From mean field to three-dimensional spin glasses
(A journey through the numerics)

Florent Krząkała

Find these slides on my webpage:
www.pct.espci.fr/~florent/

Thanks to
O.C. Martin,
T. Jörg,
J.P. Bouchaud,
H. Katzgraber,
and others...
Why studying spin glasses?
Why studying spin glasses?

Very simple model (at least to define):
A starting point to understand glasses, aging, out-of-equilibrium dynamics (and other fundamental questions of modern physics).
Why studying spin glasses?

Very simple model (at least to define):
A starting point to understand glasses, aging, out-of-equilibrium dynamics
(and other fundamental questions of modern physics).

Mean field spin glasses are useful outside physics:
Neural networks, optimization problems, random graphs theory,
error correcting codes...
Why studying spin glasses?

Very simple model (at least to define):
A starting point to understand glasses, aging, out-of-equilibrium dynamics
(and other fundamental questions of modern physics).

Mean field spin glasses are useful outside physics:
Neural networks, optimization problems, random graphs theory,
error correcting codes...

Spin glasses exists!
3d Randomly Diluted Magnets (AuFe, CuMn, etc...) 
Edwards-Anderson Hamiltonian on a 3d lattice
Why studying spin glasses?

Very simple model (at least to define):
A starting point to understand glasses, aging, out-of-equilibrium dynamics (and other fundamental questions of modern physics).

Mean field spin glasses are useful outside physics:
Neural networks, optimization problems, random graphs theory, error correcting codes...

Spin glasses exists!
3d Randomly Diluted Magnets (AuFe, CuMn, etc...) Edwards-Anderson Hamiltonian on a 3d lattice
Few rigorous results in finite dimension

- cf: Newman & Stein lectures
- Self-averaging: Variance of the Free energy grows as volume (Aizenman-Wehr 90’)
- No proof of phase transition in any finite dimension!
- Many controversies. The $10^6$ question: are finite-dimensional model “meanfieldish”? 
Few rigorous results in finite dimension

- cf: Newman & Stein lectures
- Self-averaging: Variance of the Free energy grows as volume (Aizenman-Wehr 90’)
- No proof of phase transition in any finite dimension!
- Many controversies. The 10^6$ question: are finite-dimensional model “meanfieldish”?

Perform Numerical Simulations
In order to get a feeling “what’s going on...”

Some “accepted” results from the numerics:
- Free-energy distribution is Gaussian with variance N in finite dimension
  J.-P. Bouchaud, FK, O.C. Martin PRE 02’
- Spin glass phase transition for d>=3 for Ising Spins (Heisenberg still subject of debate!)
  Young PRL 83’, Marinari Parisi & Luiz-Lorenzo 97, Palassini & Caracciolo PRL 99’, Houdayer EPJB 01’, Palassini & Young PRB’01, Jörg PRE 06’
Few rigorous results in finite dimension

- cf: Newman & Stein lectures
- Self-averaging: Variance of the Free energy grows as volume \( (\text{Aizenman-Wehr 90'}) \)
- No proof of phase transition in any finite dimension!
- Many controversies. The \( 10^6 \) question: are finite-dimensional model “meanfieldish”?

Perform Numerical Simulations
In order to get a feeling “what’s going on...”

Some “accepted” results from the numerics:
- Free-energy distribution is Gaussian with variance \( N \) in finite dimension
  \( \text{J.-P. Bouchaud, FK, O.C. Martin PRE 02’} \)
- Spin glass phase transition for \( d \geq 3 \) for Ising Spins (Heisenberg still subject of debate!)
  \( \text{Young PRL 83’, Marinari Parisi & Luiz-Lorenzo 97, Palassini & Caracciolo PRL 99’, Houdayer EPJB 01’, Palassini & Young PRB’01, Jörg PRE 06’} \)

Some which are not “accepted” yet:
- The phase diagram in presence of a field or a magnetic bias
- Presence or absence of Temperature chaos
- Nature of the spin glass phase
The questions (in this seminar)

- Is there a spin glass phase under an applied magnetic field?
- Is there temperature/disorder chaos?

A Physicist Strategy

Compute (and discuss) the prediction for (diluted) mean field systems
Discuss heuristic arguments

Compare with numerical simulations of small systems in finite dimension
The questions (in this seminar)

- Is there a spin glass phase under an applied magnetic field?
- Is there temperature/disorder chaos?

A Physicist Strategy

Compute (and discuss) the prediction for (diluted) mean field systems
Discuss heuristic arguments

Compare with numerical simulations of small systems in finite dimension

These analytical results are not yet rigorously proven and remain a challenge for mathematicians
The questions (in this seminar)

- Is there a spin glass phase under an applied magnetic field?
- Is there temperature/disorder chaos?

A Physicist Strategy

Compute (and discuss) the prediction for (diluted) mean field systems
Discuss heuristic arguments

Compare with numerical simulations of small systems in finite dimension

These analytical results are not yet rigorously proven and remain a challenge for mathematicians
Answering (at the heuristic level) the long-standing question: does 3d model are “mean-field like”? 
Ordering of the Ising Spin Glass under an applied magnetic field

T. Jörg, H. Katzgraber & FK 07, in preparation
Mean field Ising Spin glass under a field

SK: Almeida & Thouless ‘78:
A Spin glass phase exists under $T_c$ for low enough magnetic field.
The critical value of the field diverges at $T=0$.
Mean field Ising Spin glass under a field

SK: Almeida & Thouless ‘78:
A Spin glass phase exists under $T_c$
for low enough magnetic field
The critical value of the field diverges at $T=0$

Diluted model: Jörg, Katzgraber & FK 07:
A similar phase diagram with a finite $h_c(T=0)$
6-connectivity regular graph with Gaussian couplings
Finite dimensional Spin glass under a field

Finite dimension Mc Millian ‘84:

*Imrie-Ma argument*: the ground state is highly unstable under a field

Spin glass phase: existence of large low energy excitations

Consider the ground state and an excitation of size $\ell$ with excess energy $E = A\ell^\theta$.
With a field $h$, we have now $E = A\ell^\theta \pm Bh\ell^{d/2}$.
If $\theta < d/2$, the ground state is unstable for large size.
Finite dimensional Spin glass under a field

Finite dimension Mc Millian ‘84:

*Imrie-Ma argument*: the ground state is highly unstable under a field

Spin glass phase: existence of large low energy excitations

Consider the ground state and an excitation of size $\ell$ with excess energy $E = A\ell^\theta$

With a field $h$, we have now $E = A\ell^\theta \pm Bh\ell^{d/2}$

If $\theta < d/2$ the ground state is unstable for large size.
Finite dimensional Spin glass under a field

Finite dimension Mc Millian ‘84:

*Imrie-Ma argument:* the ground state is highly unstable under a field

Spin glass phase: existence of large low energy excitations

Consider the ground state and an excitation of size $\ell$ with excess energy $E = A\ell^\theta$

With a field $h$, we have now $E = A\ell^\theta \pm Bh\ell^{d/2}$

If $\theta < d/2$ the ground state is unstable for large size.

Is the Imrie-Ma argument convincing? *(even for a physicist...)*

- It applies equally well to the spin glass on a Bethe Lattice where there is an AT line!
- The same argument is used with temperature variation to suggest **Temperature Chaos** but **not the absence of a spin glass phase** in temperature!
A modified Imrie-Ma argument

- Consider a large sample with a magnetization by spin $M$ under a field $H$
- Question: are there large excitations with low energies?
- Flipping a cluster of size $\ell$:
  - Costs an energy $E_{\text{field}} \propto MH\ell^d$
  - That we try to compensate by a gain from the boundaries: $E_{J_{ij}} \propto \ell^{d_s}$
- For large “droplet”, the field energy dominates and is large!
A modified Imrie-Ma argument

- Consider a large sample with a magnetization by spin \( M \) under a field \( H \).

- Question: are there large excitations with low energies?

- Flipping a cluster of size \( \ell \):
  - Costs an energy \( E_{\text{field}} \propto MH\ell^d \)
  - That we try to compensate by a gain from the boundaries: \( E_{J_{ij}} \propto \ell^{d_s} \)

- For large “droplet”, the field energy dominates and is large!

\[
E_{\text{field}} \propto MH\ell^d
\]

It is very hard to have low energy large-scale excitation under a field.
The controversy

versus

Magnetic field

P

SG

Tc

Temperature

0  0.5  1  1.5
The controversy

Monte-Carlo simulations
Monte-Carlo simulations

- Generating a representative set of configurations (with the proper weight) for small systems
- Using Metropolis dynamics and parallel tempering (mixing different replicas at different temperatures)
- Question 1: Are we able to see the AT line for random graphs?
- Question 2: What do we observe on 3d lattices?
Spin glass transition on random graph
Spin glass transition on random graph

P

SG

Tc

0  0.5  1  1.5
Spin glass transition on random graph

Compute the spin glass susceptibility

\[ \frac{\chi_{SG}}{N} = \langle q^2 \rangle - \langle q \rangle^2 \]

From replica theory, we expect that at the transition

\[ \chi_{SG} \propto N^{1/3} \]
Spin glass transition on random graph

Compute the spin glass susceptibility

\[ \frac{\chi_{SG}}{N} = \langle q^2 \rangle - \langle q \rangle^2 \]

From replica theory, we expect that at the transition

\[ \chi_{SG} \propto N^{1/3} \]
Spin glass transition on random graph

Compute the spin glass susceptibility

\[
\frac{\chi_{SG}}{N} = \langle q^2 \rangle - \langle q \rangle^2
\]

From replica theory, we expect that at the transition

\[
\chi_{SG} \propto N^{1/3}
\]

“Accord parfait” between simulation and theory
The AT line on random graph
The AT line on random graph
Compute the spin glass susceptibility

\[ \frac{\chi_{SG}}{N} = \langle q^2 \rangle - \langle q \rangle^2 \]

From replica theory, we expect that at the transition

\[ \chi_{SG} \propto N^{1/3} \]
Compute the spin glass susceptibility

$$\frac{\chi_{SG}}{N} = \langle q^2 \rangle - \langle q \rangle^2$$

From replica theory, we expect that at the transition

$$\chi_{SG} \propto N^{1/3}$$
The AT line on random graph

Compute the spin glass susceptibility

$$\frac{\chi_{SG}}{N} = \langle q^2 \rangle - \langle q \rangle^2$$

From replica theory, we expect that at the transition

$$\chi_{SG} \propto N^{1/3}$$

"Accord parfait" between simulation and theory again! Simulations are able to see the AT line when it is there!
Spin glass transition in 3d

Magnetic field

? P

SG

Tc

Temperature
Spin glass transition in 3d

Magnetic field

\[ P \]

Temperatur
Compute the spin glass correlation length

\[ < S S_r >^2_c \propto e^{-r/\xi} \]

From usual theory of phase transition, we expect that at the transition

\[ \xi(L, T = T_c) \propto L \]
Spin glass transition in 3d

Magnetic field

Compute the spin glass correlation length
\[ \langle SS' \rangle_c^2 \propto e^{-r/\xi} \]

From usual theory of phase transition, we expect that at the transition
\[ \xi(L, T = T_c) \propto L \]
Good (and convincing) evidence for the presence of a SG transition

\[ \langle S S_r \rangle_c^2 \propto e^{-r/\xi} \]

From usual theory of phase transition, we expect that at the transition

\[ \xi(L, T = T_c) \propto L \]
Spin glass in field in 3d spin glasses?

Magnetic field

$P$

$SG$

$T_c$

Temperature
Spin glass in field in 3d spin glasses?
Spin glass in field in 3d spin glasses?

Compute the spin glass correlation length

\[ \langle SS_r \rangle_c^2 \propto e^{-r/\xi} \]

From usual theory of phase transition, we expect that at the transition

\[ \xi(L, T = T_c) \propto L \]
Compute the spin glass correlation length

\[ \langle SS_r \rangle_c^2 \propto e^{-r/\xi} \]

From usual theory of phase transition, we expect that at the transition

\[ \xi(L, T = T_c) \propto L \]
Spin glass in field in 3d spin glasses?

Compute the spin glass correlation length

\[ \langle SS_r \rangle_c^2 \propto e^{-r/\xi} \]

From usual theory of phase transition, we expect that at the transition

\[ \xi(L, T = T_c) \propto L \]

Good (and convincing) evidence for the absence of a SG transition in field
Temperature and Disorder chaos

FK & O. Martin, EPJ B 01
FK & J.-P. Bouchaud, EPL 05
H. Kaztgraber & FK, PRL 07
Random energies strike back: The Re-Rem

Let us consider $2^N$ “states” with free energies $F_i = E_i - TS_i$

$$
\rho_E(E_i) = \frac{\exp \left( - \frac{E_i^2}{N} \right)}{\sqrt{N\pi}} \quad \rho_S(S_i) = \frac{\exp \left( - \frac{S_i^2}{N^2\alpha} \right)}{\sqrt{N^2\alpha\pi}}
$$
Random energies strike back: The Re-Rem

Let us consider $2^N$ “states” with free energies $F_i = E_i - T S_i$

$$\rho_E(E_i) = \frac{\exp\left( -\frac{E_i^2}{N} \right)}{\sqrt{N\pi}}$$

$$\rho_S(S_i) = \frac{\exp\left( -\frac{S_i^2}{N^2\alpha} \right)}{\sqrt{N^{2\alpha}\pi}}$$

Temperature chaos arises from level crossings!
Random energies strike back: The **Re-Rem**

Let us consider $2^N$ “states” with free energies $F_i = E_i - TS_i$

\[
\rho_E(E_i) = \frac{\exp\left(-\frac{E_i^2}{N}\right)}{\sqrt{N\pi}}
\]

\[
\rho_S(S_i) = \frac{\exp\left(-\frac{S_i^2}{N^{2\alpha}}\right)}{\sqrt{N^{2\alpha}\pi}}
\]

**REM like**

**Re-REM like**

Temperature chaos arises from level crossings!

**Free energies being random Gaussian, the model is solvable with a mapping to the REM:**

\[
\alpha < 0.5
\]

\[
T_c = \frac{1}{2\sqrt{\ln 2}}
\]

\[
\alpha = 0.5
\]

\[
T_c = \frac{1}{\sqrt{4\ln 2 - 1}} \approx 0.75
\]

\[
\alpha > 0.5
\]

\[
T_c \rightarrow \infty
\]

$F$ non-extensive
Level crossings in the Re-Rem
Level crossings in the Re-Rem

Free-energy of the lowest state is

\[ F_0 \approx -\sqrt{2N \log 2 \sigma_f} = -N \sqrt{\log 2 \left( 1 + T^2 N^{2\alpha - 1} \right) \log 2} \]
Level crossings in the Re-Rem

Free-energy of the lowest state is

\[ F_0 \approx -\sqrt{2N \log 2\sigma_f} = -N \sqrt{\log 2(1 + T^2 N^{2\alpha - 1})} \]

Number of lowest states crossings:

\[ \mathcal{N}_N(T, T + \delta T) = N^\alpha \delta T g\left(\frac{T}{N^{0.5 - \alpha}}\right) \]

High quality numerical determination of \( g(x) \) (up to \( 2^{800} \) levels simulated)
The Re-Rem

- States to state fluctuations induces extensive level crossing
- Temperature chaos, magnetic field chaos etc etc
- The Re-Rem is the simplest “mean-field” model with T-chaos
The Re-Rem

- States to state fluctuations induces extensive level crossing
- Temperature chaos, magnetic field chaos etc etc
- The Re-Rem is the simplest “mean-field” model with T-chaos

But what about finite dimensions?
The Imrie-Ma argument again

- Consider a small change in disorder

\[ J_{ij} \rightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}}, \]

Spin glass phase: existence of large low energy excitations

Consider the ground state and an excitation of size \( \ell \) with excess energy \( E = A \ell^\theta \)

Changing the couplings, we have now \( E = A \ell^\theta \pm B \Delta J \ell^{d_s/2} \)

If \( \theta < d_s/2 \) the ground state is unstable for large size.

McKay, Berker & Kirkpatrick, PRL 82'
Fischer-Huse PRB 86'
Bray-Moore PRL 87'
The Imrie-Ma argument again

- Consider a small change in disorder

\[ J_{ij} \rightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}} \]

Spin glass phase: existence of large low energy excitations

Consider the ground state and an excitation of size \( \ell \) with excess energy \( E = A\ell^{\theta} \)
Changing the couplings, we have now \[ E = A\ell^{\theta} \pm B\Delta J\ell^{d_s/2} \]
If \( \theta < d_s/2 \) the ground state is unstable for large size.

“Chaotic” length scale:
\[ \xi_{chaos} \propto \Delta J^{-\frac{1}{d_s/2-\theta}} \]

McKay, Berker & Kirkpatrick, PRL 82’
Fischer-Huse PRB 86’
Bray-Moore PRL 87’
Disorder chaos

Ground states computations:
Two copies with couplings $J$ and $J'$

$$J_{ij} \rightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}},$$

“Chaotic” length $\Delta J^{-1/\xi}$

suggests that the overlap is just a function of

$$g(L \Delta J^{1/\xi})$$
Disorder chaos

**Ground states computations:**

Two copies with couplings $J$ and $J'$

$$J_{ij} ightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}},$$

“Chaotic” length $\Delta J^{-1/\xi}$

suggests that the overlap is just a function of

$$g(L \Delta J^{1/\xi})$$
Disorder chaos

Ground states computations:
Two copies with couplings $J$ and $J'$

$$J_{ij} \rightarrow J'_{ij} = J_{ij} + x_{ij} \Delta J \sqrt{1 + \Delta J^2},$$

“Chaotic” length $\Delta J^{-1/\xi}$ suggests that the overlap is just a function of

$$g(L\Delta J^{1/\xi})$$

2d EA, with $\xi=1$

3d EA, with $\xi=1.3$
Disorder chaos

**Ground states computations:**
Two copies with couplings \( J \) and \( J' \)

\[
J_{ij} \to J'_{ij} = J_{ij} + x_{ij} \Delta J / \sqrt{1 + \Delta J^2},
\]

“Chaotic” length \( \Delta J^{-1/\xi} \)
suggests that the overlap is just a function of

\[
g(L\Delta J^{1/\xi})
\]

---

---

**Mean field**
The Imrie-Ma argument over and over again

- Consider a small change in temperature $T + dT$

Spin glass phase: existence of large low energy excitations
Consider two temperatures and the free energy of one “droplet”

$$F(T_1) = \gamma(T_1)\ell^\theta$$

According to the droplet picture, the energy is almost $T$-independent

$$F(T_2) \approx F(T_1) + T_1 S(T_1) - T_2 S(T_2).$$

where

$$S = \sigma(T)\ell^{d_s}/2$$

Therefore, it exists again a size beyond which large droplets have to be flipped
The Imrie-Ma argument over and over again

• Consider a small change in temperature $T + dT$

Spin glass phase: existence of large low energy excitations
Consider two temperatures and the free energy of one “droplet”

$$F(T_1) = \gamma(T_1) \ell^\theta$$

According to the droplet picture, the energy is almost $T$-independent

$$F(T_2) \approx F(T_1) + T_1 S(T_1) - T_2 S(T_2).$$

where

$$S = \sigma(T) \ell^{d_s/2}$$

Therefore, it exists again a size beyond which large droplets have to be flipped

$$\ell_c = \left( \frac{\gamma(T_1)}{T_2 \sigma(T_2) - T_1 \sigma(T_1)} \right)^{1/\zeta} \quad \text{with} \quad \zeta = \frac{d_s}{2} - \theta.$$ 

“Chaotic” length scale: $\ell_c(T_1, T_2) \propto \left( T_2^{3/2} - T_1^{3/2} \right)^{-1/\zeta}$. 


Monte Carlo simulations
Two copies with couplings $J$ and $J'$

$$J_{ij} \rightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}},$$

$$Q(L, T, \Delta T) = f_1(L/l_{chaos}^{\Delta T})$$

$$Q(L, T, \Delta J) = f_2(L/l_{chaos}^{\Delta J})$$
Monte Carlo simulations

Two copies with couplings $J$ and $J'$

$$J_{ij} \rightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}}$$

$$Q(L, T, \Delta T) = f_1 \left( \frac{L}{l_{chaos}}^{\Delta T} \right)$$

$$Q(L, T, \Delta J) = f_2 \left( \frac{L}{l_{chaos}}^{\Delta J} \right)$$
Temperature and disorder chaos in 3d

Monte Carlo simulations
Two copies with couplings $J$ and $J'$

$$J_{ij} ightarrow J'_{ij} = \frac{J_{ij} + x_{ij} \Delta J}{\sqrt{1 + \Delta J^2}}$$

$$Q(L, T, \Delta T) = f_1(L/l_{chaos}^{\Delta T})$$

$$Q(L, T, \Delta J) = f_2(L/l_{chaos}^{\Delta J})$$

The two functions might even be the same! (up to a rescaling factor)
Conclusions
Conclusions

- Numerical simulations show that 3d systems look quite different from mean field one...
Conclusions

• Numerical simulations show that 3d systems look quite different from mean field one...
• ...but that some features have still to be understood
Conclusions

- Numerical simulations show that 3d systems look quite different from mean field one...
- ... but that some features have still to be understood
- Presence of temperature chaos in simulation
Conclusions

- Numerical simulations show that 3d systems look quite different from mean field one...
- ... but that some features have still to be understood
- Presence of temperature chaos in simulation
- Can temperature and disorder chaos be better characterized (from a rigorous point of view)?
Conclusions

- Numerical simulations show that 3d systems look quite different from mean field one...
- ... but that some features have still to be understood
- Presence of temperature chaos in simulation
- Can temperature and disorder chaos be better characterized (from a rigorous point of view) ?
- The Re-REM: an Interesting extension of the REM
  - Temperature chaos
  - Level Crossings
Conclusions

- Numerical simulations show that 3d systems look quite different from mean field one...
- ... but that some features have still to be understood
- Presence of temperature chaos in simulation
- Can temperature and disorder chaos be better characterized (from a rigorous point of view) ?
- The Re-REM: an Interesting extension of the REM
  - Temperature chaos
  - Level Crossings
- What can be demonstrated for random graphs ?
Conclusions

• Numerical simulations show that 3d systems look quite different from mean field one...
• ... but that some features have still to be understood
• Presence of temperature chaos in simulation
• Can temperature and disorder chaos be better characterized (from a rigorous point of view)?
• The Re-REM: an Interesting extension of the REM
  • Temperature chaos
  • Level Crossings
• What can be demonstrated for random graphs?

Final remark: A simple case where the mean field picture applies
Book on spin glasses
Book on spin glasses
Book on spin glasses
Book on spin glasses

Many states....
Book on spin glasses

Many states....

...Non trivial overlap (in titles)....
Book on spin glasses

Many states....

...Non trivial overlap (in titles)....
Many states....

...Non trivial overlap (in titles)....
Book on spin glasses

Many states....

...Non trivial overlap (in titles)....
Book on spin glasses

Many states....

...Non trivial overlap (in titles)...

...and clustering properties!