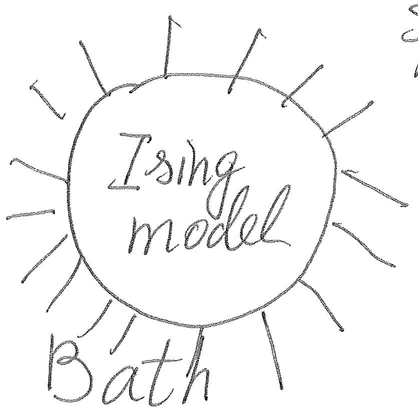
Lecture 9

Simulations of the Ising model.

Metropolis algorithm:

We consider interaction between our spin system (Ising model) and the bath.



The system state is characterised by a spin configuration

$$\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3 \ldots\ldots \sigma_N)$$

where $\sigma_n = \pm 1$, N is the number of spins.

The interaction with the bath results in a transition from one spin configuration (or microstate) to another microstate.

We numerate these microstate by index $m = 1, 2, \ldots M$.

We have transitions (random walks in the spin states space)

$$\vec{\sigma}^{(1)} \longrightarrow \vec{\sigma}^{(2)} \longrightarrow \vec{\sigma}^{(3)} \rightarrow \ldots\ldots \rightarrow \vec{\sigma}^{(M)} \rightarrow$$

If we have a physical quatity $A(\vec{\sigma})$ that depends on $\vec{\sigma}$ (energy, magnetization, susceptibility, ...), then the mean value avaraged over microstates is

$$\langle A \rangle = \frac{1}{M} \sum_{m=1}^{M} A(\vec{\sigma}^{(m)})$$

For example, a mean magetic moment is

$$< \frac{1}{N}\sum_{n=1}^{N}{}' \sigma_n > = \frac{1}{M}\sum_{m=1}^{M}{}' \left(\frac{1}{N}\sum_{n=1}^{N}{}' \sigma_n^{(m)}\right)$$

In equilibrium (with the bath), we can find the probability that the spin system is in ~~the~~ a spin configuration $\vec{\sigma}$. (this probability is proportional to frequency of transition into the state $\vec{\sigma}$). One show that the probability $\mathcal{P}(\vec{\sigma})$ is

$$\mathcal{P}(\sigma) = \frac{e^{-E(\vec{\sigma})/K_B T}}{Z}$$

where $E(\vec{\sigma})$ is the internal energy of the Ising model, and Z is the normalization factor (the partition function).

Then we obtain

$$< A(\vec{\sigma}) > = \frac{1}{M}\sum_{m=1}^{M}{}' A(\vec{\sigma}^{(m)}) \underset{M\to\infty}{=}$$

$$= \sum_{\{\vec{\sigma}\}}{}' \mathcal{P}(\vec{\sigma})\, A(\vec{\sigma}) = \sum_{\{\vec{\sigma}\}} e^{-E(\vec{\sigma})} A(\sigma)$$

Let us consider probability of a transition from a microstate ~~a state~~ α to a microstate β; We denote this probability (or frequency)

$$w(\alpha \to \beta)$$

We use <u>the detailed balance</u>.

The detailed balance assume that in the equilibrium (with the bath) the frequency of transition from α to β,

$$P(\vec{\sigma}^{(\alpha)})\, w(\alpha \to \beta),$$

is equal to the frequency of jump from β to α,

$$P(\vec{\sigma}^{(\beta)})\, w(\beta \to \alpha).$$

That is we obtain

$$P(\vec{\sigma}^{(\alpha)})\, w(\alpha \to \beta) = P(\sigma^{(\beta)})\, w(\beta \to \alpha)$$

Therefore the ratios of probability (frequencies) of transitions is

$$\frac{w(\alpha \to \beta)}{w(\beta \to \alpha)} = \frac{P(\vec{\sigma}^{(\beta)})}{P(\vec{\sigma}^{(\alpha)})} = \frac{e^{-\beta E(\vec{\sigma}^{(\beta)})}}{e^{-\beta E(\sigma^{(\alpha)})}}$$

$$= \exp\left[-\beta\left(E_\beta - E_\alpha\right)\right]$$

$$= \exp\left[-\beta\, \Delta E_{\beta\alpha}\right]$$

Thus the ratio is determined by ~~the~~ the energy difference

$$\Delta E_{\alpha\beta} = E(\sigma^{(\beta)}) - E(\sigma^{(\alpha)})$$

The basic process in ~~the~~ a spin system is a rotation of a single spin.

$$(\sigma_1, \sigma_2, \ldots \sigma_n \ldots \sigma_N) \longrightarrow (\sigma_1 \sigma_2 \ldots, -\sigma_n, \sigma_N)$$

$$\sigma_n \longrightarrow -\sigma_n$$

That is we assume that transition are due to a <u>local change</u> of a spin state.

This idea is based on an assumption that a simulteneous rotation of two or more spins is unlikely process.

The simplest way to introduce the frequensies of transitions $w(\alpha \to \beta)$ is given by the <u>Metropolis algorithm</u>

$$w(\alpha \to \beta) = \begin{cases} 1, & \text{if } E_\beta - E_\alpha \leqslant 0 \\ e^{-\beta \Delta E_{\beta\alpha}}, & \text{if } E_\beta - E_\alpha > 0 \end{cases}$$

One show that this algorithm satisfies the detailed balance condition.

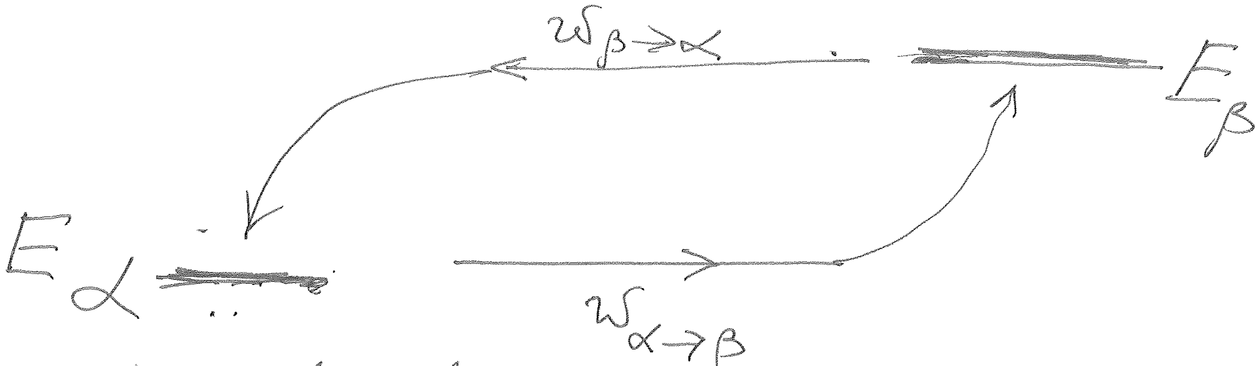
In the limit of infinite number of transition between microstates ($M \to \infty$) the statistic of the system will be the Gibbs statistic.

If we assume that every transition has a mean duration τ_0 then we can introduce "time" as $t = \tau_0 k$, where k is the number of the transitoons. The time scale τ_0 is determened by interactions between the bath and the system. This allows us to study <u>relaxaton dynamics</u> and find a relaxation time t_r

$$\Delta \text{(magnetic moment)} \propto e^{-t/t_r}$$

deviation from the equilibrium value

Energy levels



Metropolis algorithm

$$\begin{cases} w_{\alpha\to\beta} = e^{-\beta(E_\beta - E_\alpha)} \\ w_{\beta\alpha} = 1 \end{cases}$$

Ratio

$$\frac{w_{\alpha\to\beta}}{w_{\beta\to\alpha}} = e^{-\beta(E_\beta - E_\alpha)}$$

This the ~~[illegible]~~ detailed balance condition

Therefore the ratio of probabilities P_α

$$\frac{P_\beta}{P_\alpha} = \frac{w_{\alpha\to\beta}}{w_{\beta\to\alpha}} = e^{-\beta(E_\beta - E_\alpha)}$$

Thus the probability to find the system in state α ~~is~~

$$P_\alpha = \frac{e^{-\beta E_\alpha}}{Z}$$

Theoretical analysis of the relaxation time shows that, when a spin system tends to the critical point the relaxation time diverges

$$t_{\tau} \propto \frac{1}{|T - T_c|}$$

This phenomenon is called as "critical slowing down".

In the critical point $t_{\tau} = \infty$. and it means that the system relaxes following a power law

$$m(t) \propto \frac{1}{t^{z}}$$

where z is a dynamical exponent.

This result means that the more close we are to T_c, the longer time we need to reach the equilibrium state.

This phenomenon must be taken into account in simulations by increasing the number of microstates

It leads to a deviation of simulations from the theoretical formulas that were derived for the infinite number of microstates