2. Tools of statistical mechanics of disordered systems (Cavity method)

Tools/ideas/concepts there may be many but I'd like to focus on two of them:

* cavity method
* replica method

To illustrate them I need a nice, simple, nontrivial model:
ferromagnetic model of random Poissonian graphs

We want to study thermodynamical properties of

$$\mathcal{H}(\vec{\sigma}) = -\sum_{(i,j)\in G} J_{ij}\sigma_i\sigma_j - \sum_{i=1}^{N} h_i\sigma_i$$

with $\vec{\sigma} = (\sigma_1, \dots, \sigma_N)$ $\sigma_i \in \{-1, 1\}$

$G = (V, E)$

$V = \{1, \dots, N\}$ set of nodes

$E \subseteq V \times V$ set of vertices

$J_{ij} \equiv$ coupling constant,
exchange interaction
strength interaction
$\in \mathbb{R}$

If $J_{ij} > 0 \implies$ ferromagnetic interaction
$J_{ij} < 0 \implies$ antiferromagnetic interaction

$h_i \to$ local external magnetic fields

Let's consider for simplicity $J_{ij} > 0$.
Recall that thermodynamical properties of the system are microscopically captured by the Gibbs-Boltzmann probability distribution

$$P(\vec{\sigma}) = \frac{1}{Z} e^{-\beta \mathcal{H}(\vec{\sigma})}$$

$$Z \equiv \sum_{\vec{\sigma}} e^{-\beta \mathcal{H}(\vec{\sigma})}$$

is the partition function

$$-\beta F = \log Z$$

F is free energy. Observables of interest will have expectation values

$$\mathcal{O}(\vec{\sigma}) \equiv \text{some observable of interest}$$

$$\langle \mathcal{O}(\vec{\sigma}) \rangle \equiv \sum_{\vec{\sigma}} P(\vec{\sigma}) \, \mathcal{O}(\vec{\sigma})$$

Examples

1) $\mathcal{O}(\vec{\sigma}) \equiv M(\vec{\sigma}) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i$

↳ instantaneous magnetization

2) local ones

$$\mathcal{O}_i(\vec{\sigma}) = \sigma_i$$

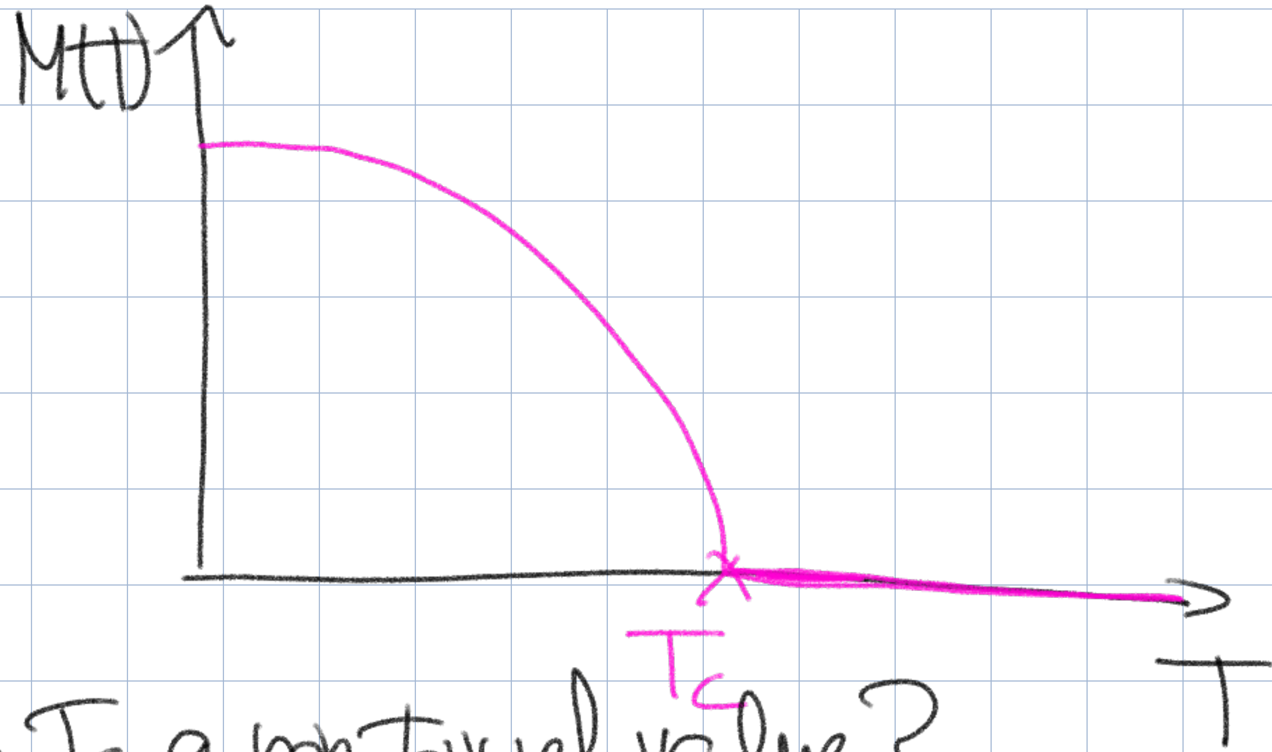
$$\mathcal{O}_{ij}(\vec{\sigma}) = \sigma_i \sigma_j$$

$$\mathcal{O}(\vec{\sigma}) = \mathcal{H}(\vec{\sigma})$$

Thermodynamical magnetization

$$M(T) = \langle M(\vec{\sigma}) \rangle$$

which behavior do we expect?



Has T_c a non-trivial value?
(Of course there are other, much more interesting question related to critical phenomena, but that is not the point of these lectures)

To find $M(T)$ I need to do the following

$$M(T) = \sum_{\vec{\sigma}} P(\vec{\sigma}) \frac{1}{N} \sum_{i=1}^{N} \sigma_i$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{\vec{\sigma}} P(\vec{\sigma}) \sigma_i$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{\sigma_i} P_i(\sigma_i) \sigma_i$$

$$= \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle$$

where

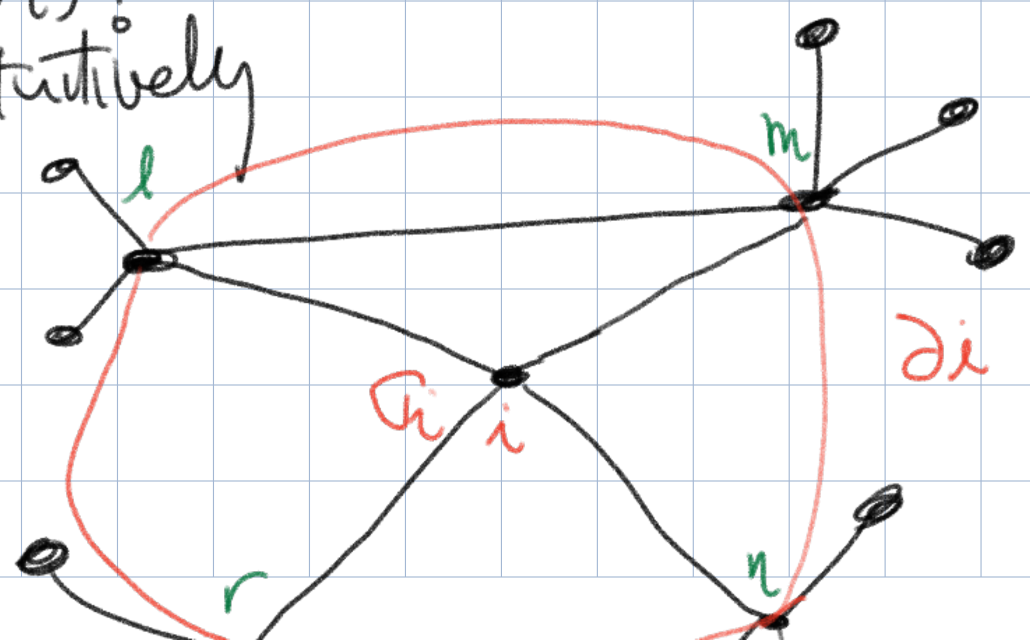
$$P_i(\sigma_i) \equiv \sum_{\sigma_{\setminus i}} P(\vec{\sigma})$$

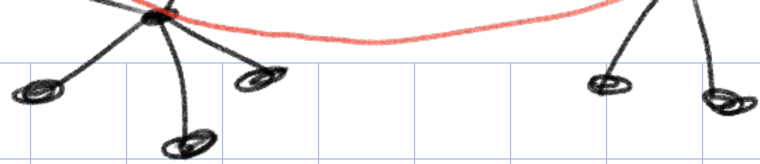
→ one-variable marginal distribution

The previous result makes perfect sense: If I want to calculate expectation values of local quantities I do not need the whole Gibbs-Boltzmann distribution only its one-variable marginals

Can I find simple expressions for $P_i(\sigma_i)$?

Intuitively





$\partial i \equiv$ the set of nodes which are neighbors to node i

→ in our example: $\partial i = \{l, m, r, n\}$

Somehow $P_i(\sigma_i)$ must depend on $P_{\partial i}(\sigma_{\partial i})$ and $P_{\partial i}(\sigma_{\partial i})$ must depend on the probabilities of the following neighbors, etc... There is of course a hierarchical structure of equations that related marginals of higher order (e.g. stat mech. is difficult)

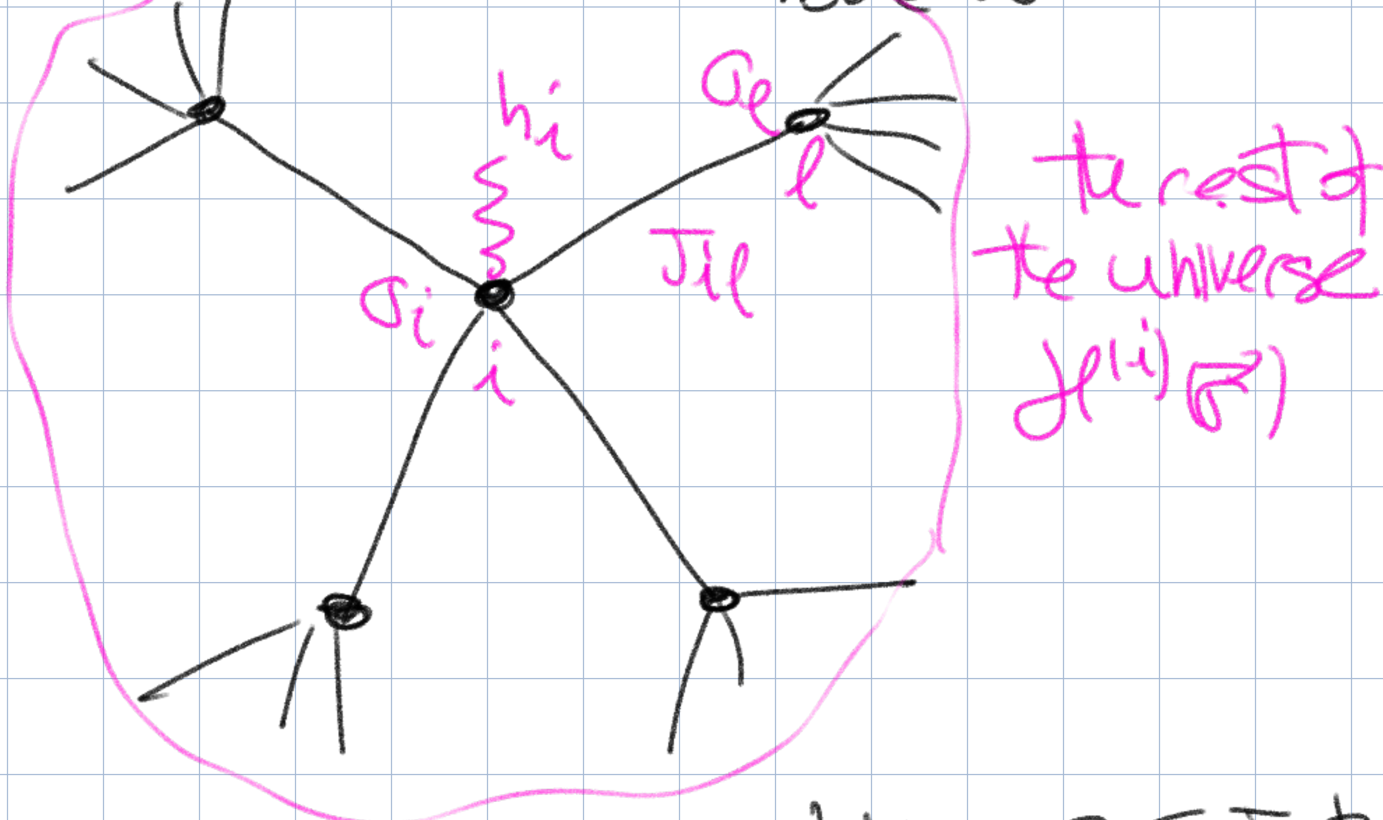
Let's write down the hierarchical structure more explicitly for the previous Hamiltonian

$$P_i(\sigma_i) = \sum_{\vec{\sigma}_{\setminus i}} P(\vec{\sigma}) = \frac{1}{Z} \sum_{\vec{\sigma}_{\setminus i}} e^{-\beta \mathcal{H}(\vec{\sigma})}$$

Let's write the Hamiltonian $\mathcal{H}(\vec{\sigma})$ as follows

$$\mathcal{H}(\vec{\sigma}) = -h_i\sigma_i - \sigma_i \sum_{l\in\partial i} J_{il}\sigma_l + \mathcal{H}^{(\backslash i)}(\vec{\sigma})$$

$\rightsquigarrow$ Hamiltonian without node i



thus $$P_i(\sigma_i) = \frac{1}{Z}\sum_{\vec{\sigma}_{\backslash i}} e^{\beta h_i\sigma_i + \beta\sigma_i \sum_{l\in\partial i} J_{il}\sigma_l} \times e^{-\beta\mathcal{H}^{(\backslash i)}(\vec{\sigma})}$$

$$= \frac{1}{Z} e^{\beta h_i \sigma_i} \sum_{\sigma_{\partial i}} e^{\beta\sigma_i \sum_{l\in\partial i} J_{il}\sigma_l} \sum_{\sigma_{\backslash i\cup\partial i}} e^{-\beta\mathcal{H}^{(\backslash i)}(\vec{\sigma})}$$

$$= \frac{Z^{(\backslash i)}}{Z} e^{\beta h_i\sigma_i} \sum_{\sigma_{\partial i}} e^{\beta\sigma_i \sum_{l} J_{il}\sigma_l}$$

$$\times \left\{ \frac{1}{Z^{(i)}} \sum_{\vec{\sigma}_{i \backslash \partial i}} e^{-\beta \mathcal{H}^{(i)}(\vec{\sigma})} \right\}$$

with $Z^{(i)} = \sum_{\vec{\sigma}_{i}} e^{-\beta \mathcal{H}^{(i)}(\vec{\sigma})}$

this is rather simply

$$P^{(i)}(\sigma_{\partial i}) = \frac{1}{Z^{(i)}} \sum_{\vec{\sigma}_{i \backslash \partial i}} e^{-\beta \mathcal{H}^{(i)}(\vec{\sigma})}$$

denote also $Z^{(i)}/Z = \frac{1}{Z_i}$

so we get

$$P_i(\sigma_i) = \frac{1}{Z_i} e^{\beta h_i \sigma_i} \sum_{\sigma_{\partial i}} e^{\beta \sigma_i \sum_{\ell} J_{i\ell} \sigma_\ell} P^{(i)}(\sigma_{\partial i})$$

which is perfectly intuitive and reasonable. Of course, now we would do the same for the object $P^{(i)}(\sigma_{\partial i})$ and so on and so forth. If you don't find this expression intuitive do the following

$$P_i(\sigma_i) = \frac{e^{\beta h_i \sigma_i}}{Z_i} \int d\theta \, \rho_{\partial i}^{(i)}(\theta) \, e^{\beta \theta \sigma_i}$$

$$\rho_{\partial i}^{(i)}(\theta) = \sum_{\sigma_{\partial i}} P^{(i)}(\sigma_{\partial i}) \, \delta\left(\theta - \sum_{\ell} J_{i\ell}\sigma_\ell\right)$$

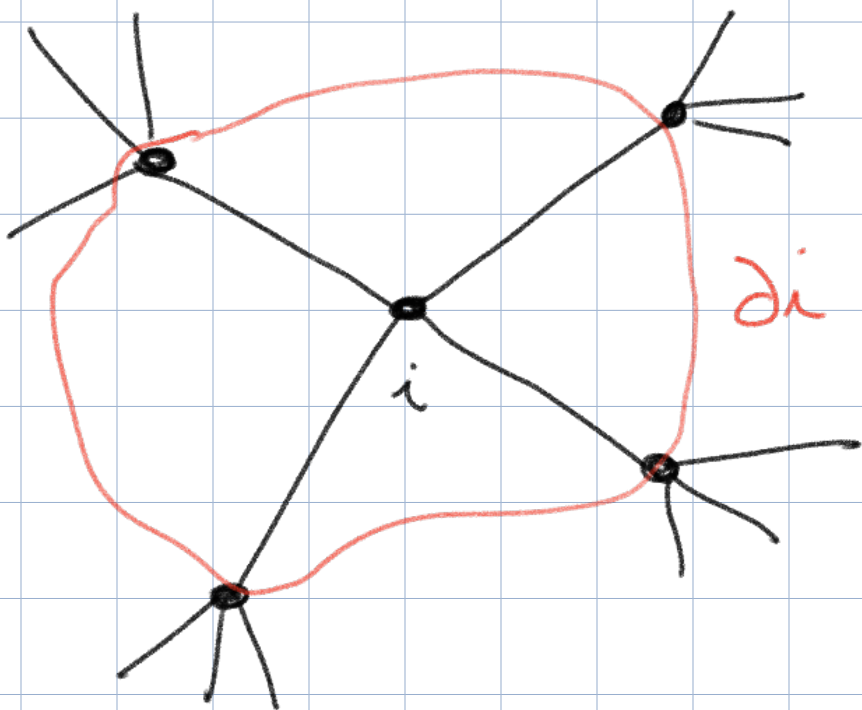
↳ probability that the neighbours of i, ∂i, generate an effective field acting on σ_i equal to θ

So, this hierarchy for the marginals is something difficult to deal with; possibilities

* truncate it and close "manually

→ depending on the place of truncation you have
basic mean field theory
1st order mean field theory
...

For certain types of models the function occurs naturally!
Suppose that G is a "tree"



If we remove i then the neighbours of i, ∂i are statistically independent. This mean

$$P^{(u)}_{\partial i}(\sigma_{\partial i}) = \prod_{\ell \in \partial i} P^{(u)}_{\ell}(\sigma_{\ell})$$

When graph is tree-like or maybe we want to use this as an approximation this is called the Bethe-Peierls approximation

$$P^{(i)}_{\partial i}(\sigma_{\partial i}) \simeq \prod_{\ell \in \partial i} P^{(i)}_{\ell}(\sigma_{\ell})$$

↳ Bethe-Peierls approximation

Using Bethe-Peierls expression / approximation we have

$$P_i(\sigma_i) = \frac{1}{Z_i} e^{\beta h_i \sigma_i} \prod_{\ell \in \partial i} \sum_{\sigma_\ell} e^{\beta \sigma_i J_{i\ell} \sigma_\ell} P^{(i)}_{\ell}(\sigma_\ell)$$

↳ physical/real one-variable marginals

cavity/auxiliary one variable marginals

cavity method ≡ see how the system behaves when removing certain objects

Notice that although $P_i(\sigma_i)$ and $P^{(i)}_{\ell}(\sigma_\ell)$ are single-variable marginals, they are not of the same nature ⇒ This is not a system of closed equations. How to close it?

start from $P_i^{(j)}(\sigma_i)$ with $j \in \partial i$ and do the same type of derivation: you will find that

$$\boxed{P_i^{(j)}(\sigma_i) = \frac{e^{\beta h_i \sigma_i}}{Z_i^{(j)}} \prod_{\ell \in \partial i \setminus j} e^{\beta J_{i\ell} \sigma_i \sigma_\ell} P_\ell^{(i)}(\sigma_\ell)}$$

this are the so-called cavity equations

Recall I want and efficient way to obtain $M(T)$. Let's introduce the following parametrization

$$P_i^{(j)}(\sigma_i) = \frac{e^{\beta \tilde{h}_i^{(j)} \sigma_i}}{2\cosh(\beta \tilde{h}_i^{(j)})} \quad \text{and} \quad \tilde{h}_i^{(j)} \equiv \text{are cavity fields}$$

$$P_i(\sigma_i) = \frac{e^{\beta \tilde{h}_i \sigma_i}}{2\cosh(\beta \tilde{h}_i)}$$

Then

$$M(t) = \frac{1}{N}\sum_{i=1}^{N} \tanh(\beta \tilde{h}_i) \quad (\cancel{**a})$$

with

$$\tilde{h}_i = \theta_i + \sum_{\ell \in \partial i} u(J_{i\ell}, h_\ell^{(i)}) \quad (\cancel{aa})$$

$$h_i^{(j)} = \theta_i + \sum_{\ell \in \partial i / j} u(J_{i\ell}, h_\ell^{(i)}) \quad (*)$$

cavity equation

and

$$u(x,y) = \frac{1}{\beta} \operatorname{atanh}\left[\tanh(\beta x)\tanh(\beta y)\right]$$

We solve the problem B

I. Iterate (*) until convergence this is called the belief propagation algorithm

2. Use solution in ($\cancel{**}$) to obtain $\{\tilde{h}_i\}$

3. Use the solution of $\{\tilde{h}_i\}$ in ($\cancel{aaa}$) to obtain M(t)

Of course, one can use this method of the cavity (seeking to generate statistical independence of objects) to calculate other thermodynamic quantities: I leave as an exercise for you to use this method to find expressions of

- internal energy in terms of cavity marginals/fields
- free energy in terms of cavity marginals

Also I leave as an exercise to consider the case of an homogeneous system on random regular graphs to see how far you can go with the cavity equations