

One Dimensional Ising model - Mean Field Approximation

Consider N atom in a z directed magnetic field. Each atom has a spin $\pm\frac{1}{2}$. $\rightarrow S_i = \pm 1$ (Twice the z component of atomic spin).

The total energy of is given by

$$E = -J \sum_{\langle i,j \rangle} S_i S_j - \mu H \sum_{i=1}^N S_i$$

J \rightarrow Exchange energy

S_i \rightarrow Spin of the i^{th} atom

H \rightarrow Applied magnetic field

μ \rightarrow Atomic moment

The following observations can be made from the equation.

- First term in right shows that overall energy is less when spins are aligned.
- This is mostly due to Pauli's exclusion principle.

Let us find out the energy of the i^{th} atom.

$$e_i = -\frac{J}{2} \sum_{k=1}^z S_k S_i - \mu H S_i$$

Note that we have introduced an extra $\frac{1}{2}$ term to account for the double counting when we estimate total energy ($\sum_i^n e_i$). Energy belongs to a pair of atoms.

$$e_i = -\mu S_i \left[\frac{J}{2\mu} \sum S_k + H \right]$$
$$e_i = -\mu H_{eff} S_i$$

• H_{eff} consist of two terms. The first term is the internal field generated by the neighbouring atoms and the second term is the external magnetic field.

Now let us try to find the mean spin of the system. The system is in thermal equilibrium at all stages and there is no exchange of particles, so the appropriate way to solve this is by the canonical ensemble.

Mean spin can be defined by:

$$\bar{s} = \frac{\sum_{S_i=\pm 1} S_i e^{-\beta e_i}}{\sum e^{-\beta e_i}} = \frac{\sum_{S_i=\pm 1} S_i e^{-\beta \mu H_{eff} S_i}}{\sum e^{-\beta \mu H_{eff} S_i}}$$
$$= \frac{e^{\beta \mu H_{eff}} - e^{-\beta \mu H_{eff}}}{e^{\beta \mu H_{eff}} + e^{-\beta \mu H_{eff}}} \quad (1)$$
$$= \tanh [\beta \mu H_{eff}]$$

Now, let us make an assumption that all atoms have identical spins, ie $s_i = \bar{s}$. This is known as Mean Field Approximation. With this assumption, our effective field can be written as,

$$H_{eff} = \frac{zJ\bar{s}}{2\mu} + H$$

$$\bar{s} = \tanh \left[\beta\mu H + \frac{\beta z J \bar{s}}{2} \right]$$

Define critical temperature,

$$T_c = \frac{Jz}{2k_B}$$

and critical field,

$$H_c = \frac{k_B T_c}{\mu} = \frac{Jz}{2\mu}$$

$$\frac{T_c}{H_c} = \frac{\mu}{k_B}$$

Now,

$$\begin{aligned} \bar{s} &= \tanh \left[\frac{\mu H}{k_B T} + \frac{z J \bar{s}}{2 k_B T} \right] \\ &= \tanh \left[\frac{\mu}{k_B T} \left[H + \frac{Jz}{2\mu} \bar{s} \right] \right] \\ &= \tanh \left[\frac{\mu}{k_B T} [H + H_c \bar{s}] \right] \tag{2} \\ &= \tanh \left[\frac{T_c}{H_c T} [H + H_c \bar{s}] \right] \\ \bar{s} &= \tanh \left[\frac{T_c}{T} \left[\bar{s} \frac{H}{H_c} \right] \right] \end{aligned}$$

As you can see, this is a transcendental function and can be easily solved using any efficient numerical method.

Net magnetization

$$M = \mu \sum_{i=1}^N s_i = \mu N \bar{s}$$

Net energy

$$\begin{aligned} E &= \sum_{i=1}^N e_i \\ &= \sum_{i=1}^N -\mu H_{eff} s_i \\ &= -\mu H_{eff} \bar{s} N \\ &= -\mu N \bar{s} \left[\frac{J}{2\mu} z \bar{s} + H \right] \end{aligned} \tag{3}$$

We know that $\frac{Jz}{2k_B} = T_c$ and $\frac{Jz}{2\mu} = H_c$

$$\begin{aligned} &= -\mu N [H_c \bar{s} + H] \bar{s} \\ &= -\mu N H_c \left[\frac{H}{H_c} + \bar{s} \right] \bar{s} \end{aligned}$$

Thus, energy $E = -N k_B T_c \left[\frac{H}{H_c} + \bar{s} \right] \bar{s}$