Spin Glasses and Replica Symmetry

Carlos Couto

Instituto Superior Técnico - Departamento de Física

Quantum Agora - 28th of October 2021

Introduction

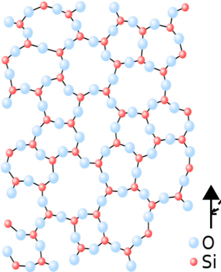
- Goal $\longrightarrow$ Expose techniques used to study spin-glass systems:
  - Replica trick;
  - Replica Symmetry Breaking.
- These methods are used to study disordered systems.
- Techniques have been useful in other fields like machine learning, enabling calculations such as knowing the storage capacity of certain models.

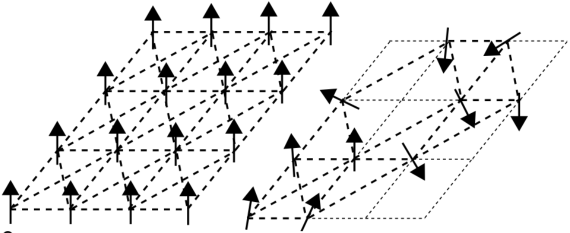
Outline

- Disordered Systems;
- Replica trick;
- The p-spin spherical model:
  - Annealed free energy
  - Replica symmetric free energy
  - Replica symmetry breaking free energy

Disordered Systems - Spin-Glasses

- The replica method is useful when studying **disordered systems**.
- Disorder $\longrightarrow$ Absence of symmetries/correlations.
- **Spin-glasses** are famous examples of this, belonging to the class of *quenched disordered* systems.





As an example take the Edwards-Anderson model:

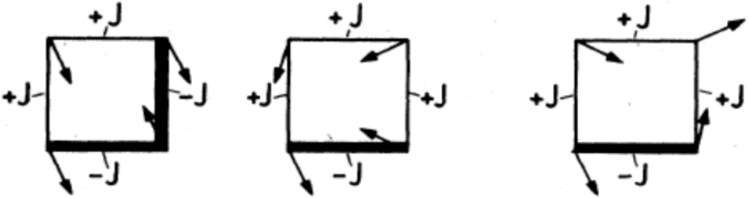
$$H = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j \tag{1}$$

Or the Sherrington-Kirkpatrick model:

$$H = -\sum_{ij} J_{ij}\sigma_i\sigma_j \tag{2}$$

- Disorder is present via the random couplings J.
- *Quenched* $\implies$ J are constant in time (or at least at the timescale where the spins fluctuate).

- *Disorder is frustrating.*
- Frustration $\longrightarrow$ There exists loops where product of couplings is negative.
- Impossible to satisfy all couplings at the same time.
- This leads to multiplicity of states with the same energy.



- In principle, every observable is some function $O(\boldsymbol{\sigma}, \boldsymbol{J})$ which depends on the specific configuration of couplings J and spins σ.
- However, for large enough systems we expect that physical properties do not depend on J.
- That is, we expect physical quantities to be **self-averaging**.
- For increasingly large N the distribution for any physical quantity is **sharply peaked around its average value** and the variance goes to zero.

Free energy

- The free energy of a given system, in the thermodynamic limit is:

$$F = \lim_{N\to\infty} -\frac{1}{\beta N} \int dJ p(J) \log \int d\sigma e^{-\beta H(\sigma,J)} \qquad (3)$$

- This is a quenched average. For each realization of the system we first compute the free energy and then we average it out over J.
- One way of solving integrals like the above is through the replica trick.
- A simpler, crude approximation is given by

$$F = -\frac{1}{\beta N} \log \int dJ p(J) \int d\sigma e^{-\beta H(\sigma,J)} \qquad (4)$$

which is called the annealed approximation, valid for high temperatures.

Replica trick

- The replica trick stems from the following remark:

$$\overline{\log Z} = \lim_{n \to 0} \frac{1}{n} \log \overline{Z^n} = \lim_{n \to 0} \frac{\overline{Z^n} - 1}{n} \tag{5}$$

- The above always holds true in the real numbers.
- The *trick* is to promote n to an integer, meaning that

$$\overline{Z^n} = \int d\sigma_1 \cdots d\sigma_n \overline{e^{-\beta H(\sigma_1, J) - \cdots - \beta H(\sigma_n, J)}} \,. \tag{6}$$

- Performing the above calculation is only valid for integers, however we will perform an analytical continuation of the results to realize the limit.

- On disordered systems, at low temperature and in the thermodynamic limit we can have **ergodicity breaking**.
- It is useful to split these parts into "pure states" and if to each configuration we can assign one pure state then

$$\langle A\rangle = \frac{1}{Z}\int D\sigma e^{\beta H(\sigma)} A(\sigma) = \frac{1}{Z}\sum_{\alpha}\int_{\sigma\in\alpha} D\sigma e^{\beta H(\sigma)} A(\sigma) = \sum_{\alpha} w_{\alpha}\langle A\rangle_{\alpha} \tag{7}$$

- An alternative form of the replica trick is:

$$\overline{\langle A\rangle} = \lim_{n\to 0}\int D\sigma_1\cdots D\sigma_n A(\sigma_1)\overline{e^{-\beta H(\sigma_1,J)-\cdots-\beta H(\sigma_n,J)}}$$

- The Hamiltonian is given by:

$$H = -\sum_{i_1 > \cdots > i_p = 1}^{N} J_{i_1 \cdots i_p} \sigma_{i_1} \cdots \sigma_{i_p} \quad , p \geq 3 \; ; \tag{8}$$

- To keep energy finite, the spins are continuous real variables such that $\sum_{i=1}^{N} \sigma_i^2 = N$. $\rightarrow$ **spherical constraint**
- The couplings follow a Gaussian distribution:

$$p(J) = \exp\left(-\frac{1}{2} J^2 \frac{2N^{p-1}}{p!} \right) \tag{9}$$

Notice that the variance goes to zero in the thermodynamic limit.

- Annealed Free Energy $\rightarrow$ Average of the partition function over the disorder:

$$\overline{Z} = \int D\sigma \int \prod_{i_1 > \cdots > i_p \geq 1} dJ^N_{i_1 \cdots i_p} \exp\left[-J^2_{i_1 \cdots i_p} \frac{N^{p-1}}{p!} + J_{i_1 \cdots i_p} \beta \sigma_{i_1} \cdots \sigma_{i_p} \right] \tag{10}$$

- The integral over the spins **is over a spherical surface** (remember the constraint!).
- The integrals on the couplings are **Gaussian integrals**.

Sidenote

We can ignore the normalization constants as they will disappear when we take the logarithm and the thermodynamic limit.

- Performing the Gaussian integration for each coupling leaves us with:

$$\overline{Z} = \int D\sigma \exp\left[\frac{\beta^2}{4N^{p-1}} p! \sum_{i_1 > \cdots > i_p \geq 1}^{N} \sigma_{i_1}^2 \cdots \sigma_{i_p}^2\right] \tag{11}$$

- As $N \to \infty$, we have that $p! \sum_{i_1 > \cdots > i_p \geq 1}^{N} \approx \sum_{i_1 \cdots i_p = 1}^{N}$. This simplifies to:

$$\overline{Z} = \int D\sigma \exp\left[\frac{\beta^2}{4N^{p-1}} \left(\sum_{i=1}^{N} \sigma_i^2\right)^p\right] = \exp\left[\frac{N\beta^2}{4}\right] \Omega \tag{12}$$

where Ω is the surface of the sphere.

Free Energy per site

$$F = -\beta/4 - \frac{\log \Omega}{\beta N}$$

- To make use of the replica trick we need to calculate $\overline{Z^n}$. We will make use of indices a, b to signify the replicas.

$$\overline{Z^n} = \int D\sigma_i^a \int \prod_{i_1 > \cdots > i_p \geq 1}^{N} dJ_{i_1 \cdots i_p}^N \exp\left[-J_{i_1 \cdots i_p}^2 \frac{N^{p-1}}{p!} + J_{i_1 \cdots i_p} \beta \sum_{a=1}^{n} \sigma_{i_1}^a \cdots \sigma_{i_p}^a \right] \tag{13}$$

- Performing the Gaussian integration and using the thermodynamic limit to swap the sums yields:

$$\overline{Z^n} = \int D\sigma_i^a \exp\left[\frac{\beta^2}{4N^{p-1}} \sum_{a,b=1}^{n} \left(\sum_{i=1}^{N} \sigma_i^a \sigma_i^b \right)^p \right] \tag{14}$$

- We **start with coupled sites** and **decoupled replicas** and after averaging over the disorder we **decoupled the sites** and **coupled the replicas**.

Overlap and self-overlap of spin configurations

Overlap of spin configurations

An useful quantity to measure the similarity between two different spin configurations σ and τ is their overlap:

$$q_{\sigma\tau} = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tau_i \tag{15}$$

The **self-overlap** is given by $q_{\sigma\sigma} = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^2$.

- With Ising spins, $s_i = \pm 1$ the overlap can be:
  - $1 \rightarrow$ Configurations are completely correlated
  - $-1 \rightarrow$ Configurations are completely anti-correlated
  - $0 \rightarrow$ Configurations are uncorrelated
- In our case, the overlaps between replicas will be represented by Q_{ab}. The spherical constraint ensures that $Q_{aa} = 1$.
- Furthermore we have that $-1 \leq Q_{ab} \leq 1$.

- An useful property of the Dirac delta is:

$$\int_{\mathbb{R}^N} f(\boldsymbol{x})\delta(g(\boldsymbol{x}))d\boldsymbol{x} = \int_{g^{-1}(0)} \frac{f(\boldsymbol{x})}{|\nabla g|} d\sigma(\boldsymbol{x}) \ , \tag{16}$$

  where $\sigma(\boldsymbol{x})$ is a surface measure of $g^{-1}(0)$.
- **Strategy** $\rightarrow$ pass the spherical integral to an integral over all possible spins using $g(\sigma_i^a) = N - \sum_i (\sigma_i^a)^2 \implies |\nabla g| = 4N$.
- Pass to the Fourier representation of the Dirac delta.
- We also have that:

$$1 = \int dQ_{ab}\delta\left(NQ_{ab} - \sum_i \sigma_i^a\sigma_i^b\right) = \int dQ_{ab} \int d\lambda_{ab} e^{\lambda_{ab}\left(NQ_{ab} - \sum_i \sigma_i^a\sigma_i^b\right)} \tag{17}$$

Replica Calculation

- Using the Dirac delta property from the previous slide and introducing the integrals over Q_{ab} for $a \neq b$ we have:

$$\overline{Z^n} = \int DQ_{ab} \int D\lambda_{ab} \int D\sigma_i^a \exp\left[\frac{\beta^2 N}{4} \sum_{a,b=1}^{n} Q_{ab}^p + N \sum_{a,b=1}^{n} \lambda_{ab} Q_{ab} - \sum_{i=1}^{N} \sum_{a,b=1}^{n} \lambda_{ab} \sigma_i^a \sigma_i^b\right] \tag{18}$$

- We can perform the integral over the spins, which is an n-dimensional Gaussian integral, yielding:

$$\overline{Z^n} = \int DQ_{ab} \int D\lambda_{ab} \exp\left[-NS(Q,\lambda)\right] \tag{19}$$

with

$$S(Q,\lambda) = -\frac{\beta^2}{4} \sum_{a,b=1}^{n} Q_{ab}^p - \sum_{a,b=1}^{n} \lambda_{ab} Q_{ab} + \frac{1}{2} \log\det(2\lambda) \tag{20}$$

Some caveats

Caveat 1

The Free energy is given by:

$$F = -\lim_{N\to+\infty}\lim_{n\to 0}\frac{1}{n\beta N}\log\int DQ_{ab}D\lambda_{ab}\exp\left[-NS(Q,\lambda)\right] \quad (21)$$

but we are unable to calculate the above unless we swap the limits.

Caveat 2

- We need to know which saddle point is the correct one.
- **Criterion** $\rightarrow$ First correction to the saddle point method is a Gaussian integral, which should be well defined.
- Thus the eigenvalues of Hessian of $S(Q,\lambda)$ must all be positive.

The saddle point calculation

- Using the formula $\frac{\partial}{\partial \lambda_{ab}} \log \det \lambda = (\lambda^{-1})_{ab}$ the saddle point equations for λ_{ab} and Q_{ab} are:

$$2\lambda_{ab} = (Q^{-1})_{ab}$$
$$0 = \frac{\beta^2 p}{2} Q_{ab}^{p-1} + (Q^{-1})_{ab}$$

- Using the above and performing the integral, we get

Free energy after saddle point calculation

$$F = -\lim_{n\to 0} \frac{1}{2n\beta} \left(\frac{\beta^2}{2} \sum_{a,b=1}^{n} Q_{ab}^p + \log \det Q \right) \tag{22}$$

Replica Symmetry Ansatz

- As all replicas are equivalent, it is not far-fetched to assume a **replica symmetric form** for Q:

$$Q_{ab} = q_0 + (1 - q_0)\delta_{ab} \tag{23}$$

- As for the inverse matrix elements we have:

$$(Q^{-1})_{ab} = \frac{1}{1 - q_0}\delta_{ab} - \frac{q_0}{(1 - q_0)[1 + (n - 1)q_0]} \tag{24}$$

- This makes the saddle point equation

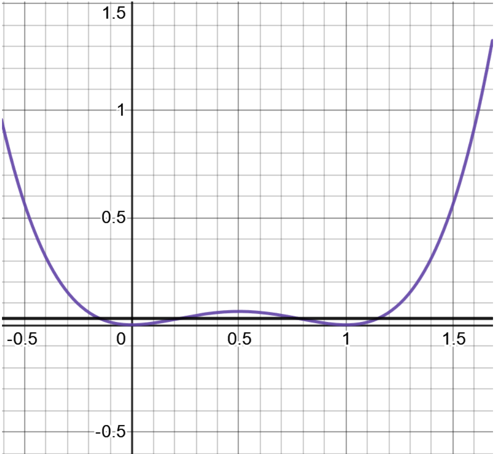
$$\frac{\beta^2 p}{2} q_0^{p-1} - \frac{q_0}{(1 - q_0)^2} = 0 \tag{25}$$

- $q_0 = 0$ is the paramagnetic solution, making it so that $F = -\frac{\beta}{4}$, the result obtained in the annealed calculation!

- We can rewrite the saddle point equation as

$$q_0^{p-2}(1-q_0)^2 = \frac{2}{\beta^2 p} \tag{26}$$

- For large β, the solutions are associated with negative eigenvalues.



Edwards-Anderson order parameter

$$q^{(1)} = \frac{1}{N}\sum_i \overline{\langle\sigma_i\rangle^2}$$

- We can rewrite the order parameter as:

$$q^{(1)} = \frac{1}{N}\sum_{i,\alpha\beta} \overline{w_\alpha w_\beta \langle\sigma_i\rangle_\alpha \langle\sigma_i\rangle_\beta} = \sum_{\alpha\beta} \overline{w_\alpha w_\beta q_{\alpha\beta}} = \int dq \overline{P(q)} q \qquad (27)$$

  where $P(q) = \sum_{\alpha\beta} w_\alpha w_\beta \delta(q - q_{\alpha\beta})$ is **the overlap distribution**.
- Similarly we find:

$$q^{(k)} = \frac{1}{N^k}\sum_{i_1\cdots i_k} \overline{\langle\sigma_{i_1}\cdots\sigma_{i_k}\rangle^2} = \int dq \overline{P(q)} q^k \qquad (28)$$

- We can also use the replica trick to compute the order parameter:

$$\frac{1}{N}\sum_i \overline{\langle\sigma_i\rangle^2} = \lim_{n\to 0} \overline{\int D\sigma_i^a \frac{1}{N}\sum_i \sigma_i^1 \sigma_i^2 e^{-\beta\sum_a H(\sigma^a)}} = \cdots = \lim_{n\to 0} Q_{12}^{SP}$$

- If there is no replica symmetry then it could be that $Q_{12}^{SP} \neq Q_{34}^{SP}$. **Nonsense!** Choice of indices should not matter!
- There may be other saddle points with the same free energy which correspond to the several choices of indices we can make.
- As such, we should average all these saddle points, yielding:

$$q^{(1)} = \lim_{n \to 0} \frac{2}{n(n-1)} \sum_{a>b} Q_{ab}^{SP} \tag{29}$$

and similarly we can generalize

$$q^{(k)} = \lim_{n \to 0} \frac{2}{n(n-1)} \sum_{a>b} (Q_{ab}^{SP})^k \tag{30}$$

Connecting the physics with the replicas

- The previous equations leads us to conclude that

$$\int dq\overline{P(q)}f(q) = \lim_{n\to 0}\frac{2}{n(n-1)}\sum_{a>b} f(Q_{ab}^{SP}) \tag{31}$$

- With $f(q) = \delta(q - q')$ we get:

$$\overline{P(q)} = \lim_{n\to 0}\frac{2}{n(n-1)}\sum_{a>b}\delta(Q_{ab}^{SP} - q) \tag{32}$$

- The entries of Q_{ab}^{SP} are the possible overlaps between pure states. The total number of equal elements is related to the probability of such an overlap occurring.

Revisiting the replica symmetric ansatz

- The average overlap distribution is $\overline{P(q)} = \delta(q - q_0)$.
- The overlap distribution also contains the self-overlaps of the pure states.
- As there is only one possible overlap this must be **the self-overlap of the only existing pure state**, the paramagnetic state.
- Assuming a replica symmetric ansatz $\implies$ System only has one equilibrium state.
- If there is ergodicity breaking at low temperatures we must search for a **replica symmetry breaking form for the matrix** in order to have more than one equilibrium state.

Replica symmetry breaking

- **Overlap between replicas is related to overlap between states.**
- The self-overlap of a state is the average overlap between configurations of said state.
- We expect that the overlap between configurations of the same state is greater than the one with configurations from different states.
- **What is the simplest possible ergodicity breaking we can have?**
    - Have the overlap between configurations of the same state be $q_1 < 1$.
    - Have the overlap between configurations of different states be q_0, with $q_1 > q_0$.

- **Replicas are like configurations**! Let us cluster them into "states". Replicas may belong to the same state or not.
- Assuming a clustering of $m = 3$ replicas per group we have:

$$Q_{ab} = \begin{bmatrix} 1 & q_1 & q_1 & & & & \\ q_1 & 1 & q_1 & & q_0 & & \cdots \\ q_1 & q_1 & 1 & & & & \\ & & & 1 & q_1 & q_1 & \\ & q_0 & & q_1 & 1 & q_1 & \\ & & & q_1 & q_1 & 1 & \\ & \vdots & & & & & \ddots \end{bmatrix} \tag{33}$$

- This is called the **one step replica symmetry breaking**, or **1RSB**.

- The associated overlap distribution is:

$$\overline{P(q)} = \frac{m-1}{n-1}\delta(q-q_1) + \frac{n-m}{n-1}\delta(q-q_0) \tag{34}$$

with $1 \leq m \leq n$.

- Taking the $n \to 0$ limit we obtain

$$\overline{P(q)} = (1-m)\delta(q-q_1) + m\delta(q-q_0) \tag{35}$$

- It is clear then that for $\overline{P(q)}$ to remain a probability distribution we must have $0 \leq m \leq 1$, after taking the limit $n \to 0$.
- Thus we have three parameters, the two values of the overlaps q_0 and q_1 and the parameter m, which controls the probability of each overlap.

- Knowing the structure of the matrix Q_{ab} if we calculate its eigenvalues and their multiplicity we are able to simplify the free energy to:

$$
\begin{aligned}
-2\beta F_{1RSB} = & \frac{\beta^2}{2}[1+(m-1)q_1^p - mq_0^p] + \frac{m-1}{m}\log(1-q_1)+ \\
& + \frac{1}{m}\log[m(q_1-q_0)+(1-q_1)] + \frac{q_0}{m(q_1-q_0)+(1-q_1)}
\end{aligned}
$$

- Both the $q_1 \to q_0$ as well as the $m \to 1$ limits lead to the same free energy one would obtain in the replica symmetric ansatz.
- The only remaining thing to do is to solve the saddle point equations with respect to the parameters m, q_0, q_1.

- The equation $\partial_{q_0} F = 0$ gives $q_0 = 0$. As we are in the absence of external magnetic field we expect the distribution of states across phase space to be symmetric, with all states being orthogonal to each other.
- The other two equations are:

$$(1-m)\left(\frac{\beta^2}{2} p q_1^{p-1} - \frac{q_1}{(1-q_1)[(m-1)q_1+1]}\right) = 0 \quad (36)$$

$$\frac{\beta^2}{2} q_1^p + \frac{1}{m^2}\log\left(\frac{1-q_1}{1-(1-m)q_1}\right) + \frac{q_1}{m[1-(1-m)q_1]} = 0 \quad (37)$$

- We can solve the first equation by setting $m = 1$. There we find a non-trivial stable solution q_s at a temperature T_s.
- Note that $q_1 = 0$ is also a solution, leaving m undetermined. $\rightarrow$ paramagnetic phase

- For $T > T_s$ we only have one state and $P(q) = \delta(q - q_0)$.
- At $T = T_s$ we already have $q_s \neq 0$, thus the states are already well formed.
- Lowering the temperature gives a solution with $m < 1$ and $q_1 > q_s$.
- However, $m = 1$ makes it so that the probability of these states is zero, growing as we continue to decrease the temperature.

$$\overline{P(q)} = (1 - m)\delta(q - q_1) + m\delta(q - q_0) \tag{38}$$

Concluding Remarks

- The 1RSB has been proven to be exact. If we were to perform additional steps we would obtain trivial contributions from the saddle point equations.
- Using the 1RSB we found a transition between the paramagnetic phase and a spin-glass phase at low temperature.
- The reason why the states are well-formed at the transition has to do with the existence of metastable states above T_s. These are not captured by this static analysis.

The end.

Any questions?

Main References

- Castellani, T., & Cavagna, A. (2005). Spin-Glass Theory for Pedestrians. Journal of Statistical Mechanics: Theory and Experiment, 2005(05), P05012. https://doi.org/10.1088/1742-5468/2005/05/P05012
- Crisanti, A., & Sommers, H.-J. (1992). The spherical p-spin interaction spin glass model: The statics. Zeitschrift Für Physik B Condensed Matter, 87(3), 341–354. https://doi.org/10.1007/BF01309287
- Morone, F., Caltagirone, F., Harrison, E., & Parisi, G. (2014). Replica Theory and Spin Glasses. ArXiv:1409.2722 [Cond-Mat]. http://arxiv.org/abs/1409.2722