 2\beta J = 1$$

$\beta^* = 1/(2J)$ defines the *critical temperature* $T^* = 1/\beta^*$. For high temperatures $\beta < \beta^*$ ($T > T^*$) we will have only one solution $m^* = 0$, meaning that the system has no overall magnetization. For $\beta = \beta^*$ there are *three* coincident solutions at $m^* = 0$, and in the small temperature limit ($\beta \to \infty$), we will have $2\beta J > 1$, leading to other two solutions $\pm m^*$ with $|m^*| \neq 0$, meaning that the system will *spontaneously magnetize*.

0.4 Random Field Ising Model (RFIM)

We now *randomize* the field h_i experienced by every particle:

$$H = -\frac{J}{N}\sum_{ij} S_i S_j - \sum_i h_i S_i$$

Intuitively, the random fluctuations of h from a particle to another will have an effect *similar* to thermal noise. So we expect that, even at 0 temperature, the system may not exhibit a ferromagnetic phase if the h_i are sufficiently strong.
Explicitly, let's set the distribution of h_i to be gaussian with 0 mean and δ^2 variance (so that then we can evaluate *gaussian integrals*):

$$\mathbb{P}(h_i) = \frac{1}{\sqrt{2\pi\delta^2}} \exp\left(-\frac{h_i^2}{2\delta^2}\right)$$

($\sigma \to \delta$ everywhere)
We consider the scale ratios $2J/\delta$ (ferromagnetic coupling to disorder) and T/δ (temperature to disorder), and plot the *phase diagram* with respect to these axes.
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The *ferromagnetic* phase starts at $T = 0$ for a sufficiently high $2J/\delta$, and the boundary tends to the diagonal as $2J/\delta$ and T/δ both increase (as in the ordered Ising model). So, even at $T = 0$, if J is low enough, the system will be *paramagnetic* (not magnetized).
To see this, we start by writing the partiition function:

$$Z_h = \sum_S e^{-\beta H_h}$$

where the sum is over all possible configurations $S \in \{S_i\}$, and the energy H is computed over a choice of random fields $h = \{h_i | i = 1, \ldots, N\}$, with N being the number of spins.
To compute the *free energy*, we can first compute the partition function Z and average it, or *average the free energy itself*. The *physical solution* is the second one, i.e. to average the free energy, as this is a *physical measurable quantity* (and not a mathematical construct like Z). We denote the "average over disorder" as $\bar{X}$, leading to:

$$\bar{X} = \int \prod_i \mathrm{d}h_i \, \mathbb{P}(h_i) X_h \qquad h = \{h_i\} = \{h_1, \ldots, h_N\}$$

And so, for the free energy:

$$\bar{F}_h = -k_B T \overline{\ln Z_h}$$

Dropping the h:

$$\bar{F} = -k_B T \overline{\ln Z}$$

However, practically it is easier to deal with $\overline{Z^n}$, $n \in \mathbb{N}$ than $\overline{\ln Z}$. So we compute $\bar{F}$ with the "replica trick".
The idea is to consider n replicas of the system, all with the *same* quenched disorder (same choice of $\{h_i\}$). Then:

$$\overline{\ln Z} = \lim_{n\to 0} \frac{\overline{Z^n} - 1}{n} = \lim_{n\to 0} \frac{1}{n} \ln \overline{Z^n} = \frac{\partial}{\partial n} \overline{Z^n} \Big|_{n=0} \qquad n \in \mathbb{R}$$

Intuitively, letting the number of replicas n to be 0 *does not make sense*. However this is usually mathematically, as we now see.

The previous identity is derived by Taylor expansion of the exponential:

$$\lim_{n\to 0} \frac{Z^n - 1}{n} = \lim_{n\to 0} \frac{e^{n \ln Z} - 1}{n} = \lim_{n\to 0} \frac{n \ln Z + \frac{1}{2!}(n \ln Z)^2 + \dots}{n} = \ln Z$$

Rearranging:

$$Z^n \approx 1 + n \ln Z$$

Taking the average, thanks to linearity we can write:

$$\overline{Z^n} \approx 1 + n\overline{\ln Z} \tag{1}$$

Now consider the second expression:

$$A = \lim_{n\to 0} \frac{1}{n} \log\big(\overline{Z^n}\big) \tag{2}$$

Substituting (1) in (2) we get:

$$A = \lim_{n\to 0} \frac{1}{n} \ln\big(1 + n\overline{\ln Z}\big)$$

As $n \to 0$, we can use $\ln(1 + x) \approx x + O(x^2)$ $(x \to 0\ )$, leading to:

$$A = \overline{\ln Z}$$

So we proved that:

$$\overline{\ln Z} = \lim_{n\to 0} \frac{\overline{Z^n} - 1}{n} = \lim_{n\to 0} \frac{1}{n} \ln \overline{Z^n}$$

The third expression evaluates (again, thanks to linearity) to:

$$\frac{\partial}{\partial n} \overline{Z^n} \Big|_{n=0} = \frac{\partial}{\partial n} \exp\big(n\overline{\log Z}\big) \Big|_{n=0} = Z^n \overline{\log Z} \Big|_{n=0} = \overline{\log Z}$$

We define an index $a = 1, \ldots, n$. Then:

$$\overline{Z^n} = \overline{\sum_{S^a} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a\right) \exp\left(\beta \sum_i \sum_a S_i^a h_i\right)} =$$
$$\underset{(a)}{=} \sum_{S^a} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a\right) \overline{\exp\left(\beta \sum_i \sum_a S_i^a h_i\right)} =$$
$$= \sum_{S^a} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a\right) \overline{\exp\left(\sum_i h_i \lambda_i\right)} \qquad \lambda_i = \beta \sum_a S_i^a$$

where the sum is over all the possible configurations of a replicas of the system, and S_i^a is the spin of the i-th particle in the a-th replica.
In (a) we note that the disorder is only present in the h_i, and so we can restrict the average. Every term summed inside the last exponential can be evaluated using gaussian integrals:

$$\overline{\exp\left(\lambda_i h_i\right)} = \int \mathrm{d}h_i \, \mathbb{P}(h_i) e^{\lambda_i h_i} = \exp\left(\frac{\delta^2 \lambda_i^2}{2}\right)$$

Substituting back:

$$\overline{Z^n} = \sum_{S^a} \exp\left(\frac{\beta J}{N} \sum_a \left(\sum_i S_i^a\right)^2\right) \exp\Big(\frac{\delta^2 \beta^2}{2} \underbrace{\sum_i \left(\sum_a S_i^a\right)^2}_{\sum_i \lambda_i^2}\Big)$$

where we used:

$$\sum_{ij} S_i^a S_j^a = \left(\sum_i S_i^a\right)\left(\sum_j S_j^a\right) = \left(\sum_i S_i^a\right)^2$$

Note that now the disorder apparently "disappears" (is only contained in the variance δ), and the separate replicas *interact* from each other.
To remove the squares we use the **Hubbard-Stratonovich transformation** (just another kind of gaussian integral):

$$\exp\left(\pm \frac{b}{2} z^2\right) = \frac{1}{\sqrt{2\pi b}} \int_{-\infty}^{+\infty} \exp\left(-\frac{x^2}{2b} - \sqrt{\pm 1} z x\right) \mathrm{d}x$$

where the *self-interaction* z^2 disappears, and we have instead zx, where x, in a certain sense, can be seen as a "mediating field" with Gaussian distribution. Physically, the idea is to convert interactions between particles to interactions of each particle with a common field.