The Potts model

We have seen that the Ising model is a 2-states model, and its generalisation to spin-1 variables, for example the Blume-Capel and the Blume-Emery-Griffiths models are 3-state systems.

The natural generalisation is the so-called "Potts model".

In the Potts model each site is occupied by a variable that can take q different variables. Neighboring site then interact with strengths that depend on the states of the two variables.

In its simplest form, the Potts model is:

$$H = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} - h \sum_i \delta_{\sigma_i, 0}$$

h a field that breaks permutation symmetry

where $\sigma_i = 0, \dots, q-1$ and $\delta_{\sigma_i,\sigma_j}$ is the Kroeneker's delta.

What is the physics of this model?

We use a mean-field approach, which is a good way to approach a new model (of course you can also approach them computationally, for example using Monte Carlo techniques).

We recall that one way to do mean-field is by writing the free-energy in terms of probabilities:

$$F = U - TS$$

with

$$U = \sum_{\{\sigma_i\}} H(\{\sigma_i\}) P(\{\sigma_i\})$$

$$S = -k_B \sum_{\{\sigma_i\}} P(\{\sigma_i\}) \ln P(\{\sigma_i\})$$

Then mean-field means forgetting about correlations:

$$P(\{\sigma_i\}) = \prod_i P(\sigma_i)$$

and

$$U = \sum_{\{\sigma_i\}} \left(-J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j} - h \sum_i \delta_{\sigma_i, 0} \right) \prod_k P_k(\sigma_k) =$$

$$= \sum_{\{\sigma_i\}} \left(-J \prod_{k \neq i,j} P_k(\sigma_k) \sum_{\langle i,j \rangle} P_i(\sigma_i) P_j(\sigma_j) - h \prod_{k \neq i} P_k(\sigma_k) \sum_i P_i(0) \right)$$

Then we can sum over all possible values of each variable that is not i or j for the interaction and not i for the field. We obtain

$$U = -J \sum_{\langle i,j \rangle} \sum_{l=0}^{q-1} p_i(\sigma_l) p_j(\sigma_l) - h \sum_i p_i(0)$$

We then assume that there is translational invariance:

$$p_i(\sigma_i) = p(\sigma_i) \quad \forall i$$

and we obtain

$$U = -J \frac{z}{2} N \sum_{\sigma=0}^{q-1} p^2(\sigma) - h N p(0)$$

We look for a phase transition where, above a given temperature, all states are equiprobable, and below it one of them, say 0, dominates.

Then we define an order parameter s such that

$$p_0 = \frac{1}{q}\left(1 + (q-1)s\right)$$

$$p_l = \frac{1}{q}(1 - s) \qquad l = 1, \dots, q-1$$

When $s=0$ then $p_\ell = \frac{1}{q}$ $\ell = 0, \dots, q-1$

while $s=1$ then $p_0 = 1$ $p_\ell = 0$ $\ell = 1, \dots, q-1$

The entropy is

$$S = -k_B \sum_{\{\sigma_i\}} P(\{\sigma_i\}) \ln P(\{\sigma_i\}) =$$

$$= -k_B \sum_{\{\sigma_i\}} \prod_k p_k(\sigma_k) \ln \prod_i p_i(\sigma_i) =$$

$$= -k_B \sum_{\{\sigma_i\}} \sum_i \prod_{k \neq i} p_k(\sigma_k) \left[p_i(\sigma_i) \ln p_i(\sigma_i) \right] =$$

$$= -k_B \sum_{\{\sigma_i\}} p_i(\sigma_i) \ln p_i(\sigma_i) = -k_B N \sum_{\sigma=0}^{q-1} p(\sigma) \ln p(\sigma)$$

At last the free-energy is

$$F = N \Big\{ -\frac{J z}{2q^2} \left[\left(1 + (q-1)s\right)^2 + (1-s)^2 (q-1) \right] +$$

extensive as it should

$$- \frac{h}{q}\left(1 + (q-1)s\right) \Big\} + k_B T \frac{1}{q} \Big[\left(1 + (q-1)s\right) \ln\left(1 + (q-1)s\right) +$$

$$+ (1-s) \ln(1-s) \Big] \Big\}$$

Let's see what are the first terms of an expansion for small s:

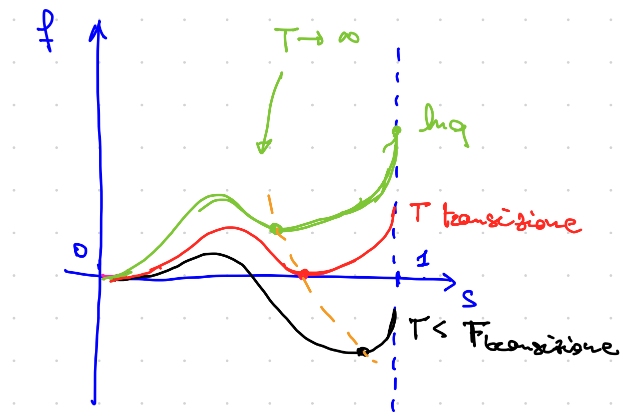
$$\underset{\color{red}{1/k_BT}}{\beta} f = \frac{\beta F}{N} \approx \frac{q-1}{2q}\left(q - \beta\frac{Jz}{2}\right) s^2 \underbrace{- \frac{1}{6}(q-1)(q-2)\, s^3}_{\text{cubic term always negative}} + \dots$$

while for $s \to 1$ we have

$$\beta f = \frac{\beta F}{N} \doteq -\beta\frac{Jz}{2} - h\beta + \ln q$$

with positive ∞ derivative

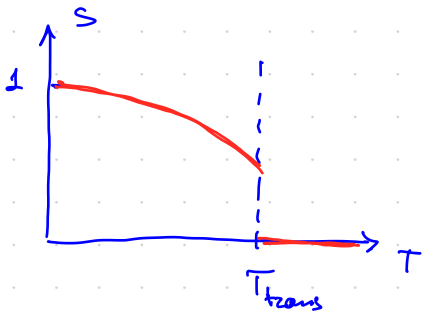
Graphically:



There is a second minimum, but if its free energy is higher than the one in $s=0$, the $s=0$ is the equilibrium state

As temperature decreases, the free energy of the second minimum also decreases and at some point it becomes to the one of the minimum in $s=0$

At even lower temperatures, the second minimum has an even lower free energy, and the system switches abruptly the order parameter, from 0 to a finite value: it is a first order phase transition!



The only case when this does not happen is $q=2$, because in this case the cubic term disappears and we are left with a simple picture of a second order phase transition.