The replica method for computational problems with randomness: principles and illustrations

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The Nobel Prize in Physics 2021

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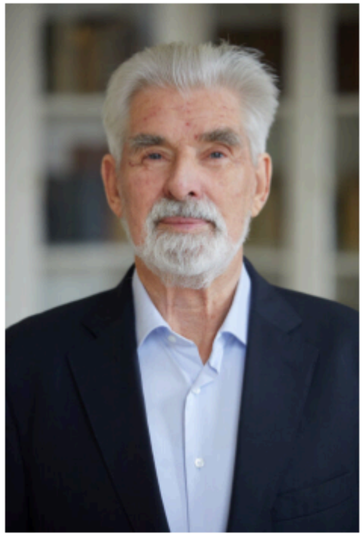
Syukuro Manabe
Prize share: 1/4



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The Nobel Prize in Physics 2021 was awarded "for groundbreaking contributions to our understanding of complex physical systems" with one half jointly to Syukuro Manabe and Klaus Hasselmann "for the physical modelling of Earth's climate, quantifying variability and reliably predicting global warming" and the other half to Giorgio Parisi "for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales."

Around 1980, Giorgio Parisi discovered hidden patterns in disordered complex materials. His discoveries are among the most important contributions to the theory of complex systems. They make it possible to understand and describe many different and apparently entirely random materials and phenomena, not only in physics but also in other, very different areas, such as mathematics, biology, neuroscience and machine learning.

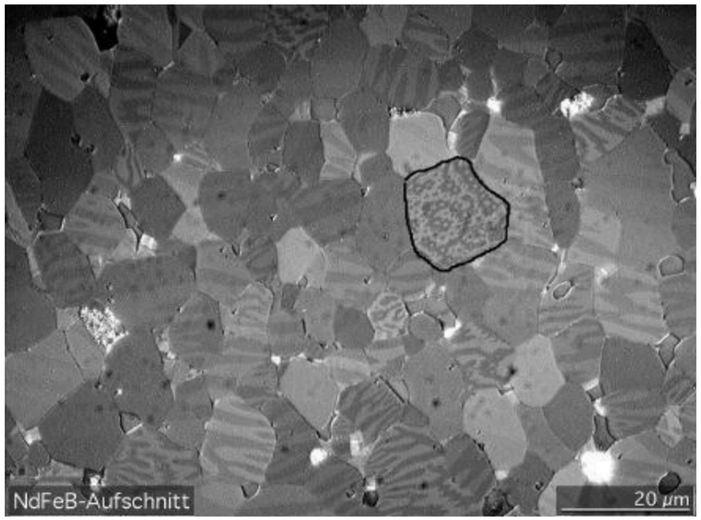
- Randomness in physics and historical background

- The replica method: definitions and meaning

- Illustration on an exactly solvable model
    - without replicas (today)
    - with replicas (tomorrow)

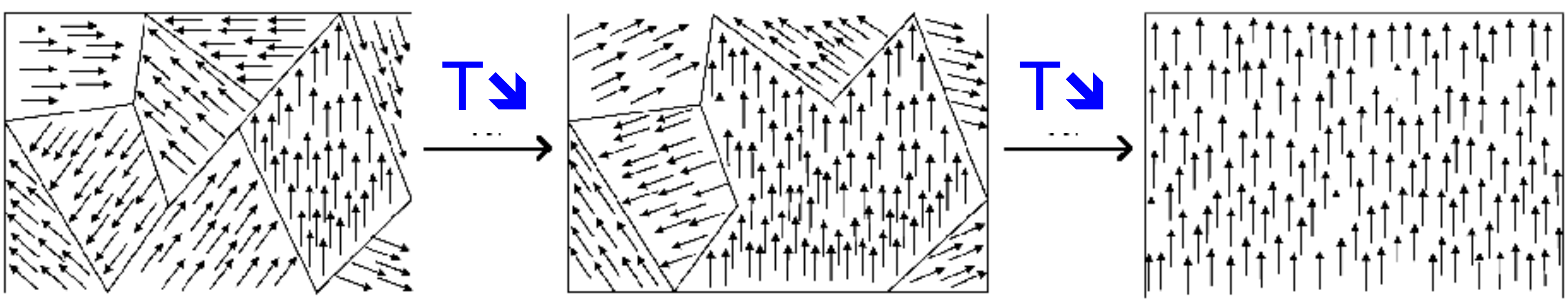
- Next lectures:
  applications to supervised/unsupervised problems
  connections with representations in neuroscience

Magnetic domains



Magnetic materials are made of small domains, in which electronic magnetic moments (carried out by spins) are oriented along the same direction. Different domains point in unrelated directions.

Al low enough temperature, all spins point in a unique direction
-> magnets



Models for magnetic materials

- Magnetic moments are vectors $\vec{S}_i$ of unit norms attached to the sites *i* of the lattice (case of 1-dim vectors: $S_i = \pm 1$)

- The probability density of a configuration of the moments is

$$p\left(\vec{S}_1,\vec{S}_2,\ldots,\vec{S}_N\right)=\frac{1}{Z}\exp\left(J\sum_{<i,j>}\vec{S}_i\cdot\vec{S}_j/T\right)$$

where J is the interaction between neighbours on the lattice
T is the temperature

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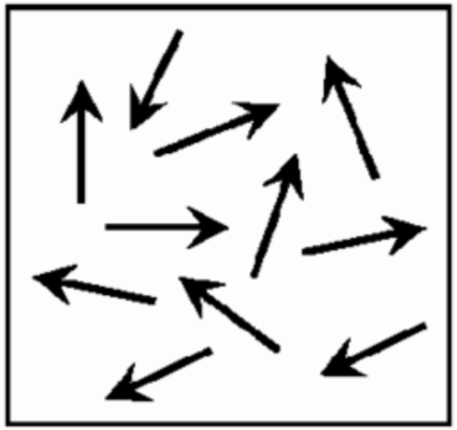
High *T*



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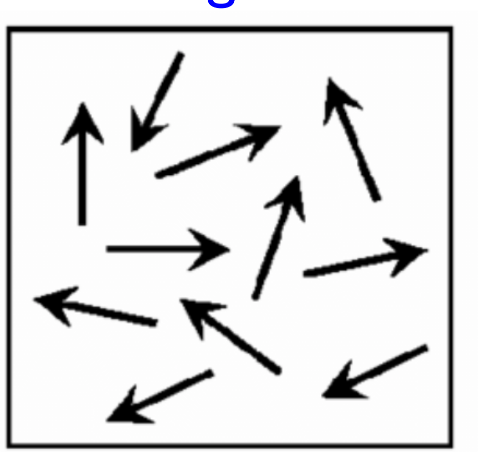
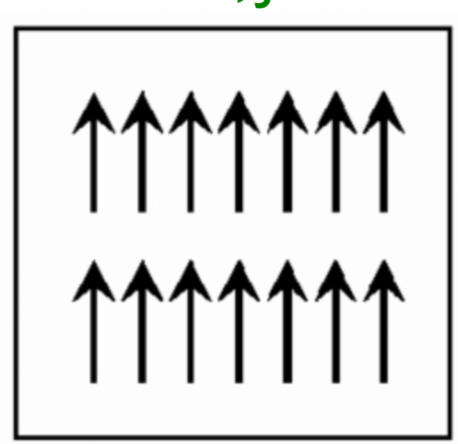


Low *T*, *J* > 0



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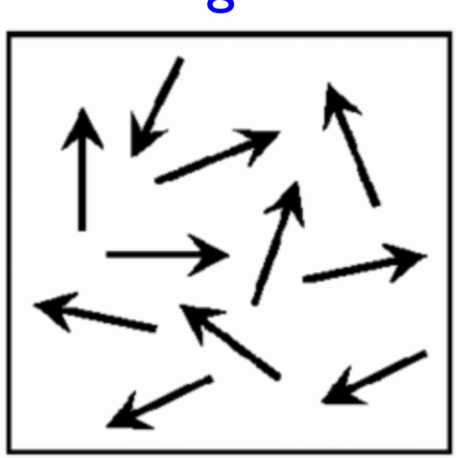

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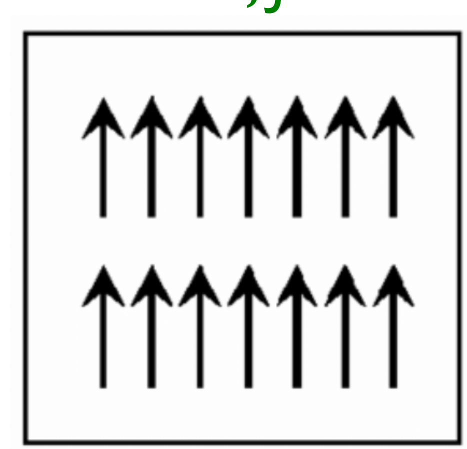
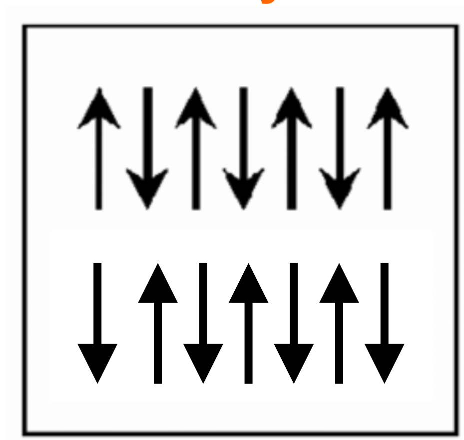
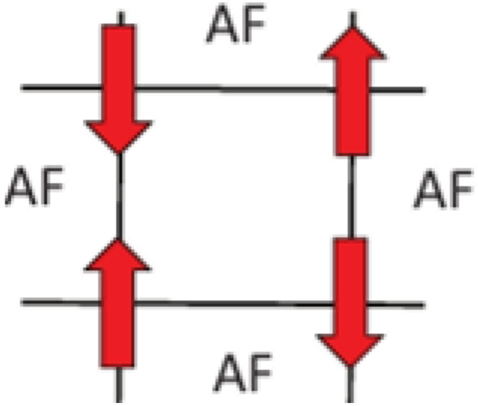


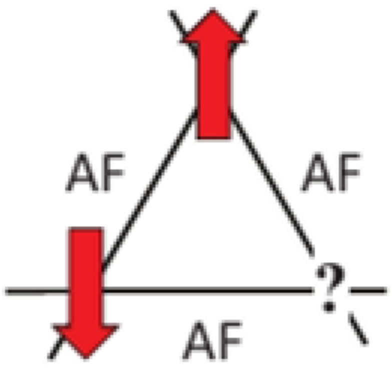
Low *T*, *J* < 0



Frustration



Square lattice

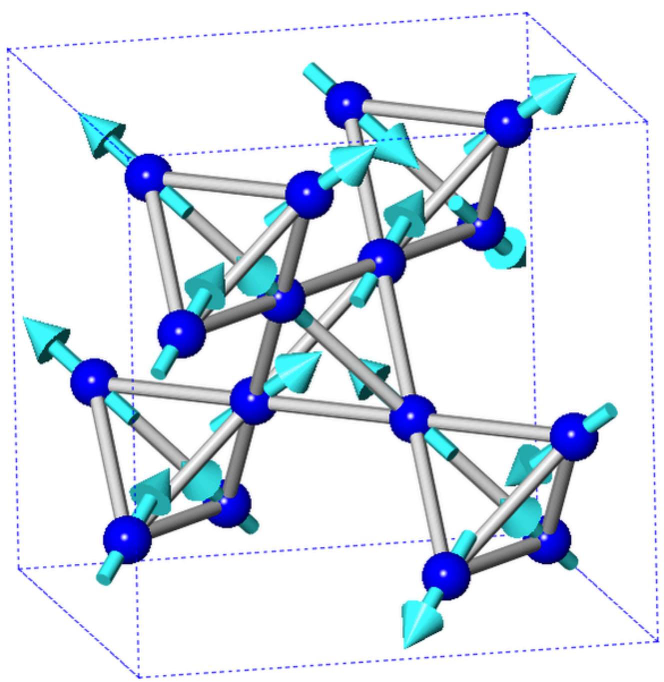


Triangular lattice

- Greedy search does not necessarily provide best configuration, i..e minimizing energy

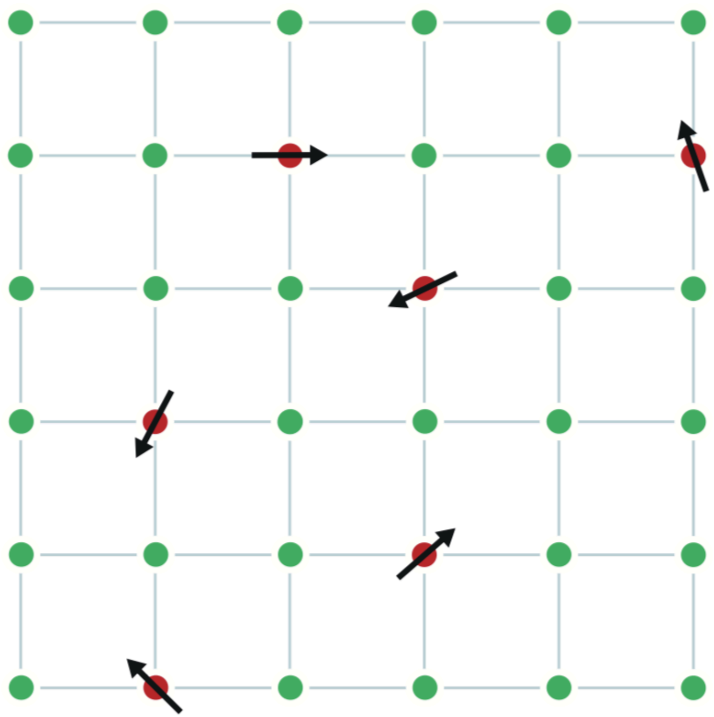
$$E = -J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$

- Best configurations can be highly degenerate: exponential number of configurations have equal (or almost equal) probabilities



Pyrochlore lattice : Dysprosium titanate $Dy_2Ti_2O_7$ (Dy carry magnetic moments, Ti and O atoms not shown)

« Dirty » magnetic materials: spin glasses

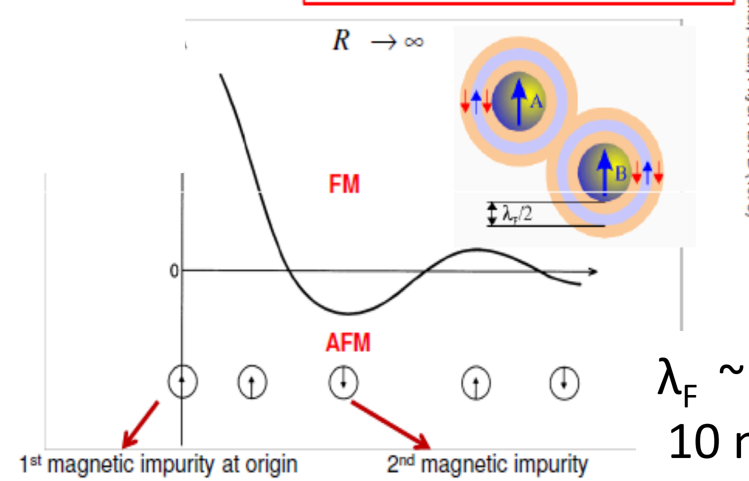


Spin glass

A spin glass is a metal alloy where iron atoms, for example, are randomly mixed into a grid of copper atoms. Each iron atom behaves like a small magnet, or spin, which is affected by the other magnets around it. However, in a spin glass they are frustrated and have difficulty choosing which direction to point. Using his studies of spin glass, Parisi developed a theory of disordered and random phenomena that covers many other complex systems.

- Iron
- Copper

$$J \propto (2k_F R)^{-2} \sin(2k_F R)$$



λ_F ~ qq 10 nm

RKKY interaction:
(Ruderman-Kittel-Kasuya-Yoshida)

$$p\left(\vec{S}_1,\vec{S}_2,\ldots,\vec{S}_N\right) = \frac{1}{Z\left[\left\{J_{ij}\right\}\right]}\exp\left(\sum_{<i,j>} J_{ij}\ \vec{S}_i \cdot \vec{S}_j / T\right)$$

??

Systems with quenched disorder

- Quenched random variables: interactions J_{ij} between spins, which are drawn at random (positive or negative) and quenched (they do not vary for a given system or « sample »)

- Thermal variables: spins $\vec{S}_i$ drawn from the *J*-dependent distribution

$$p\left(\vec{S}_1, \vec{S}_2, \ldots, \vec{S}_N \middle| \left\{J_{ij}\right\}\right) = \frac{1}{Z\left[\left\{J_{ij}\right\}\right]} \exp\left(\sum_{<i,j>} J_{ij} \; \vec{S}_i \cdot \vec{S}_j / T\right)$$

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- A historically important illustration: interactions J_{ij} drawn from a Gaussian (zero mean), and spins $s_i = \pm 1$ (Sherrington et Kirkpatrick, 1974)

Machine-learning related examples

Supervised learning:

data set of inputs and corresponding outputs: $D = \left\{ \vec{x}_\mu , \vec{y}_\mu \right\}$

quenched variables

parametric model: $\vec{y} = f(\vec{x}, \boxed{\theta})$

thermal variables

loss : $L(\theta, D) = \sum_\mu \left(\vec{y}_\mu - f(\vec{x}_\mu, \theta) \right)^2$

(similar to energy)

distribution over parameters
during training (at low *T*):

$$p\left(\theta \middle| D\right) = \frac{1}{Z\left[D\right]} \exp\left(-L(\theta, D) / T \right)$$

Machine-learning related examples

Unsupervised learning of a generative model:

data set of items: $D = \left\{ \vec{x}_\mu \right\}$

likelihood (parametric model): $p(\vec{x} | \theta)$, prior: $p_{prior}(\theta)$

- **Training** $$p_{post}\left(\boxed{\theta} \;\middle|\; \boxed{D} \right) \propto p_{prior}(\theta) \times \prod_\mu p(\vec{x}_\mu | \theta)$$

thermal variables quenched variables

- **Sampling** $$p\left(\boxed{\vec{x}} \;\middle|\; \boxed{\theta^{MAP}(D)} \right)$$

The replica method

- Suppose we want to compute the expectation value of some observable *O* over thermal variables:

$$\langle O \rangle (J) = \sum_S O(S)\; p(S|J) = \sum_S O(S)\; \frac{e^{-E[S,J]}}{Z[J]}$$

NB : Similar formulas for higher moments

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$$\overline{\langle O \rangle} = \sum_S O(S) \overline{\left(\frac{e^{-E[S,J]}}{Z[J]} \right)}$$

Not easy, interactions are present both at numerator and denominator

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- Replica method: $\frac{1}{Z[J]} = \lim_{n \to 0} Z[J]^{n-1} = \lim_{n \to 0} \sum_{S_2} \sum_{S_3} \dots \sum_{S_n} e^{-\sum_{a=2}^{n} E[S_a, J]}$

Thus $\overline{\langle O \rangle} = \lim_{n \to 0} \sum_S \sum_{S_2} \sum_{S_3} \dots \sum_{S_n} O(S)\, \overline{e^{-\left[E[S,J] + \sum_{a=2}^{n} E[S_a, J] \right]}}$

1 + (n-1) = n ➔ 0 replicas of the system, i.e. with same quenched variables!

The replica method: effective landscape

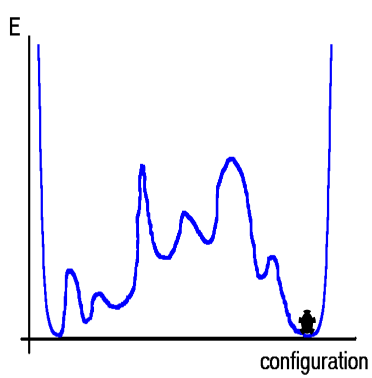
Observable we want to compute

$$\overline{\langle O \rangle} = \lim_{n\to 0} \sum_{S} \sum_{S_2} \sum_{S_3} \ldots \sum_{S_n} O(S) \;\; \overline{e^{-\beta\left[E[S,J]+\sum_{a=2}^{n} E[S_a,J]\right]}}$$

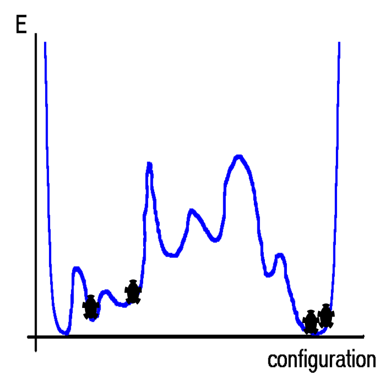
Sum over n ➔ 0 thermal configurations of the same system

Effective energy obtained after averaging over quenched variables

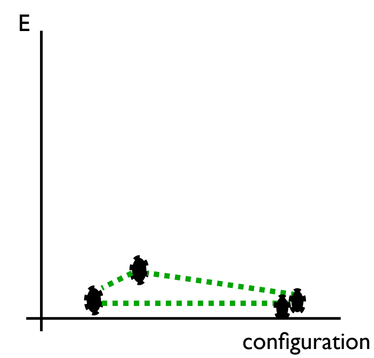
$$= e^{-E_{eff}[S,S_2,S_3,\ldots,S_n]}$$



1 configuration in quenched landscape



n independent configurations in same quenched landscape

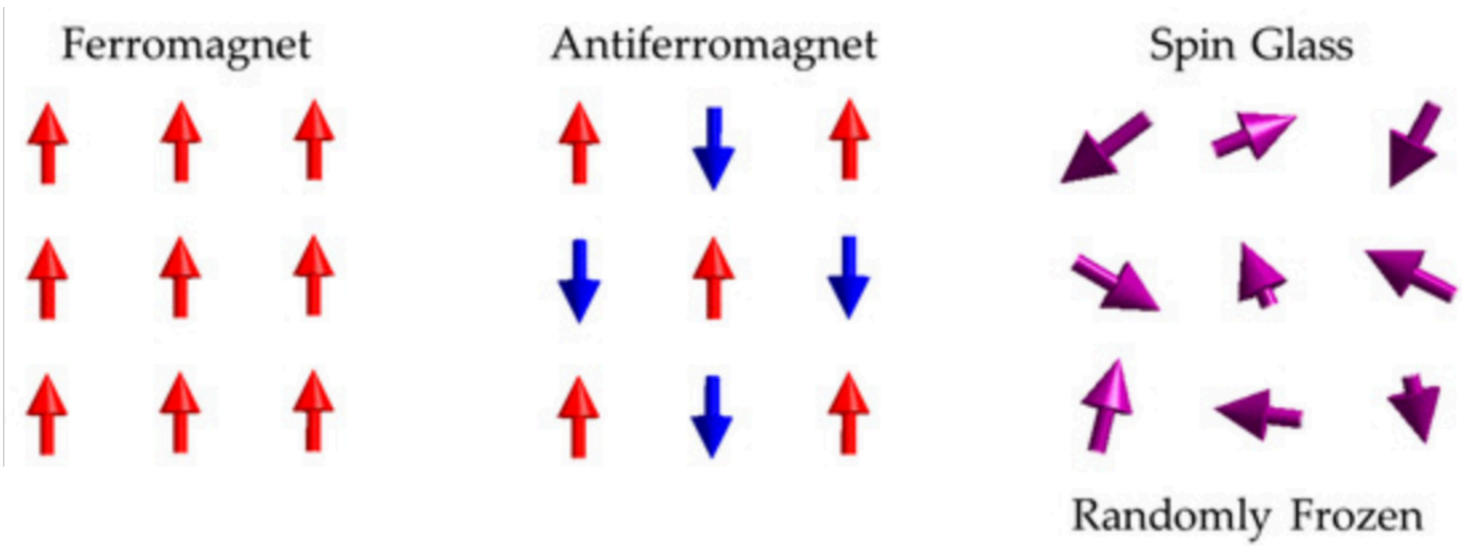


n interacting configurations

How similar are these configurations?

Notice this question makes senses also when n≠0 …

The replica method: order parameter



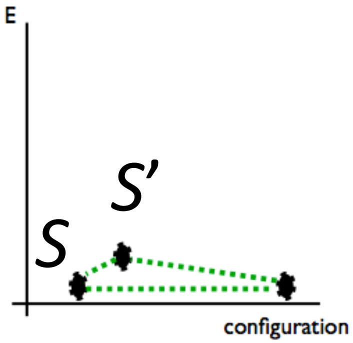
$$m = \frac{1}{N}\sum_{x,y} s_{x,y}$$

$$m^* = \frac{1}{N}\sum_{i} (-1)^{x+y} s_{x,y}$$

$$m = \frac{1}{N}\sum_{x,y} s_{x,y}\ t_{x,y}$$

Reference state *t* is unknown,
and there are plenty of them …

The replica method: order parameter



n interacting configurations

Measure of similarity between two configurations = overlap

$$q(S,S') = \frac{1}{N}\sum_i s_i s'_i$$

Thermal expectation

$$\langle q\rangle(J) = \sum_{S,S'} q(S,S')\ p(S|J)\ p(S'|J) = \sum_{S,S'} q(S,S')\ \frac{e^{-E[S,J]}}{Z[J]}\frac{e^{-E[S',J]}}{Z[J]}$$

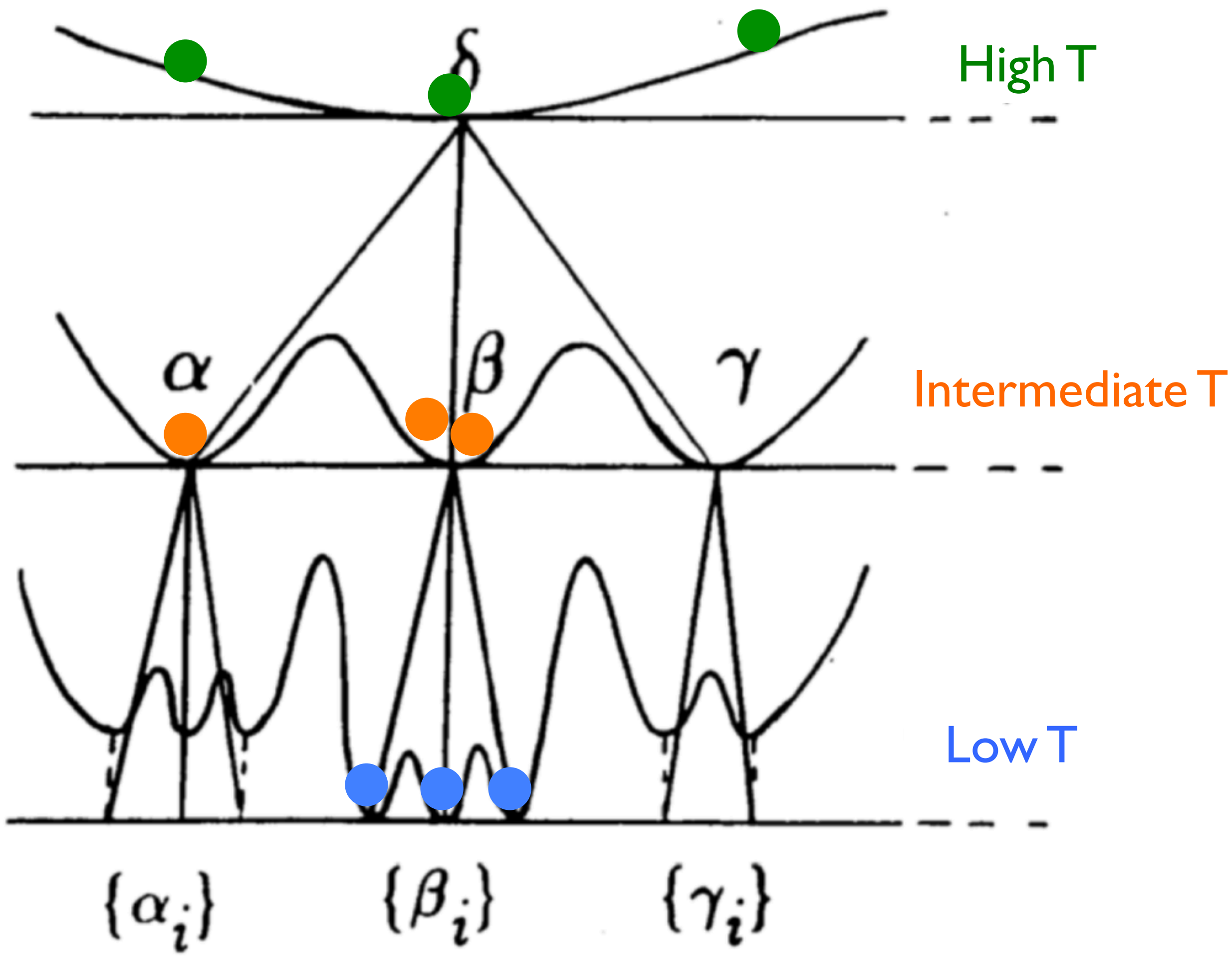
We introduce n-2 replicas

$$\frac{1}{Z[J]^2} = \lim_{n\to 0}\sum_{S_3}\sum_{S_4}\ldots\sum_{S_n} e^{-\sum_{a=3}^{n} E[S_a,J]}$$

to obtain the mean overlap (similar formulas for higher moments)

$$\overline{\langle q\rangle} = \lim_{n\to 0}\sum_{S_1}\sum_{S_2}\sum_{S_3}\ldots\sum_{S_n} q(S_1,S_2)\ e^{-E_{eff}[S_1,S_2,\ldots,S_n]}$$

The replica method: distribution of similarities



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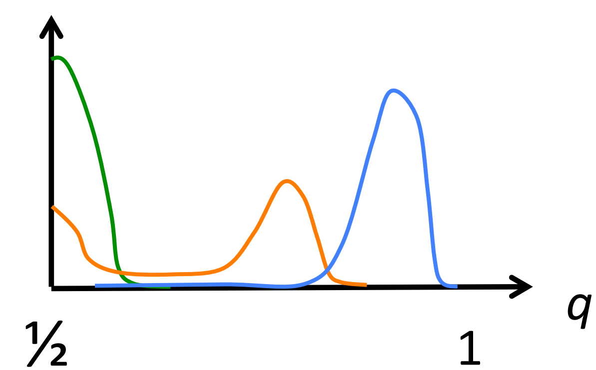
Distribution of overlaps:



This is the order parameter!

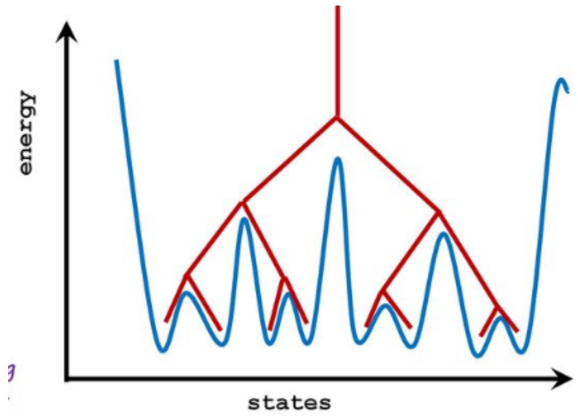
Brief historical overview

~ 1970 : first experimental studies on spin glasses

1974 : Sherrington – Kirkpatrick model

~ 1980 : **resolution of model by Parisi with the replica method**
(spectrum of linear chains of random masses & springs, F. Dyson, M. Kac)

1980-1990 : physical interpretation of Parisi's solution
(exponential number of phases,
ultrametric structure,...)



2000 : mathematical proofs of the exactness
of the solution

In parallel, applications to

1982: neuroscience (memory models)
1985: combinatorial optimization problems
1987: supervised learning (classification)
1990s: unsupervised learning