# Glasses and replicas

Marc Mézard

Bangalore, January 2010

# Glass state

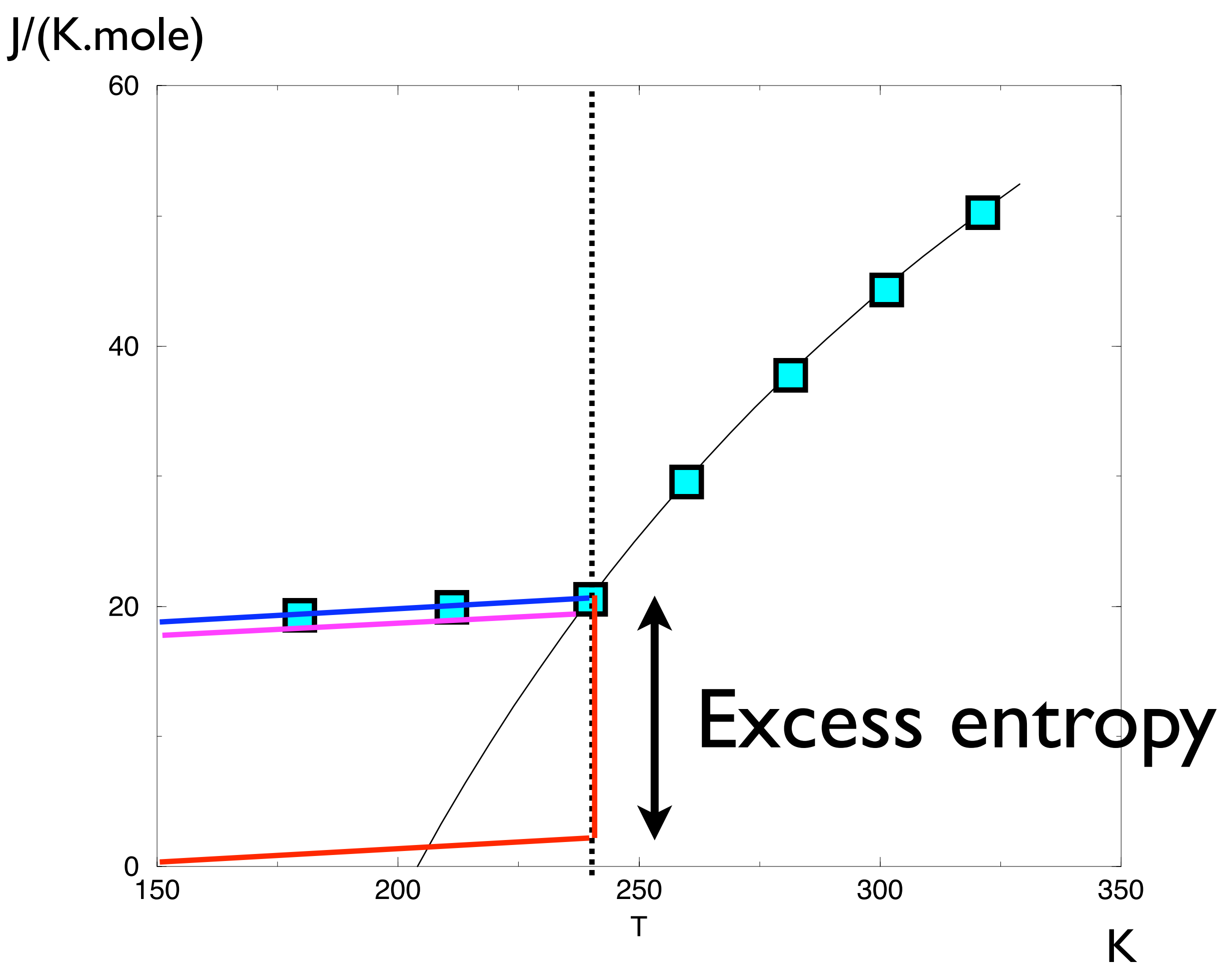
Ultimate goal: "First principles" microscopic approach: start from a microscopic Hamiltonian, understand what is the glass phase, compute its properties.

Fundamental statistical physics challenge: many, disordered states.

Other glasses: spin, electron, vortex, ..., neural networks, error correcting codes, constraint satisfaction problems, etc.

# Glasses: Relaxation time - viscosity

OTP: calorimetric entropy




Glass transition:

$$T_g = 246\ K$$

Full line: fit of liquid S:

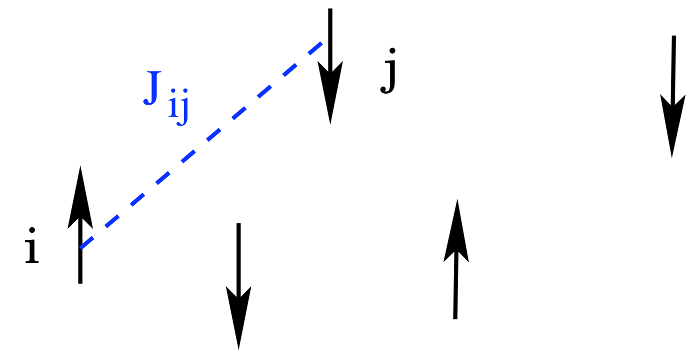
$$S = S_\infty(1 - T_K/T)$$

$$T_K = 204\ K$$

Cooling rate effects

Glass phase: specific heat $\simeq$ crystal

# Usual replica theory




Quenched disorder, e.g. spin glasses

$$E_J(s) = -\sum_{(ij)} J_{ij} s_i s_j$$

One sample = one set of couplings $J$

Boltzmann weight of the spin configuration $s$ :

$$P_J(s) = \frac{1}{Z_J} \exp\left[\beta \sum_{(ij)} J_{ij} s_i s_j\right]$$

# Usual replica theory

$$P_J(s) = \frac{1}{Z_J} \exp\left[\beta \sum_{(ij)} J_{ij} s_i s_j\right] \qquad \langle s_i \rangle_J = \sum_s P_J(s) s_i$$

Edwards-Anderson order parameter $q_{EA} = E_J \left(\langle s_i \rangle_J{}^2\right)$

Trick: $n$ non-interacting replicas:

$$q_{EA} = \lim_{n \to 0} E_J \sum_{s^1, \ldots, s^n} s_i{}^1 s_i{}^2 \exp\left[\beta \sum_{(ij)} J_{ij} \sum_{a=1}^{n} s_i{}^a s_j{}^a\right]$$

Technically: No J in the denominator. J average is often easy.

Alternatively: compute $E_J \log Z_J = \lim_{n \to 0} E_J \left(Z_J^n - 1\right)/n$

# Replicas and glasses: objections

- Structural glasses: no quenched disorder,

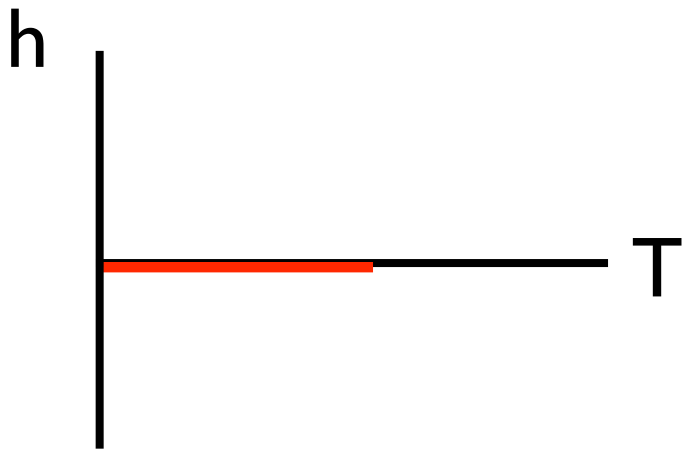
nothing like $E_J \ \log Z_J$

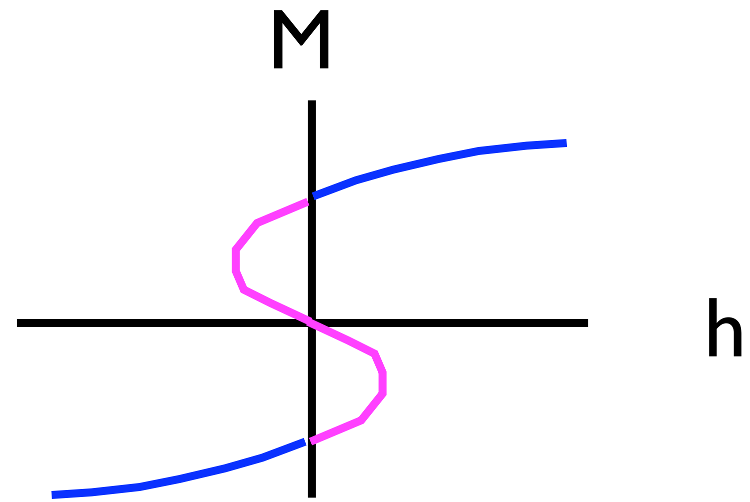
- Glass 'transition' is not an equilibrium process,

equilibrium statistical physics cannot be used

# Metastability

## Usual metastability: first order transition



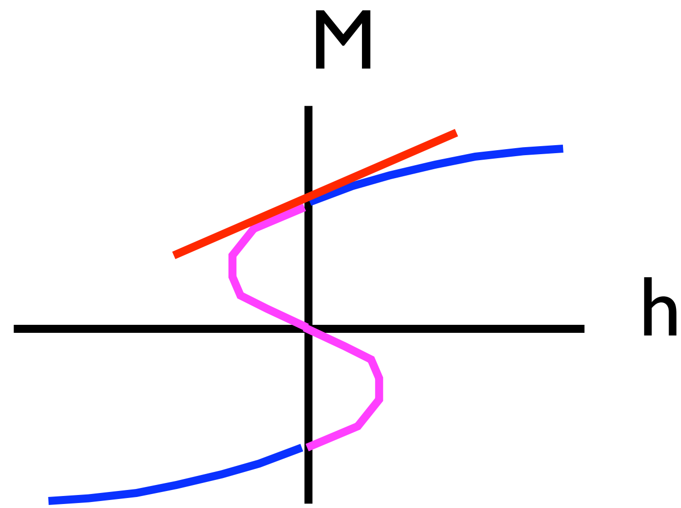

Equilibrium magnetization: $m(h) = m_s \ \mathrm{sign(h)} + \mathrm{O(h)}$

Lifetime metastable state: $\tau(h) \propto \exp(A/|h|^{\alpha})\,,\ \alpha = d - 1$

Physics of the metastable state on time scales $\ll \tau(h)$

= physics of constrained equilibrium

# Metastability




Equilibrium magnetization:

$$m(h) = m_s\ \mathrm{sign(h)} + \mathrm{O(h)}$$

Susceptibilities:

- Linear response $\chi_{LR} = \frac{1}{T} \lim_{h \to 0^+} \sum_i (\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle).$
- Equilibrium $\chi_{eq} = m_s \frac{d\ \mathrm{sign(h)}}{dh} + O(1) = \infty$

$$\chi_{eq}(h) = \chi_{LR}(h) + 2m_s\delta(h)$$

Linear response is observed when changing h, on time scales $\tau \ll \tau(h)$

# Glassiness and metastability: glasses

Hypothesis:

The main effect of the glass transition is the proliferation of states, i.e. groups of low energy configurations separated by large barriers, such that the relaxation time to jump over these barriers is larger than any experimental time, and many orders of magnitudes larger than microscopic times. Then a good starting point is to assume that these states have infinitely long lifetime (like when studying diamond)

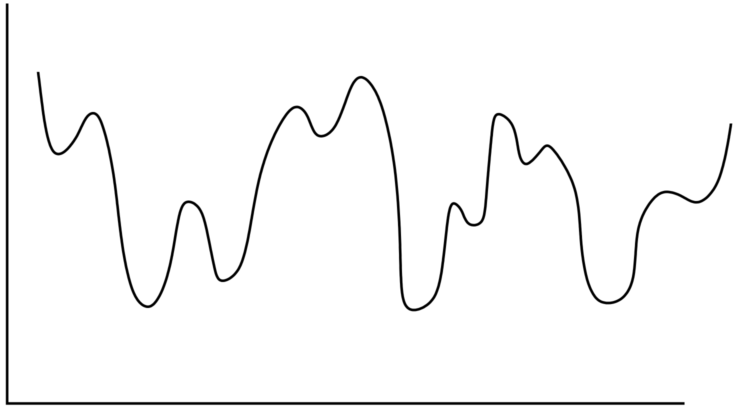
Problem: statistical physics with many states, unknown, disordered.... Replicas

# Replica Symmetry Breaking: Complicated Landscapes

$$q = \lim_{n\to 0} E_J \sum_{s^1,\ldots,s^n} {s_i}^1 {s_i}^2 \exp\left[\beta \sum_{(ij)} J_{ij} \sum_{a=1}^{n} {s_i}^a {s_j}^a\right]$$

Complicated landscape with many states. Hard for stat. phys.

Free energy




Many glasses, but many properties are self averaging

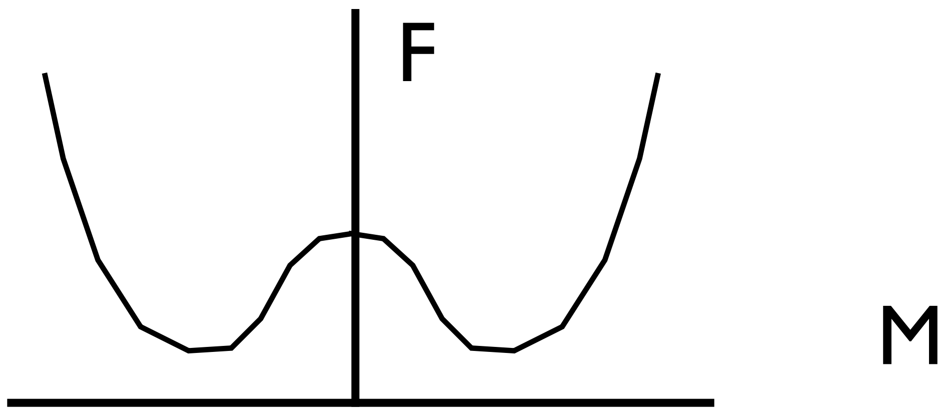
\`State' = disordered configuration. Impossible to know a conjugate field which polarizes into a state.

Each replica can condense into a different state:

$$q \to P(q)$$

# Replicas in systems without disorder

Go back to simple case of ferromagnet

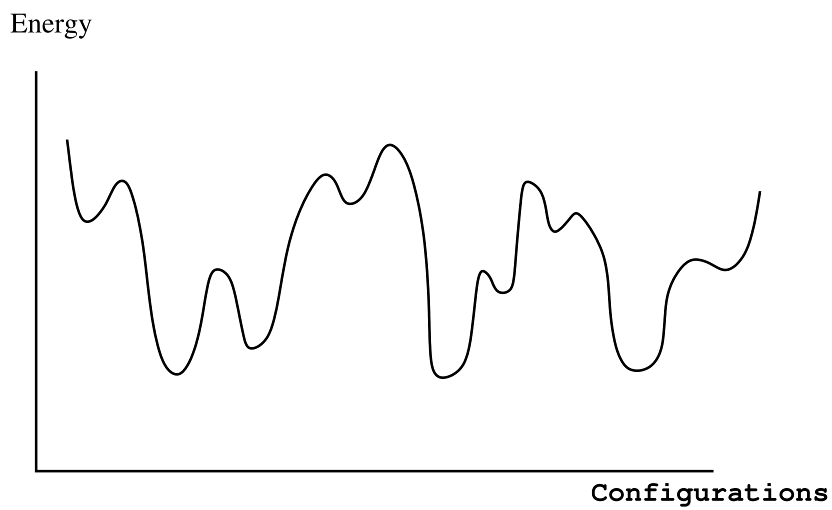


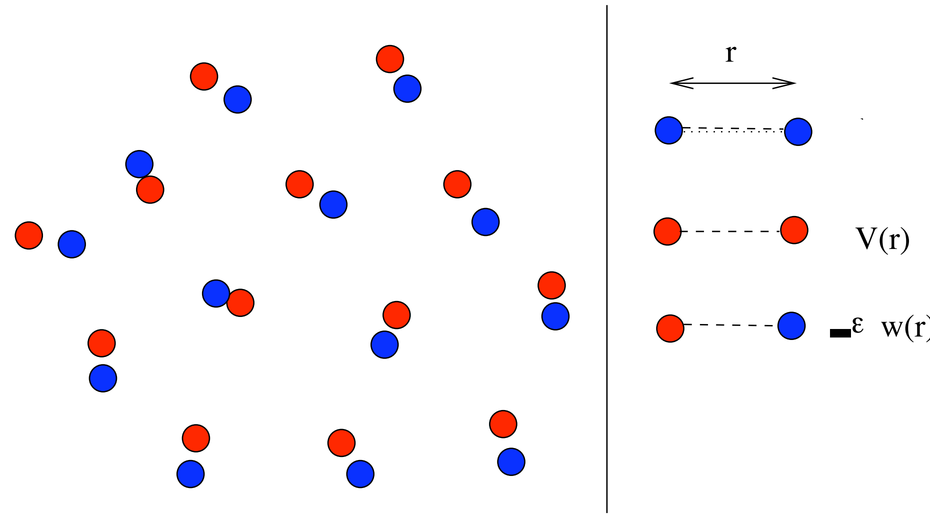

Ergodicity breaking associated with symmetry breaking. To study one of the two ferromagnetic states, add infinitesimal magnetic field:

$$M = \lim_{h \to 0} \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \langle s_i \rangle$$

# Replicas in systems without disorder

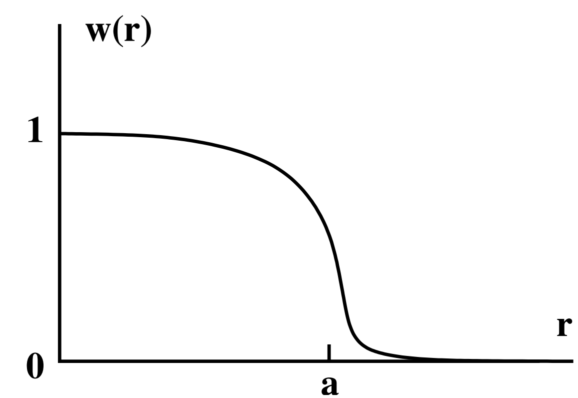
## Complicated landscape with many states. Hard for stat. phys.



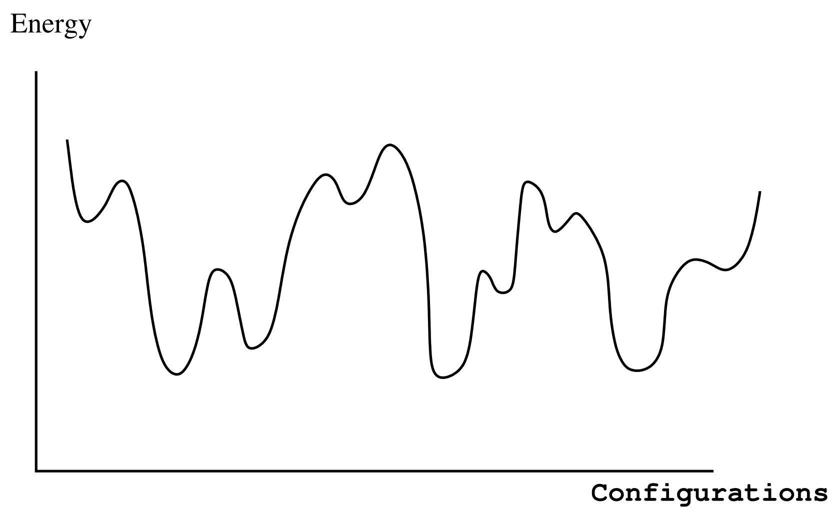

## How to choose one state? Replicas

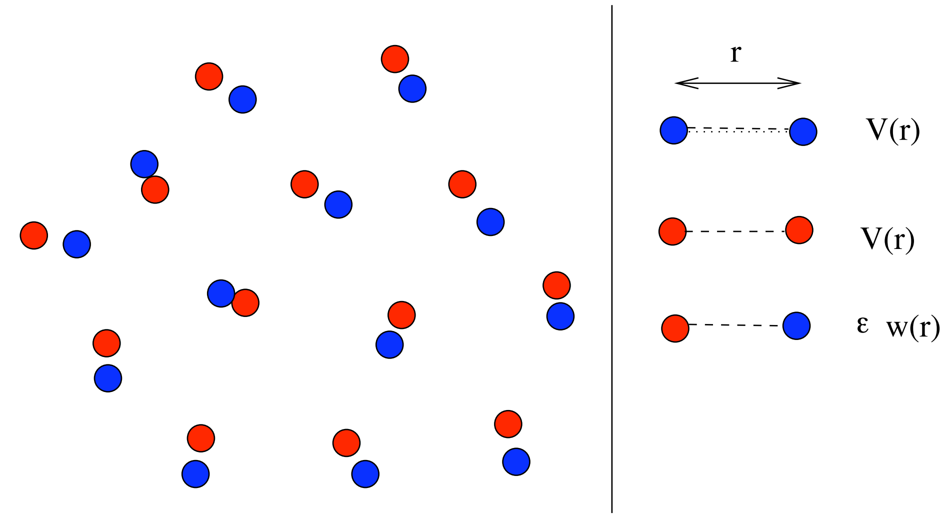
$V(r)$ : the microscopic description of your system



# Replicas in systems without disorder

Complicated landscape with many states. Hard for stat. phys.




$x$

$y$

$$H(x) + H(y) - \frac{\epsilon}{N} \sum_{i,k=1,N} w(x_i - y_k)$$

Glass = non-trivial correlations between x and y when

$$\lim_{\epsilon \to 0} \lim_{N \to \infty}$$

Replicas=conjugate field.

## To be done next:

- Statistical physics with many states: general approach and definition of the complexity function
- Solvable examples: spin glasses with p-spin interactions
- How to compute the complexity function with replicas
- Application to liquids: replica molecular liquid theory
- A class of glasses which are easier for the theorist: lattice glasses
- Beyond....

# Statistical physics with many states

States,  valleys, ....

Part of configuration space from which the system cannot escape in the time of the experiment.

Ideally: in the large $N$ limit the system cannot escape in any finite time.

Alternative: free-energy valley, with barriers that diverge when $N \to \infty$ .   $\tau = \tau_0 \, e^{\beta \Delta F}$

## Complexity and metastable states

Metastable states,  valleys, ....

Part of configuration space from which the system cannot escape in the time of the experiment.

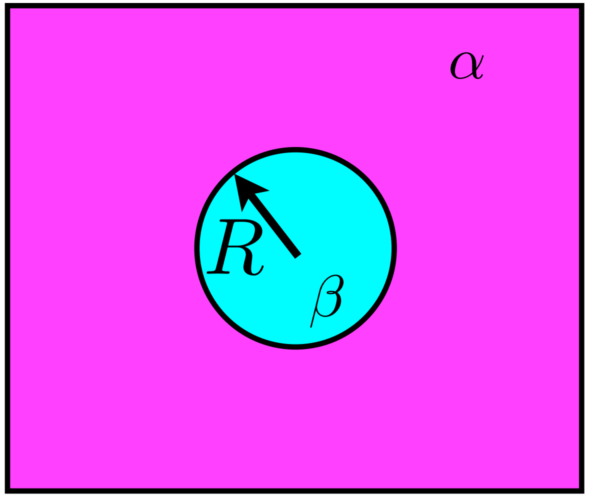
Constrained partition function (limited to the region of phase space of state $\alpha$ ): $Z_\alpha = e^{-\beta F_\alpha}$

NB: in mean field model, $F_\alpha/N$ can be larger than minimal one. Not in finite dimension:

# Complexity and metastable states

Constrained partition function (limited to the region of phase space of state $\alpha$ ): $Z_\alpha = e^{-\beta F_\alpha}$

Nucleation argument: if $F_\alpha/N > F_\beta/N$ and short range forces




$$F - F_\alpha = \frac{F_\beta - F_\alpha}{V} R^d + \sigma R^{d-1}$$

$< 0$ if $R$ is large enough

But lifetime can be very long, >> experiment time

NB: constrained partition function can always be defined (and is always used implicitly to get rid of the crystal)

# Complexity and metastable states

Constrained partition function (limited to the region of phase space of state $\alpha$ ): $Z_\alpha = e^{-\beta F_\alpha}$

$$f_\alpha = F_\alpha / N$$

Full partition function ($\beta = 1/T$ ):

$$Z \equiv \exp(-\beta N f_S) = \sum_\alpha \exp(-\beta N f_\alpha)$$

$$Z = \int df \exp(-\beta N f) \mathcal{N}(f, T, N)$$

Hypothesis:

$$\mathcal{N}(f, T, N) \approx \exp(N \Sigma(f, T))$$

Complexity function

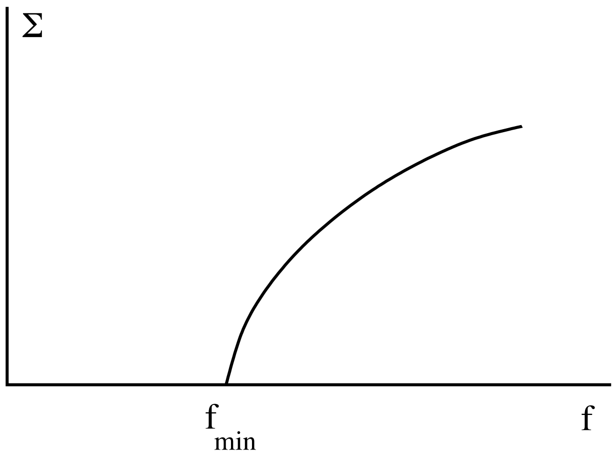
# Complexity and metastable states

## Full partition function

$$Z = \int df \, \exp(-\beta N f)\mathcal{N}(f,T,N) = \exp(-\beta N f_S)$$

$$\mathcal{N}(f,T,N) \approx \exp(N\Sigma(f,T))$$

Typically:




$$Z = \int_{f_m}^{f_M} df \, \exp(-N(\beta f - \Sigma(f,T)))$$

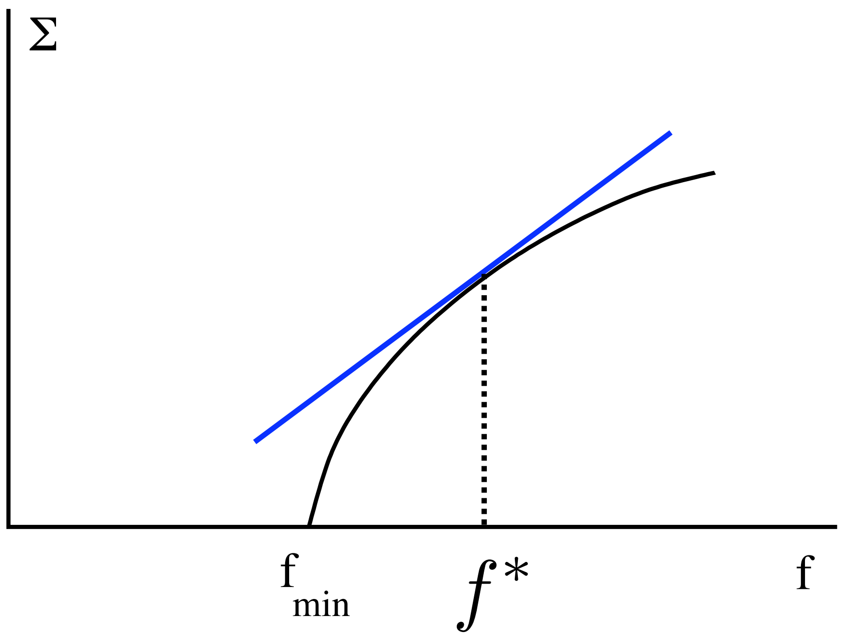
$$\beta f_S = \min_f \Phi(f) \equiv \beta f^* - \Sigma(f^*,T)$$

$$\Phi(f) \equiv \beta f - \Sigma(f,T)$$

# Complexity and metastable states

$$Z = \int_{f_m}^{f_M} df \exp(-N(\beta f - \Sigma(f,T))) = \exp(-\beta N f_S)$$

$$\beta f_S = \min_f \Phi(f) \equiv \beta f^* - \Sigma(f^*, T)$$




$$\frac{\partial \Sigma(f^*, T)}{\partial f} = \frac{1}{T}$$

$\Sigma(f^*, T)$ is finite ⟺

Exponentially many states contribute to $Z$

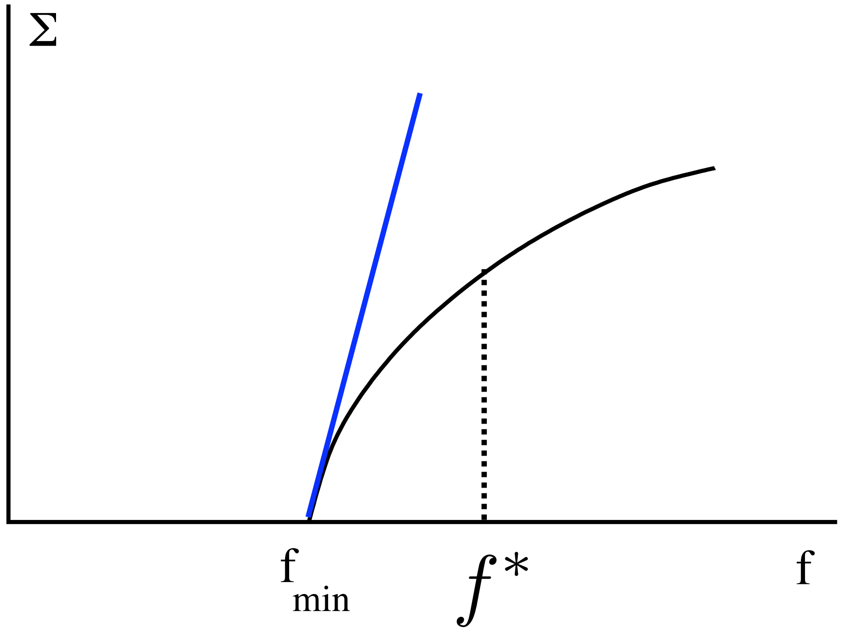
# Complexity and metastable states

$$Z = \int_{f_m}^{f_M} df \exp(-N(\beta f - \Sigma(f,T))) = \exp(-\beta N f_S)$$

$$\beta f_S = \min_f \Phi(f) \equiv \beta f^* - \Sigma(f^*,T)$$

$$\frac{\partial \Sigma(f^*,T)}{\partial f} = \frac{1}{T}$$

$$\Sigma(f^*,T) = 0$$




Condensation phenomenon: only a few states contribute to $Z$

"Replica symmetry breaking"

# Two transitions

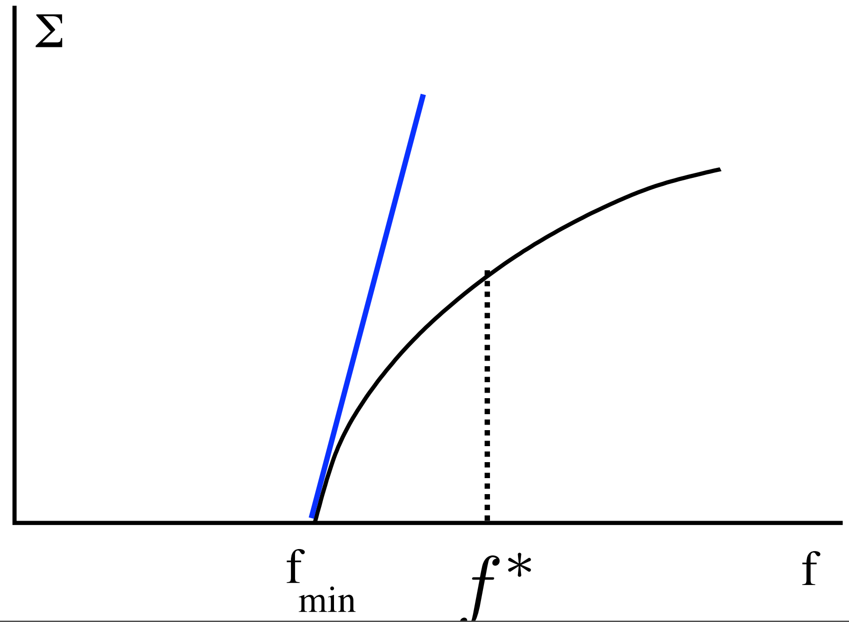
Found in broad range of spin glass mean field systems: "one step replica symmetry breaking", or "random first order theory". Two transitions when T decreases:

1) Appearance of a non trivial complexity function (appearance of long-lived valleys): $T_D$ ,"dynamical transition"

2) "Replica symmetry breaking"

$T < T_c$

Condensation phenomenon: only a few states contribute to $Z$



# One step RSB spin glasses

Random energy model (Derrida 1981)

$2^N$ energy levels, iid drawn from $e^{-E^2/N}$

$$Z = \sum_\alpha e^{-\beta E_\alpha}$$

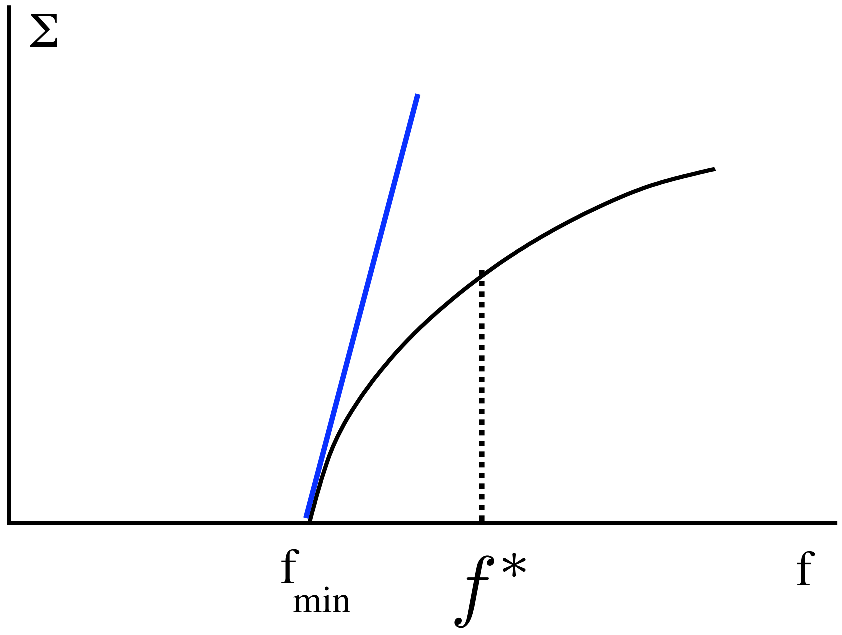
Valleys have independent energies, no internal entropy

$$\mathcal{N}(f, T, N) \approx \exp(N\Sigma(f, T))$$

$$\Sigma(f, T) = \log 2 - f^2$$

$$T_D = \infty$$

$$T_c = 1/(2\sqrt{\log 2})$$



# p-spin glasses

$$E_J(s) = -\sum_{(ij)} J_{ij} s_i s_j$$

$$\Rightarrow \quad E_J(s) = -\sum_{(i_1,\dots,i_p)} J_{i_1\dots i_p} s_{i_1} \dots s_{i_p}$$

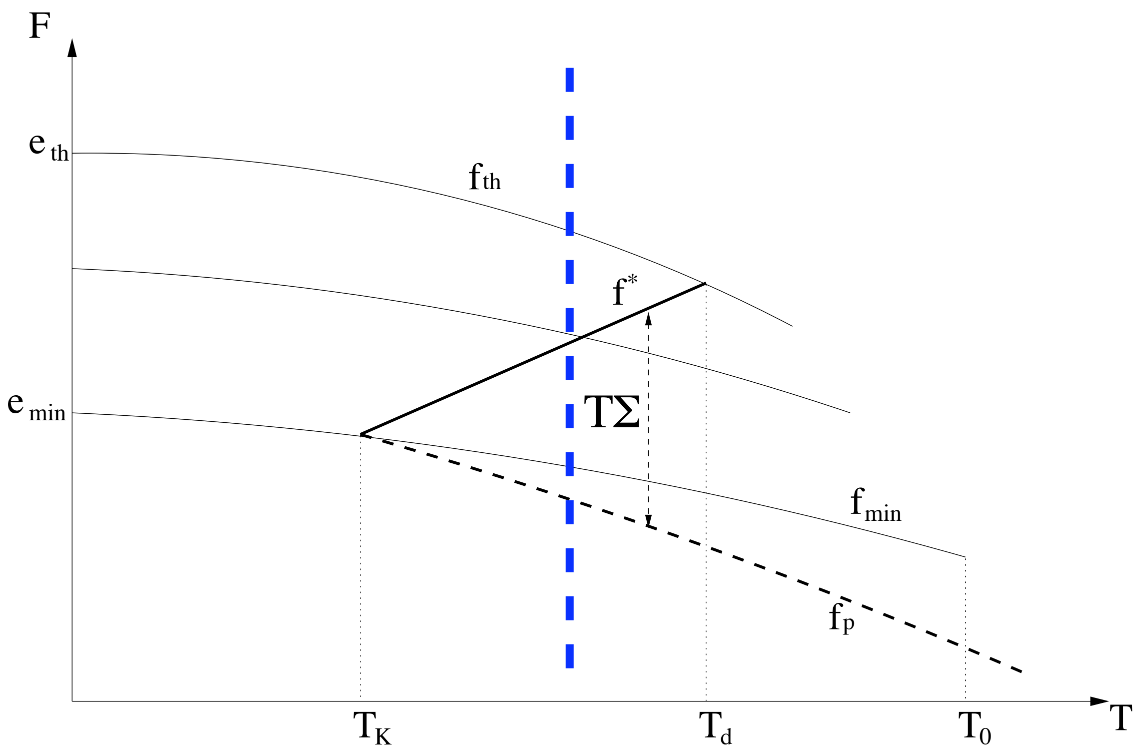
Exactly solvable for spherical spins $\sum_i s_i^2 = N$

Well understood for Ising spins, including diluted systems

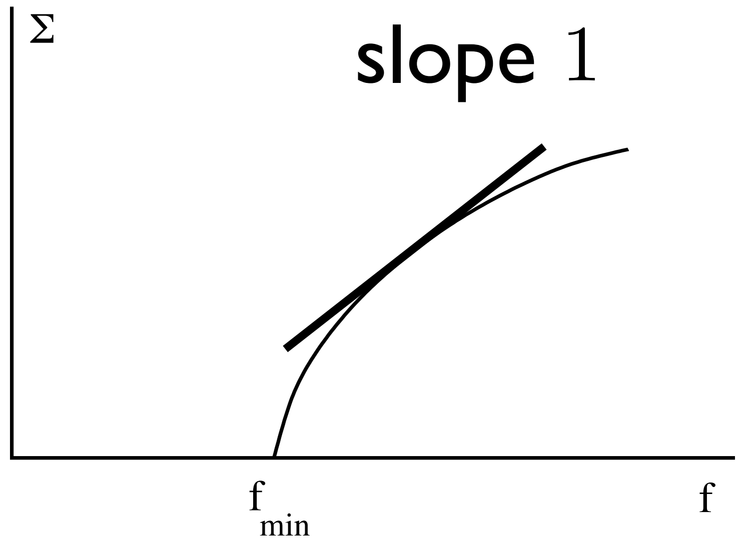
Same scenario as for the REM, just more complicated: entropy of a state is non-zero; $T_D$ and $T_c$ are finite and known

Kirkpatrick, Thirumalai, Wolynes: RFOT = good scenario of glass transition

# p-spin glasses: states




Cut along the blue line:




Many nice properties, computable...

# p-spin glasses: homework (for the theorists)

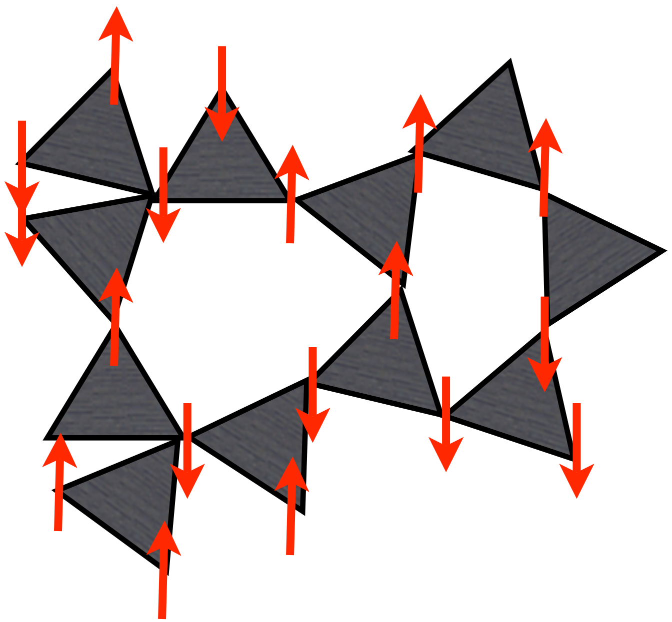
Crisanti Sommers Z. Phys. B87 (1992) 341 +...

Kurchan Parisi Virasoro J Physique 3 (1993) 1819

MM, Physica A265 (1999) 352

# Numerical experiment: diluted p-spin glass

## Ferromagnet with 3-spin interactions

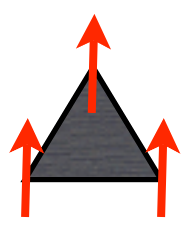
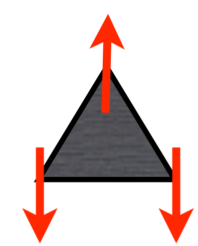


$\uparrow \quad s_i = 1$

$\downarrow \quad s_i = -1$

$$E = -\sum_{ijk} s_i s_j s_k$$

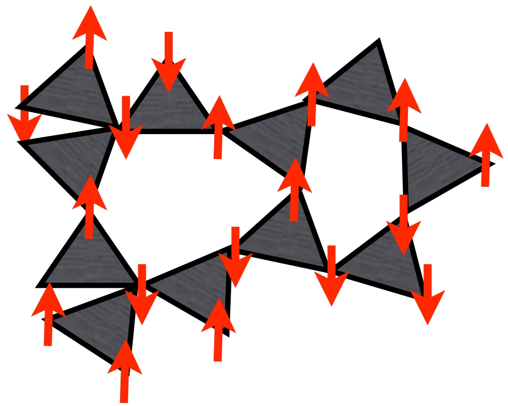
Randomly chosen triplets

Lowest E:  or  or...

Franz, M, Parisi, Ricci-Tersenghi, Weigt, Zecchina

# Trapped in a glass phase

$$E = -\sum_{ijk} s_i s_j s_k$$

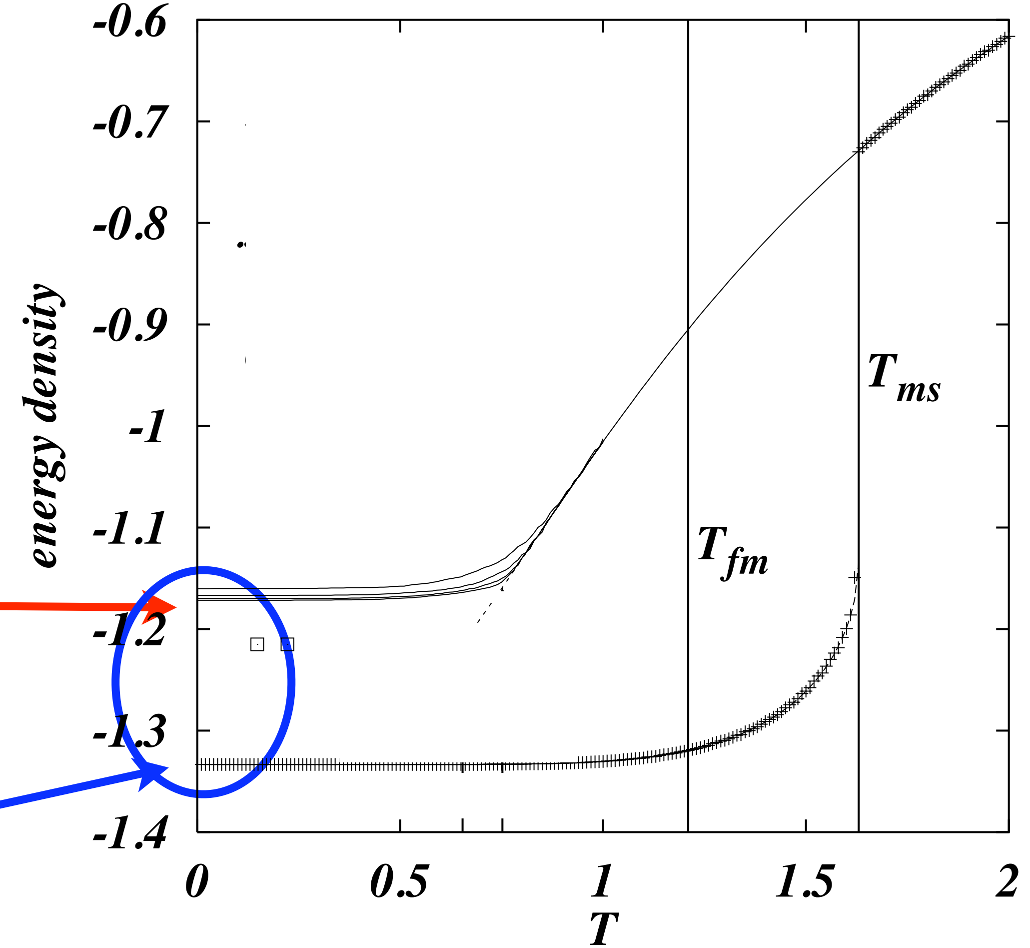


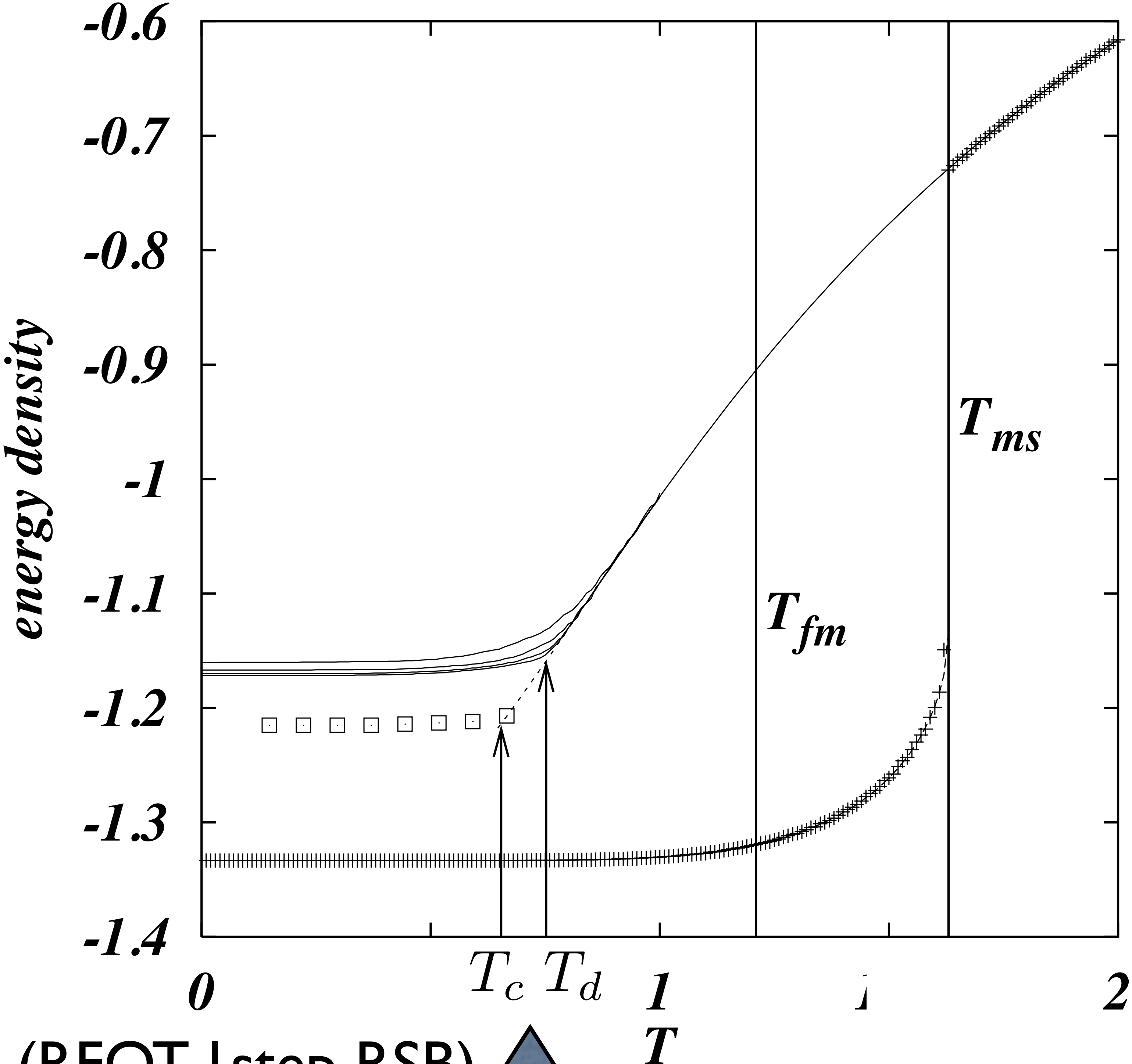
$$P(s_1, \ldots, s_N) = \frac{1}{Z} e^{-E/T}$$

$10^5$ spins, 4 triangles per spin

Metastable states found by simulated annealing $10^4$ to $10^7$ steps

Crystal state, all $s_i = 1$

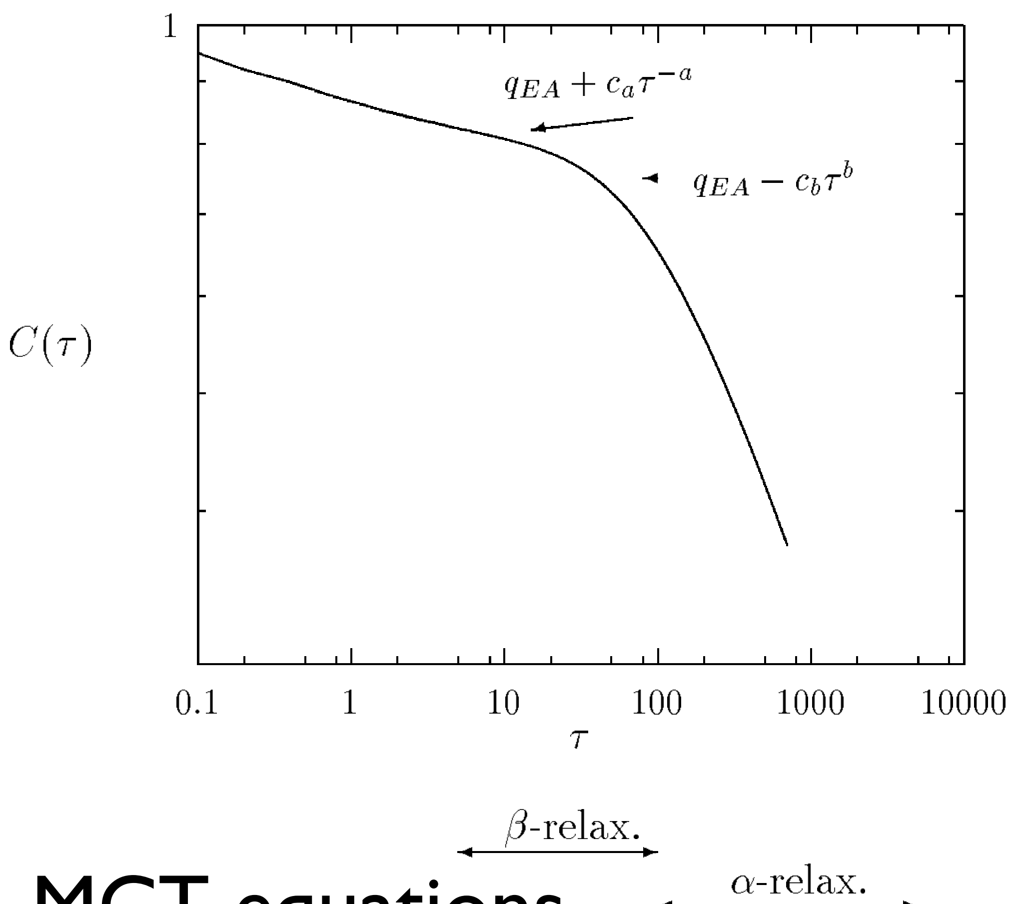





Theory (RFOT-1step RSB)

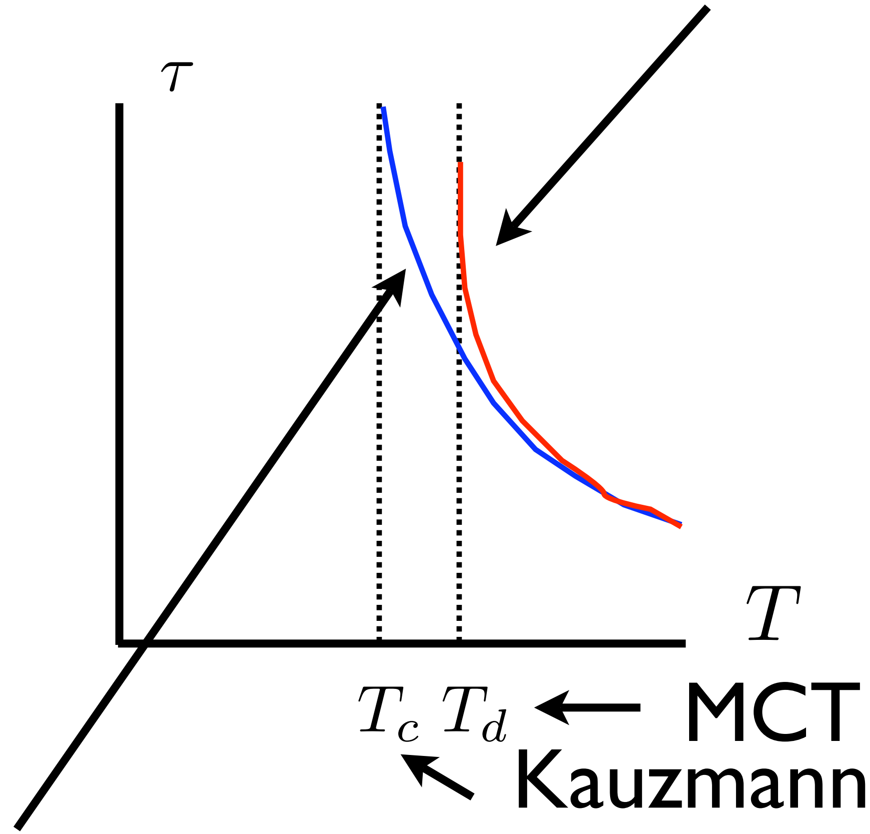
# Basic conjecture: the RFOT-1RSB transition seen in the p-spin glasses is a good mean field theory analogy for glasses

More evidence: dynamics $T > T_d$




MCT equations
+ Aging (see Kurchan)

Mean field theory




Finite dimension (nucleation) effects - conjectured. See Biroli, Franz

# Basic conjecture: the RFOT-1RSB transition seen in the p-spin glasses is a good mean field theory of glasses

Most important quantity: complexity

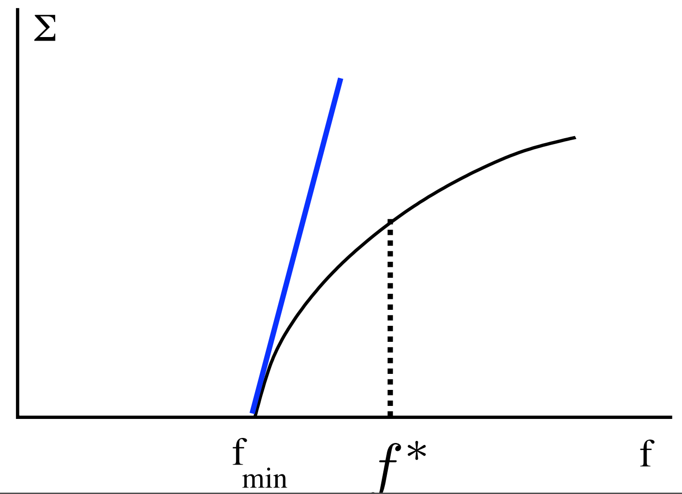
How to compute $\Sigma$ ?

$$\mathcal{N}(f,T,N) \approx \exp(N\Sigma(f,T))$$

1) Appearance of a non trivial complexity function (appearance of long-lived valleys): $T_D$ ,"dynamical transition"

2) "Replica symmetry breaking": condensation phenomenon at

$$T < T_c$$



# How to compute $\Sigma$ ?

$$Z(\beta, m) = \sum_{\alpha} e^{-\beta m N f_\alpha}$$

Partition function for $m$ replicas constrained to stay in the same state

$$Z = Z(\beta, 1)$$

$$Z = \int_{f_m}^{f_M} df \; e^{-N(\beta m f - \Sigma(f,T))} \simeq \; e^{-N(\beta m f^* - \Sigma(f^*,T))}$$

$$\frac{\partial \Sigma(f^*, T)}{\partial f} = \frac{m}{T}$$

$$\boxed{\text{New use of replicas, without quenched disorder}}$$

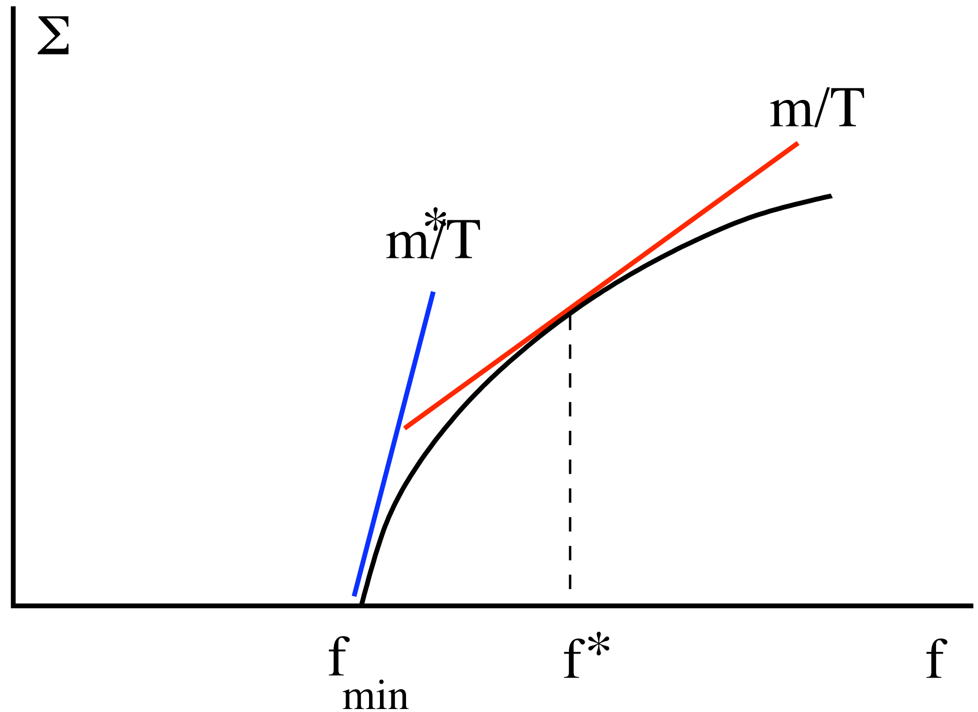
# How to compute $\Sigma$ ?

$$Z(\beta, m) \simeq \; e^{-N(\beta m f^* - \Sigma(f^*,T))}$$

$$\frac{\partial \Sigma(f^*, T)}{\partial f} = \frac{m}{T}$$

$$-\frac{1}{\beta m} \log Z(\beta, m) = \phi(\beta, m)$$

Legendre transform $\phi \longleftrightarrow \Sigma$




Fixed the temperature T. Vary the auxiliary "replica" parameter $m$. Critical value of $m$ when

Condensation at $m > m^*$

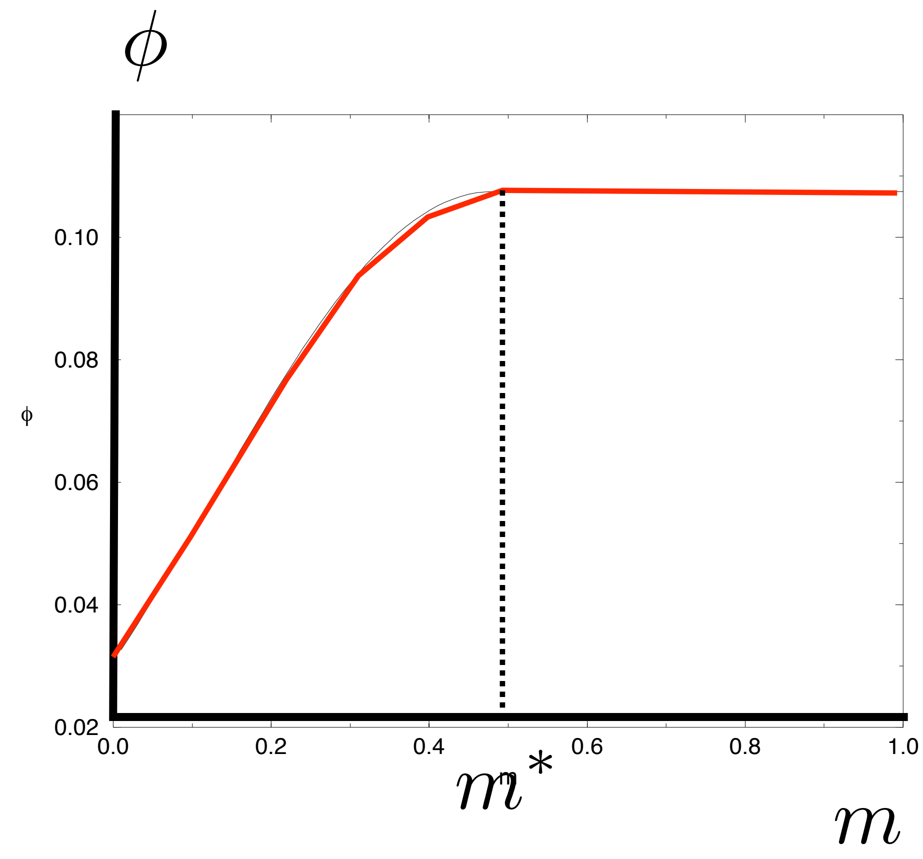
$$\frac{\partial \Sigma(f_{min}, T)}{\partial f} = \frac{m^*}{T}$$

# How to compute $\Sigma$ ?

$$Z(\beta, m) \simeq \; e^{-N(\beta m f^* - \Sigma(f^*, T))}$$

$$\frac{\partial \Sigma(f^*, T)}{\partial f} = \frac{m}{T}$$

$$-\frac{1}{\beta m} \log Z(\beta, m) = \phi(\beta, m)$$




Condensation at $m > m^*$

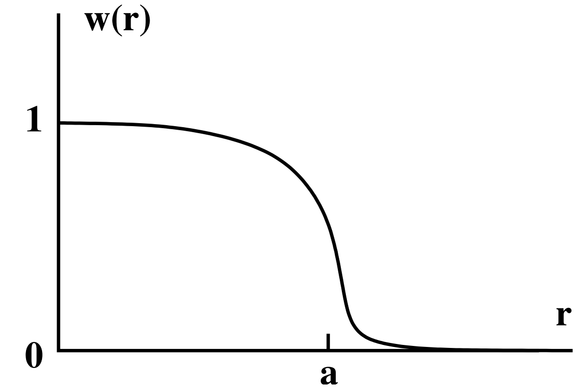
# Computing $\Sigma$ in liquids

$$H(x) = \sum_{i<j} V_{ij}(|x_i - x_j|)$$ e.g. $$V_{ij}(r) = A/r^{12} - B/r^6$$

or mixture

$$Z(\beta, m) = \sum_\alpha \exp(-\beta m N f_\alpha(\beta))$$

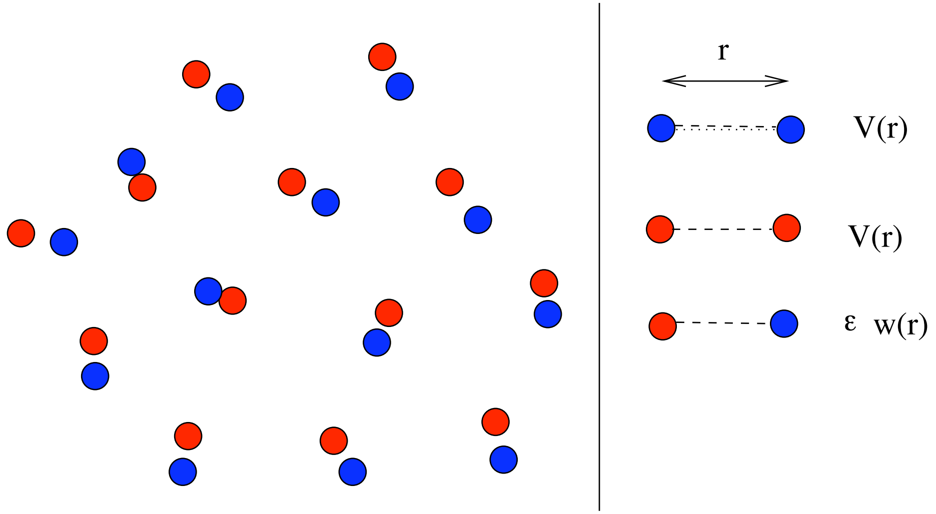
Partition function for $m$ replicas constrained to stay in the same state

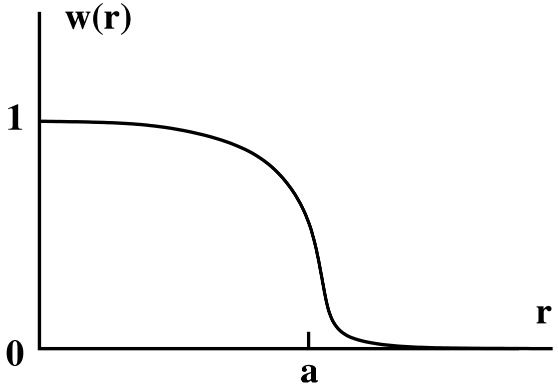



$$H_m = \sum_{1 \le i < j \le N} \sum_{a=1}^{m} V(x_i^a - x_j^a) - \epsilon \sum_{i=1}^{N} \sum_{1 \le a < b \le m} w(x_i^a - x_i^b)$$

# Molecular liquid

$$H_m = \sum_{1 \leq i < j \leq N} \sum_{a=1}^{m} V(x_i^a - x_j^a) - \epsilon \sum_{i=1}^{N} \sum_{1 \leq a < b \leq m} w(x_i^a - x_i^b)$$



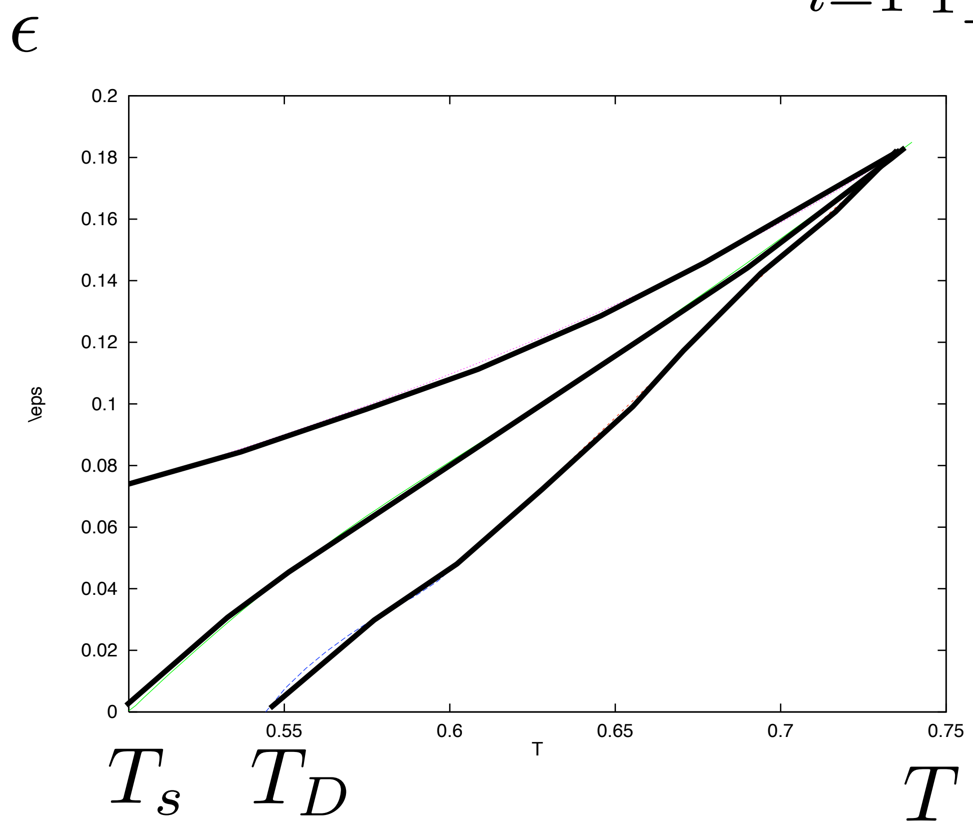



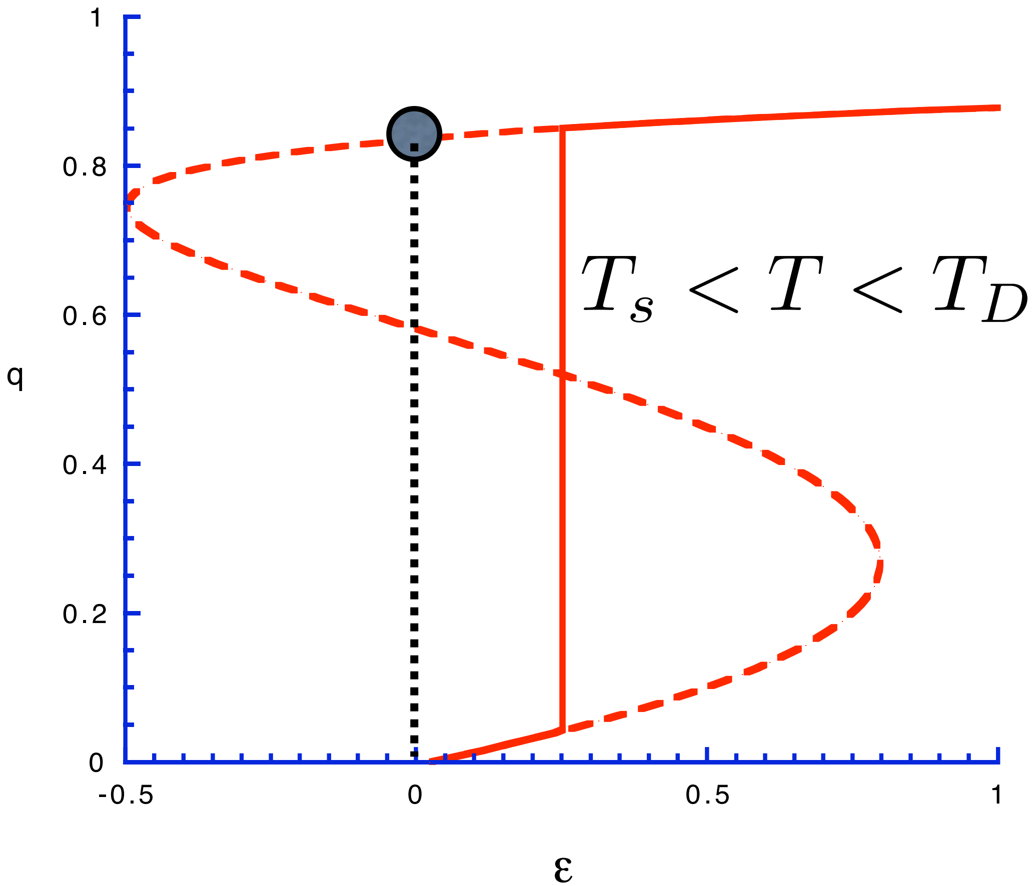

Large $\epsilon$ : molecular bound state. Take the $\epsilon \rightarrow 0$ limit:

If glass phase: molecular bound state survives.

# Molecular liquid

$$q = \frac{1}{Nm(m-1)/2} \sum_{i=1}^{N} \sum_{1 \leq a < b \leq m} \langle w(x_i^a - x_i^b) \rangle$$




NB: in finite dimensions: metastable branch. Defined only on time scales smaller than decay of the metastable state

# Molecular liquid: real study (brrrr...)

$$Z(\beta,m) = \frac{1}{N!}\int \prod_{i=1}^{N} dr_i \prod_{i=1}^{N}\prod_{a=1}^{m} du_i^a \prod_{i=1}^{N}\left(m^3\delta(\sum_a u_i^a)\right)$$
$$\exp\left(-\beta\sum_{i<j,a} v(r_i-r_j+u_i^a-u_j^a)-\beta\sum_i\sum_{a,b}W(u_i^a-u_i^b)\right)$$

Small cage expansion:

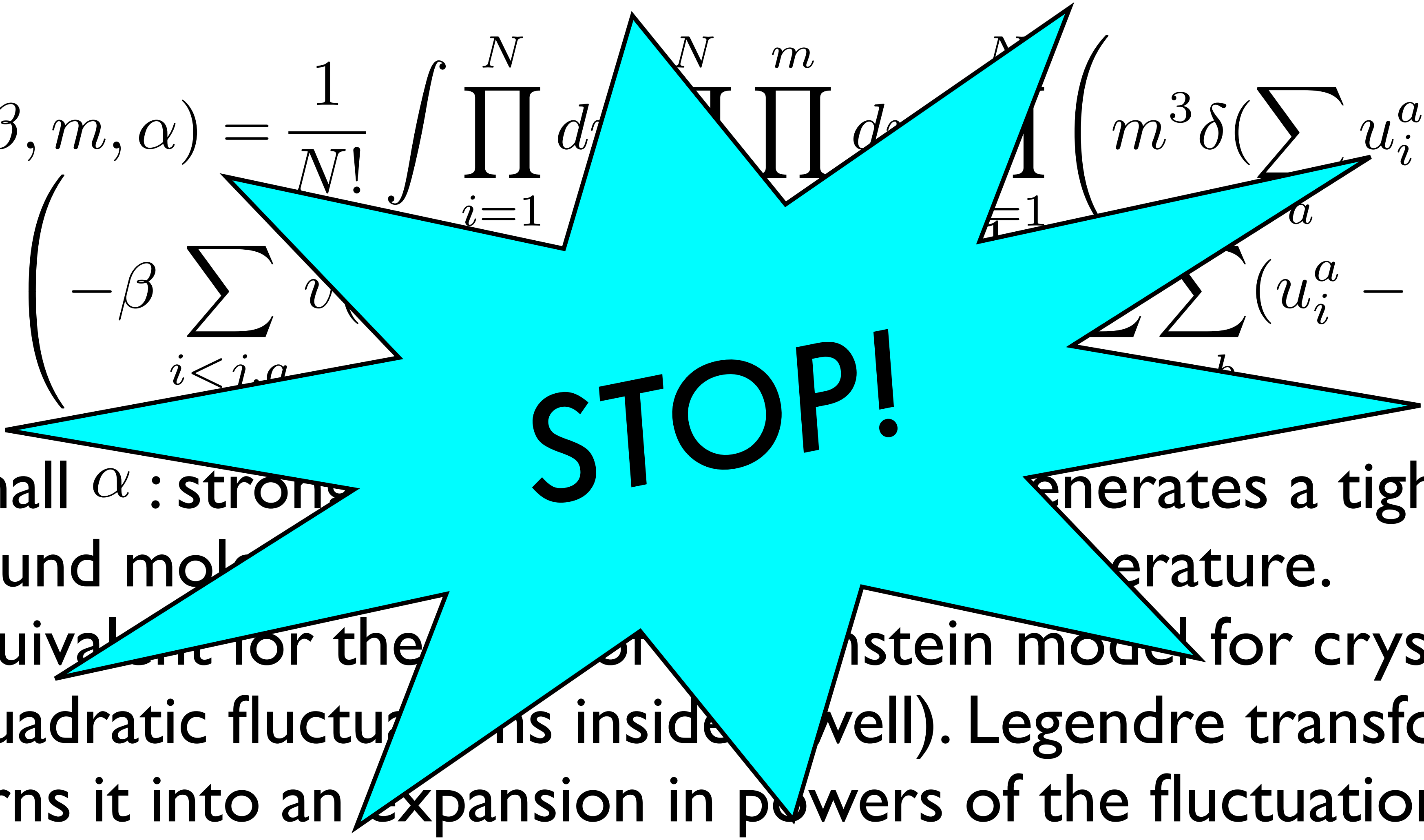
$$Z(\beta,m,\alpha) = \frac{1}{N!}\int \prod_{i=1}^{N} dr_i \prod_{i=1}^{N}\prod_{a=1}^{m} du_i^a \prod_{i=1}^{N}\left(m^3\delta(\sum_a u_i^a)\right)$$
$$\exp\left(-\beta\sum_{i<j,a} v(r_i-r_j+u_i^a-u_j^a)-\frac{1}{4\alpha}\sum_i\sum_{a,b}(u_i^a-u_i^b)^2\right)$$

# Molecular liquid: real study

Small cage expansion:

$$Z(\beta, m, \alpha) = \frac{1}{N!} \int \prod_{i=1}^{N} d \ldots \prod^{N} \prod^{m} d \ldots \prod_{\ldots=1} \left( m^3 \delta\left(\sum_a u_i^a\right) \right)$$

$$\exp\left( -\beta \sum_{i<j,a} v\left( \ldots \right. \ldots \sum \sum_{\ldots b} (u_i^a - u_i^b)^2 \right)$$

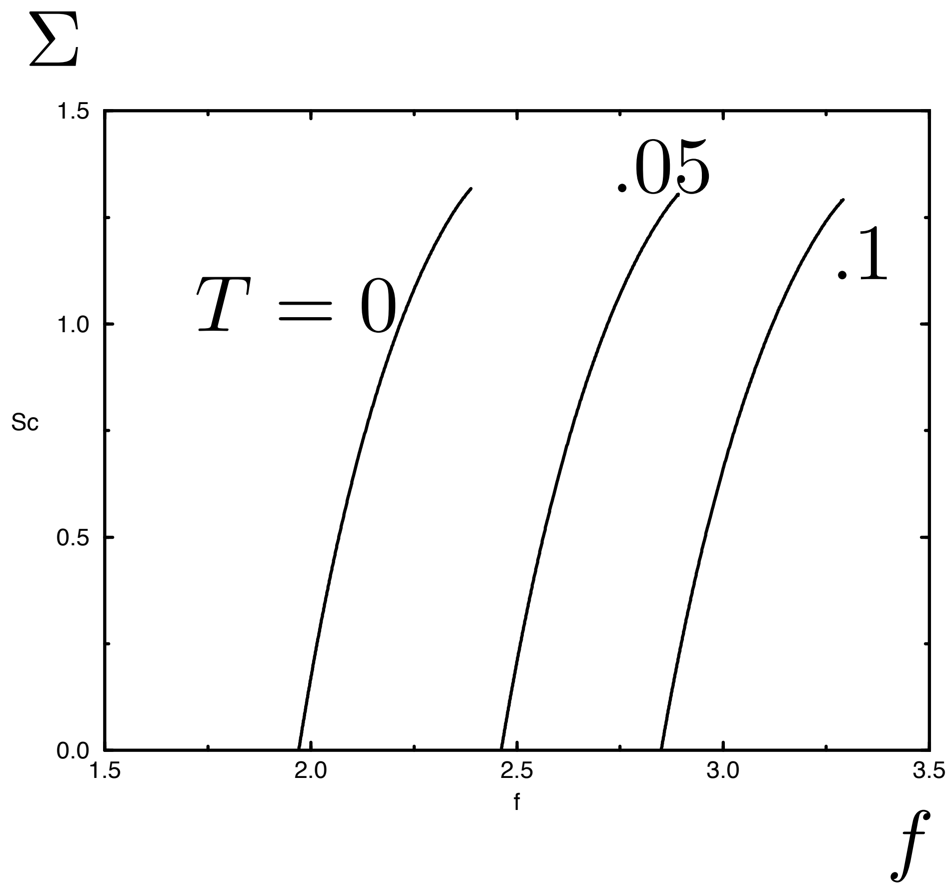



Small $\alpha$ : stron… enerates a tightly bound mol… erature. Equival… for the … nstein model for crystals (quadratic fluctu… ns inside … well). Legendre transform turns it into an expansion in p…wers of the fluctuations inside a well.

# Molecular liquid: real study

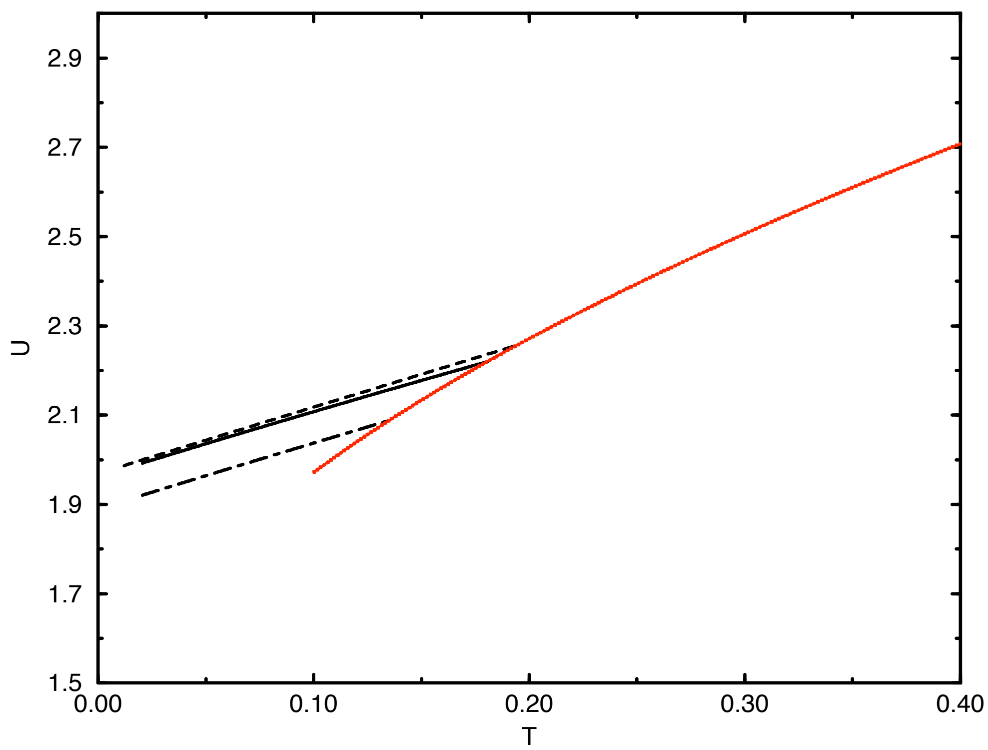
# Some results

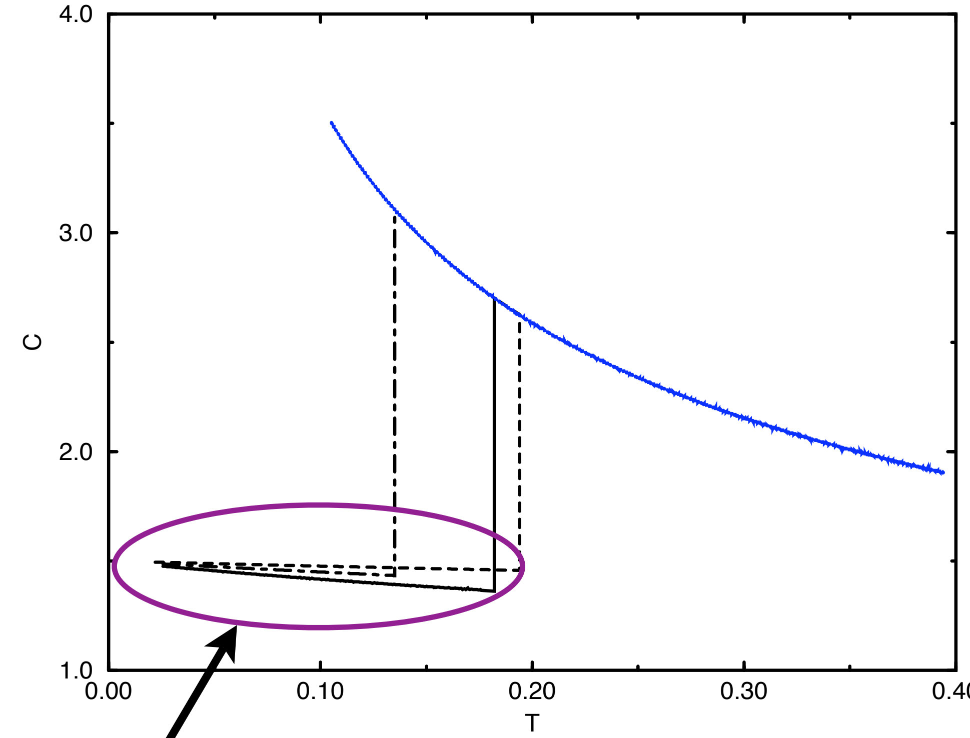
Soft spheres $V(r) = 1/r^{12}$



# Some results

Soft spheres $V(r) = 1/r^{12}$



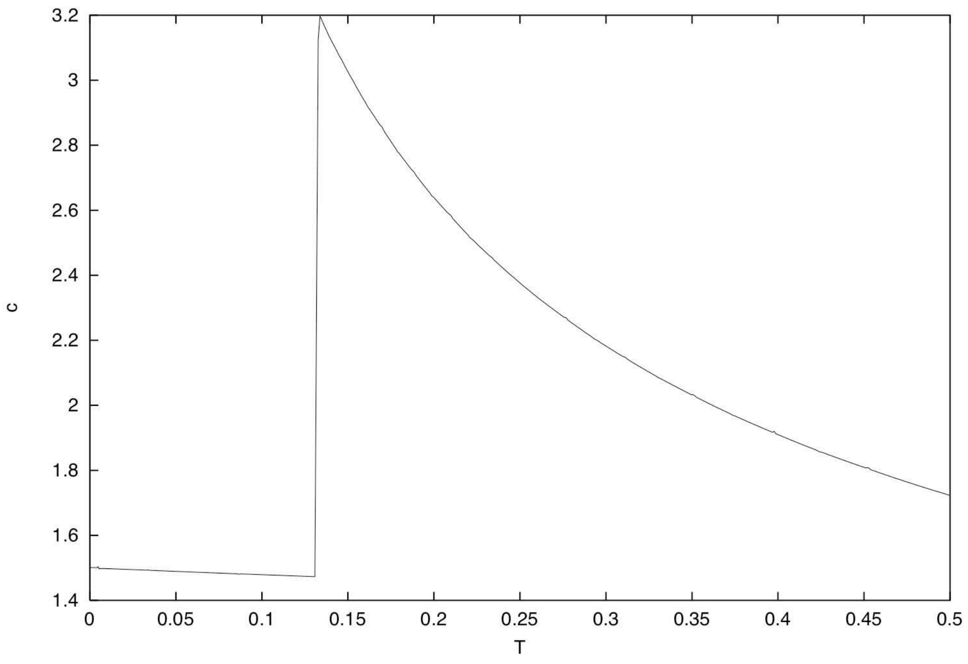



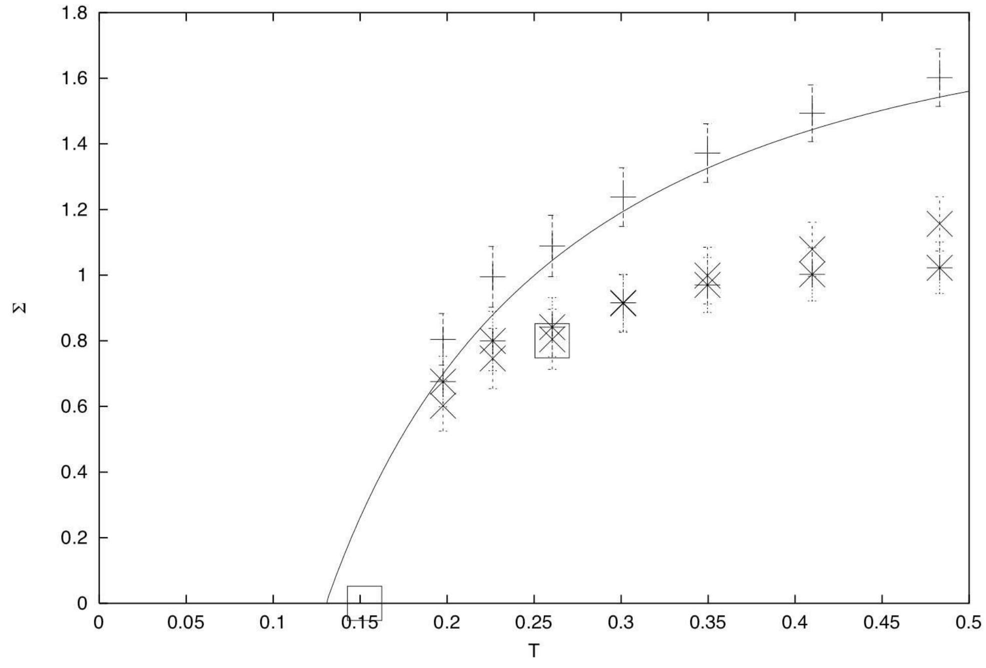

Dulong Petit (from liquid computations)!

Also binary mixtures of spheres, binary Lennard-Jones, hard spheres...

# Some results

## Binary mixtures of soft spheres

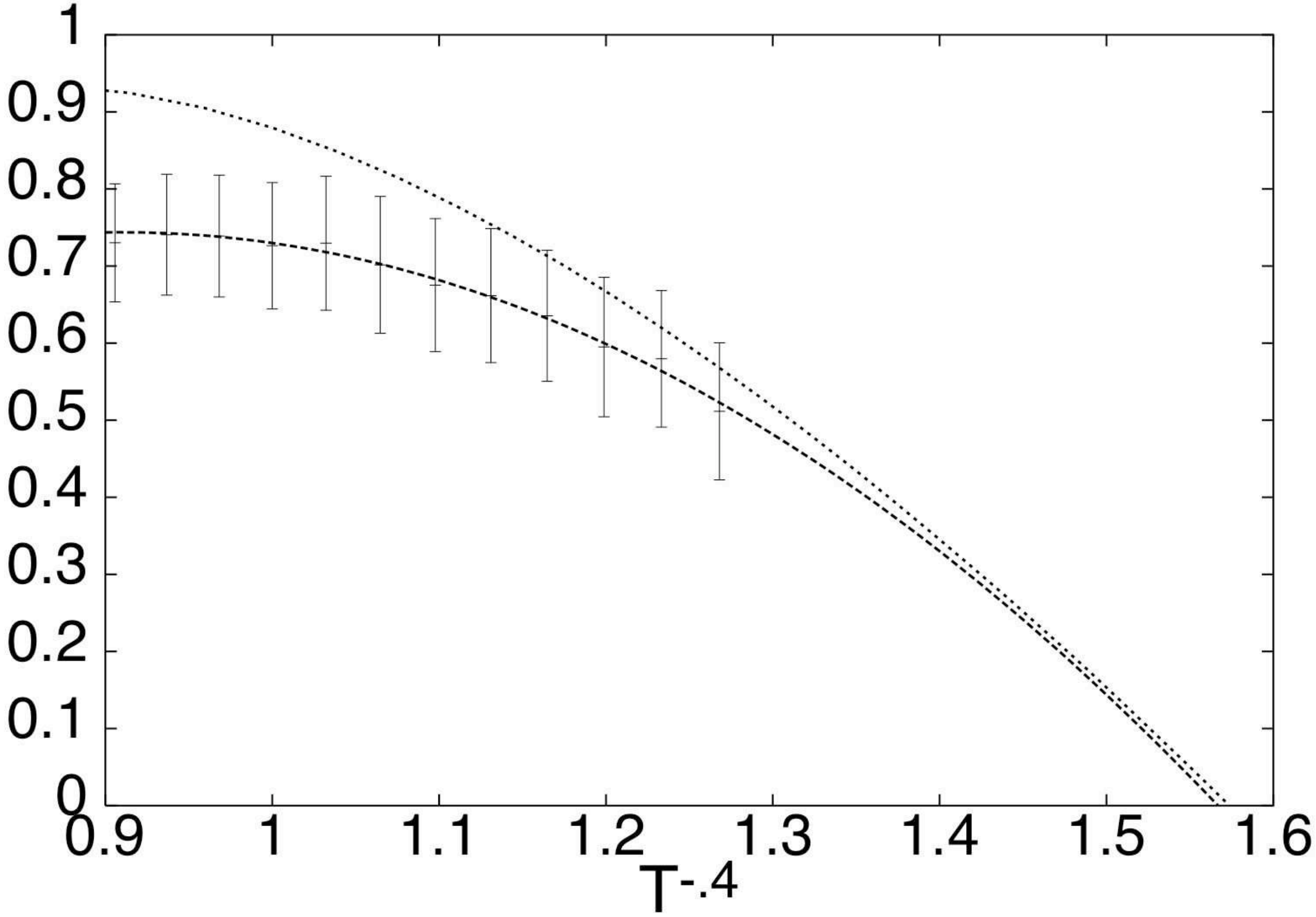



Numerical estimates of $\Sigma$ using $S_{liq} - S_{sol}$

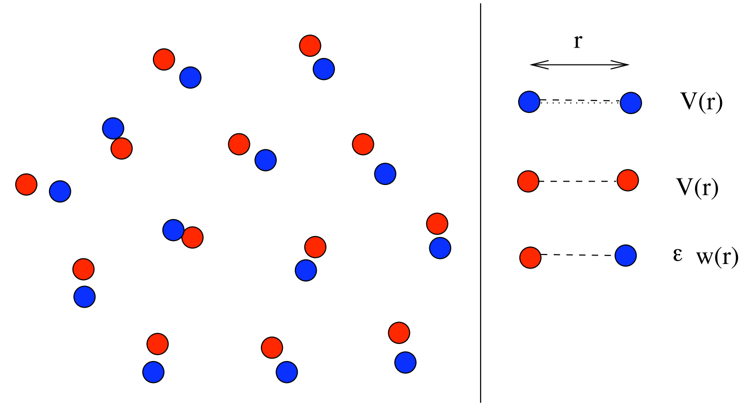
# Some results

Binary mixtures of Lennard-Jones particles (KA mixture)



# Take home message

Replica method
("new replicas")




Compute $T_d$ as the temperature where the particles remain in a molecular bound state (on your favourite time scale) in the limit $\epsilon \to 0$

Compute the complexity function, and the value of the Kauzmann temperature $T_c$

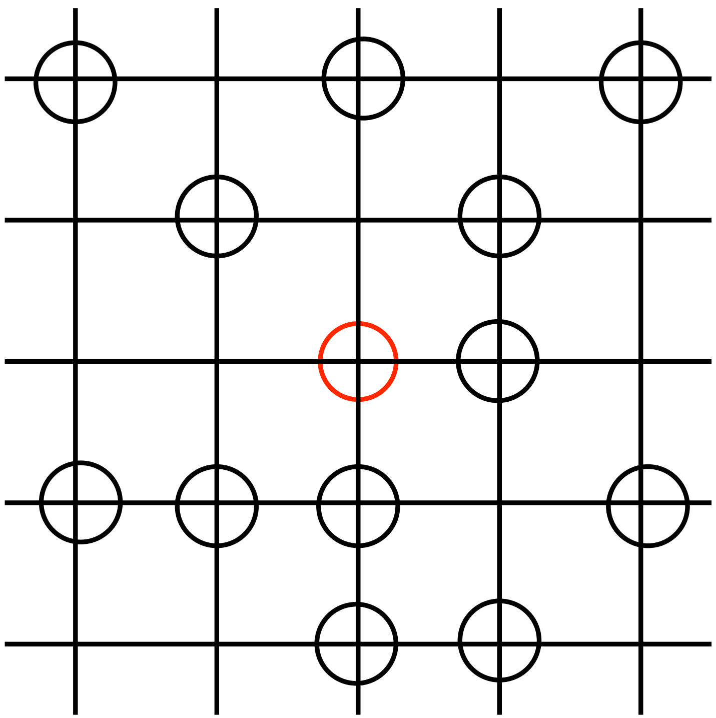
Everything is turned into liquid computations, in a molecular liquid (with $m$ atoms per molecule).

# How does it really work?

Liquids: complicated. Simpler model: lattice glass (cf gas-liquid versus lattice gas).

Biroli M, Pica Ciamarra et al., Weigt Hartmann, Darst Reichman Biroli, Rivoire Biroli Martin M, ...

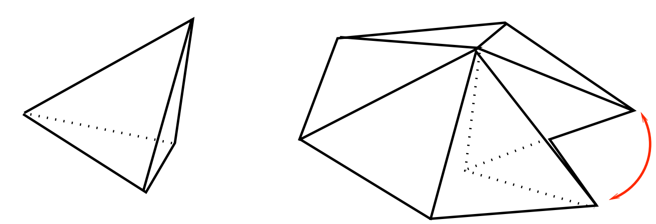
Basic idea:



DENSITY CONSTRAINT

$\leqq$ L occupied neighbours

L=2

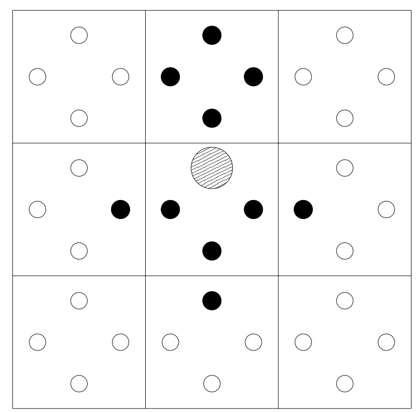


NB: different from kinematic constraints à la Kob Andersen

# Lattice glass

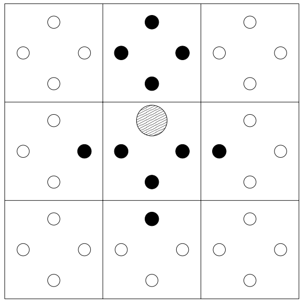
Basic model: $\left|\begin{array}{l} E = \mu \sum_i n_i \text{ if all particles have } \leq \text{ L neighbours} \\ E = \infty \quad \text{else} \end{array}\right.$

In practice, for simulations: crystallizes too easily.
Mixtures (e.g. 10% L=1, 50% L=2, 40% L=3),
or decorated unit cell

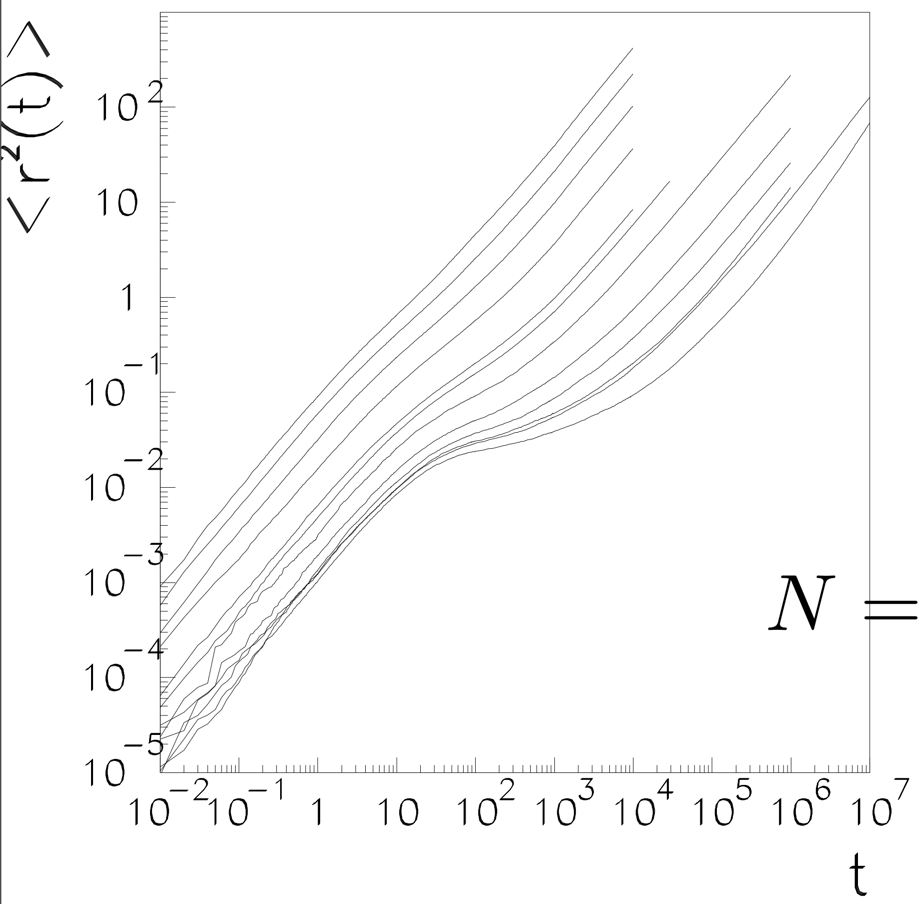


Simulations: many properties of glass forming liquids

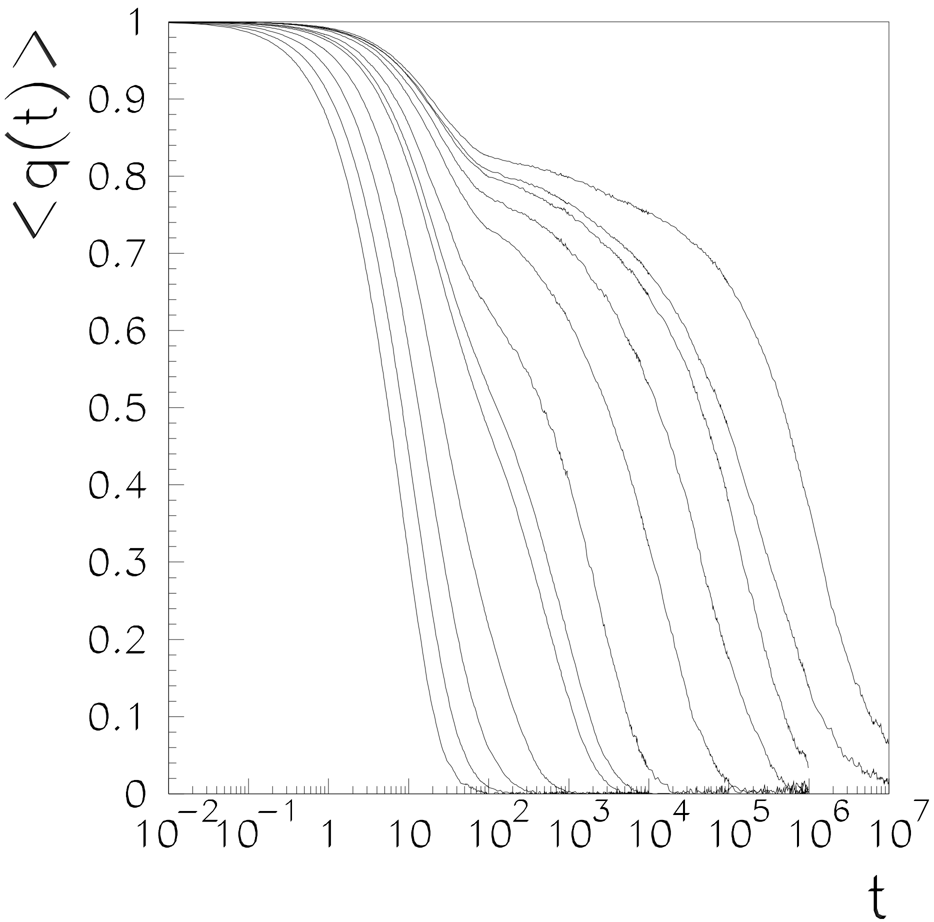
# Lattice glass: numerical results



## Dynamical simulations (Pica Ciamara)

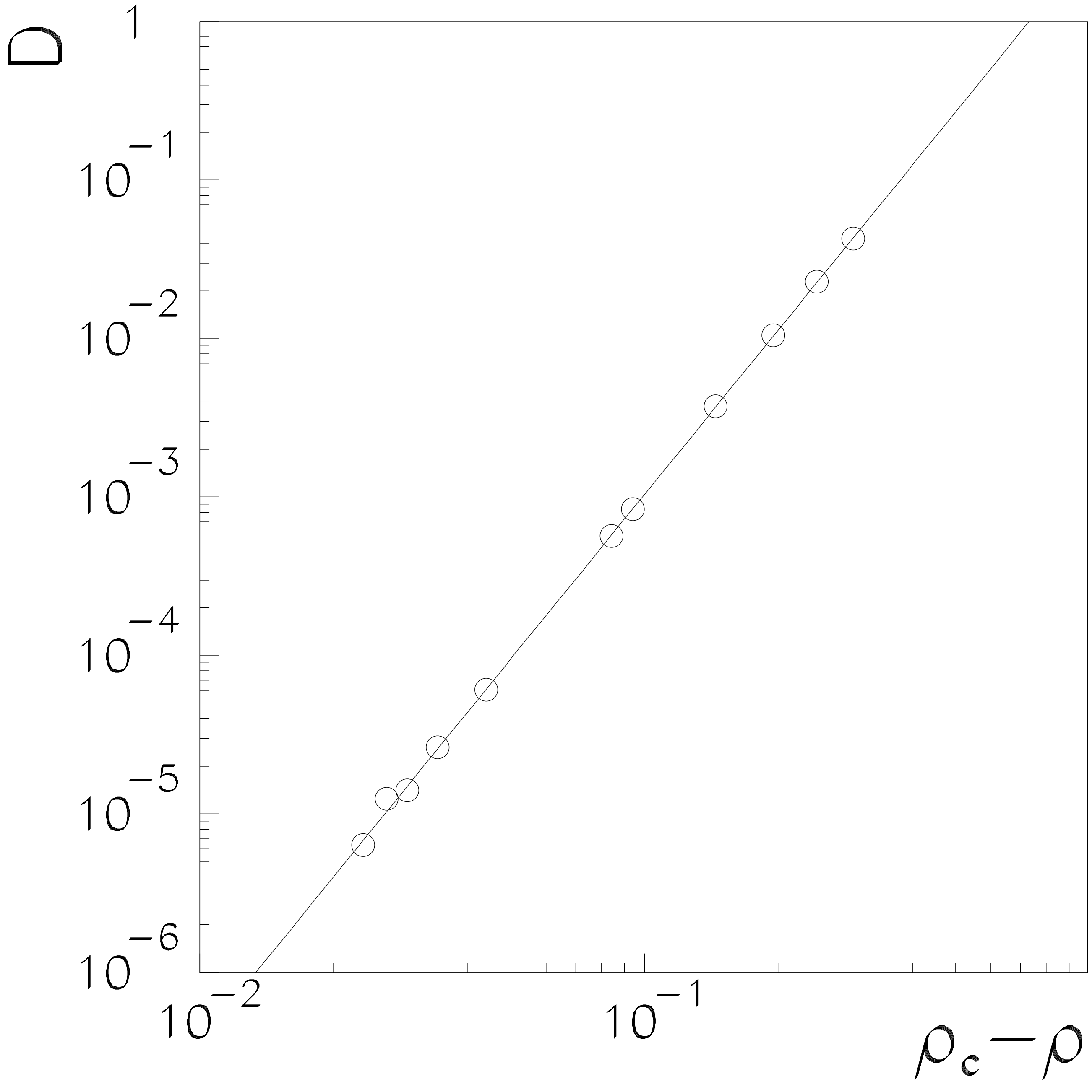


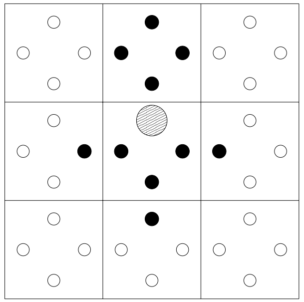

$$N = 15^3$$



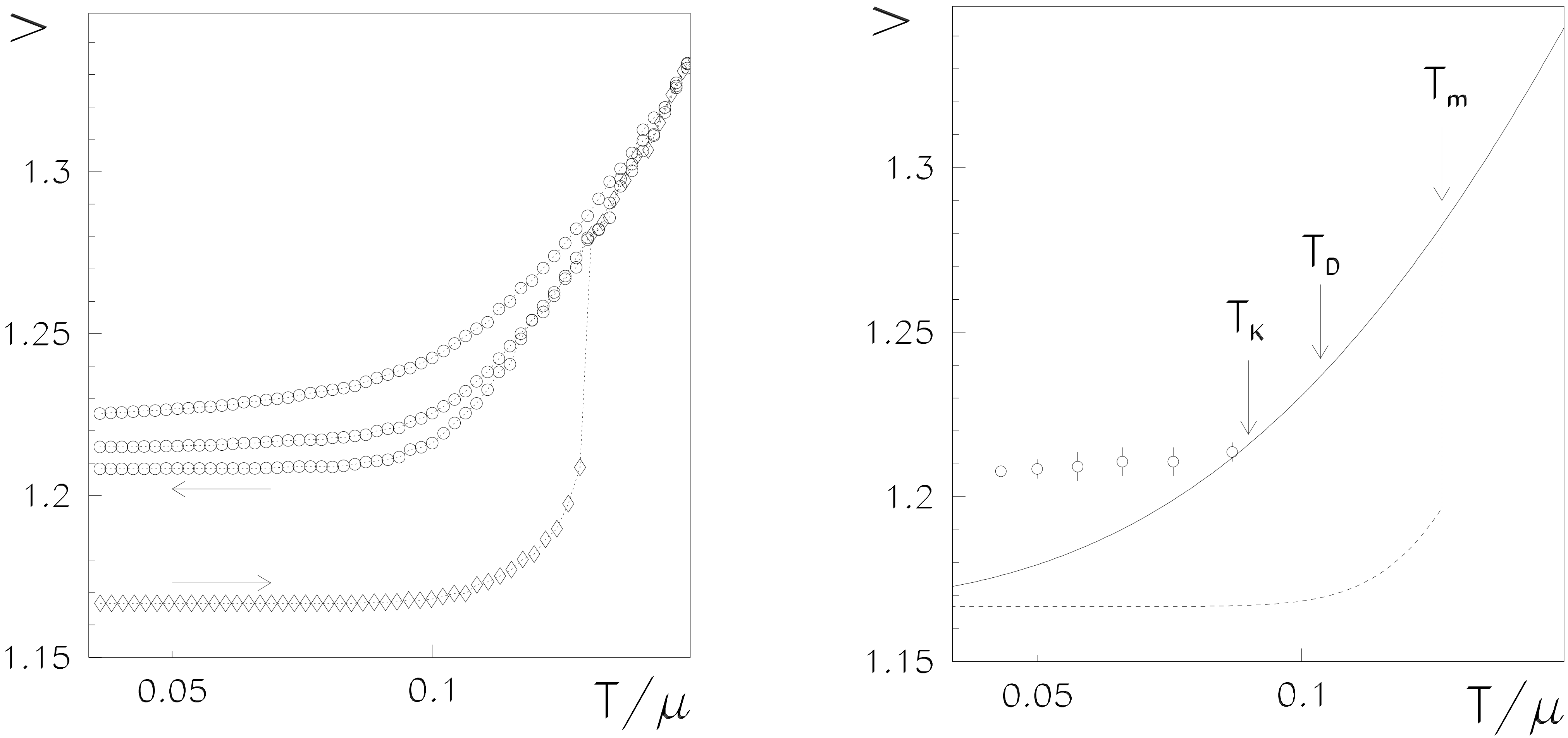

$$\rho = .55, .6, .65, .7, .75, .76, .78, .8, .81, .815, .818, .821$$

# Lattice glass: numerical results



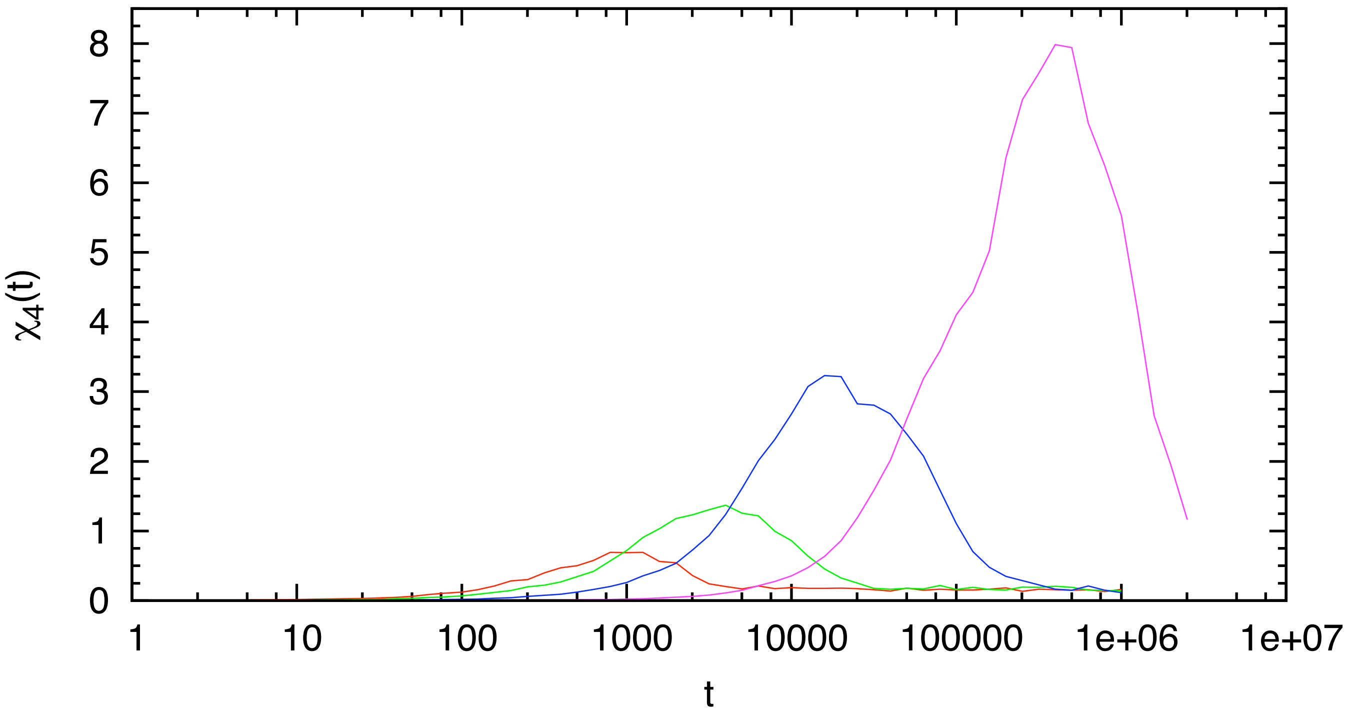



# Lattice glass: numerical results



# Lattice glass

Dynamical simulations (mixtures: Darst et al )



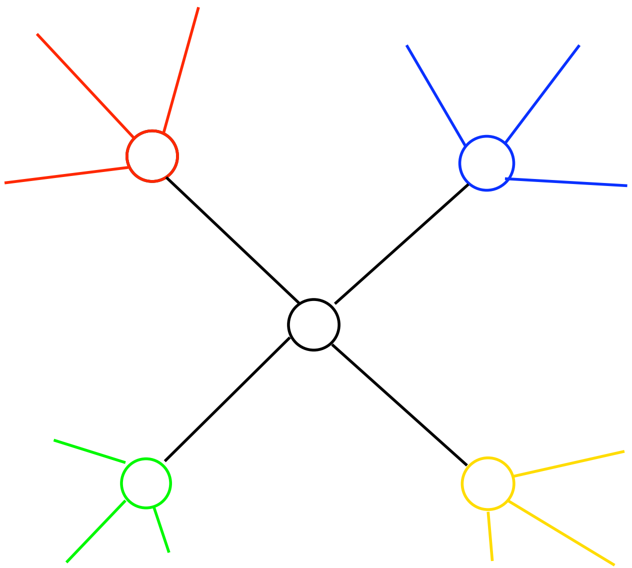
# Lattice glass: theory

$$P(n) = \frac{1}{Z(\mu)} \, e^{\mu \sum_i n_i} \, \prod_i \, I\left[ n_i \left( \sum_{j \in V(i)} n_j \right) \leq L \right]$$

Cavity method ("RS"):

Approximate locally the lattice by a tree = Bethe approximation

Take exactly into account all correlations between black site and its neighbours, but neglect the correlations between neighbours when computing their influence on the black site



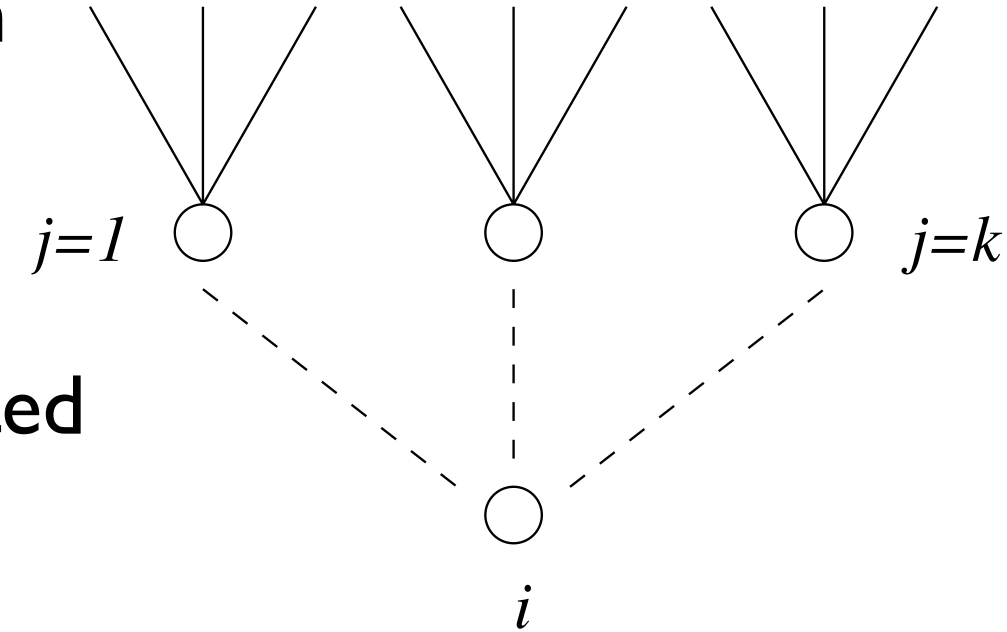
Solution on a tree = recursion

Rooted tree on $j$ :

$Z_j^e$ : root empty

$Z_j^u$ : root occupied, unsaturated

$Z_j^s$ : root occupied, saturated




$$Z_i^e = \prod_{j=1}^{k} \left( Z_j^e + Z_j^u + Z_j^s \right)$$

Recursion (here for $L = 1$ )

$$Z_i^u = e^{\mu} \prod_{j=1}^{k} Z_j^e$$

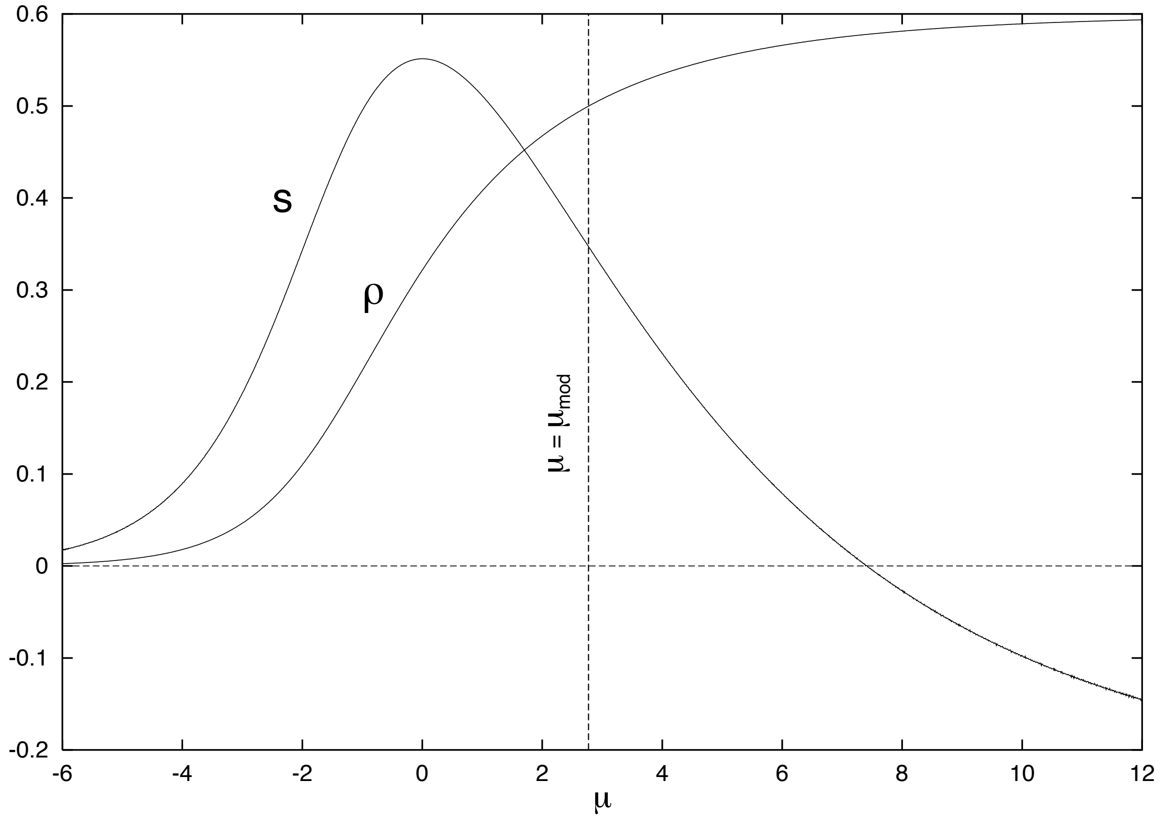
Liquid phase: homogeneous

$$\frac{Z_i^{e,u,s}}{Z_i^e + Z_i^u + Z_i^s} = p^{e,u,s}$$

$$Z_i^s = e^{\mu} \sum_{j=1}^{k} Z_j^u \prod_{r \neq j} Z_r^e$$

# Liquid phase

Solution of the equation for $p^e, p^u, p^s$, and computation of the local density by merging z rooted trees (instead of z-1 for the recursion) + computation of entropy:



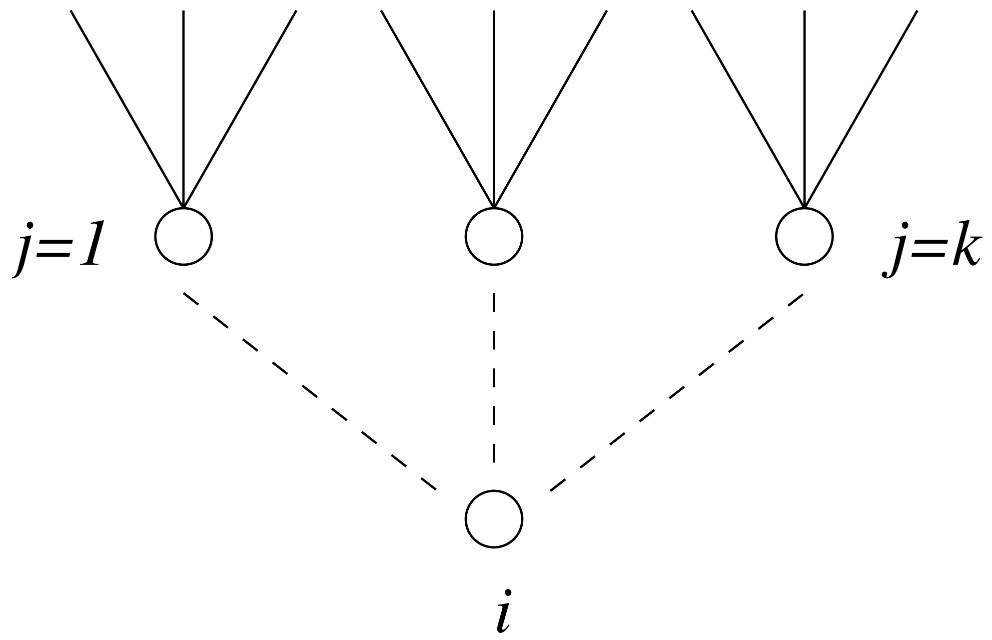
# Glass phase

$$Z_i^e = \prod_{j=1}^{k} \left(Z_j^e + Z_j^u + Z_j^s\right)$$

$$Z_i^u = e^{\mu} \prod_{j=1}^{k} Z_j^e$$

$$Z_i^s = e^{\mu} \sum_{j=1}^{k} Z_j^u \prod_{r \neq j} Z_r^e$$

$$h_i = \begin{pmatrix} Z_i^e \\ Z_i^u \\ Z_i^s \end{pmatrix} = f(\{h_j\}_{j \in \partial i_{rooted}})$$




Iterate this on a random graph: many solutions $h_i^{\alpha}$

# Glass phase: 1RSB cavity

$$h_i = \begin{pmatrix} Z_i^e \\ Z_i^u \\ Z_i^s \end{pmatrix} = f(\{h_j\}_{j \in \partial i_{rooted}})$$

Iterate this on a random graph: many solutions $h_i^\alpha$

Free energy of solution $\alpha$: $F_\alpha = N f_\alpha$

$$Z(\beta, m) = \sum_\alpha e^{-\beta m N f_\alpha}$$

$$P_i^{(m)}(h) = C \sum_\alpha \delta(h_i^\alpha - h) e^{-\beta m F_\alpha}$$

= distribution of field on a given i

$$P_i^{(m)}(h) = \mathcal{F}\left(\left\{P_j^{(m)}\right\}\right)$$

# Lattice glass RSB solution details

$$e^{-\mu a_i} = \frac{Z_i^e}{Z_i^e + Z_i^u + Z_i^s}$$

$$e^{-\mu b_i} = \frac{Z_i^e}{Z_i^e + Z_i^u}$$

$$h = (a, b) = f(h_1, h_2)$$

$$a = -\Delta F = \frac{1}{\mu} \log \left[ 1 + e^{\mu(1-a_1-a_2)} \left( e^{\mu b_1} + e^{\mu b_2} - 1 \right) \right]$$

$$b = \frac{1}{\mu} \log \left[ 1 + e^{\mu(1-a_1-a_2)} \right]$$

# Lattice glass RSB solution details

Large $\mu$ limit:


$a = \max\,[0,$

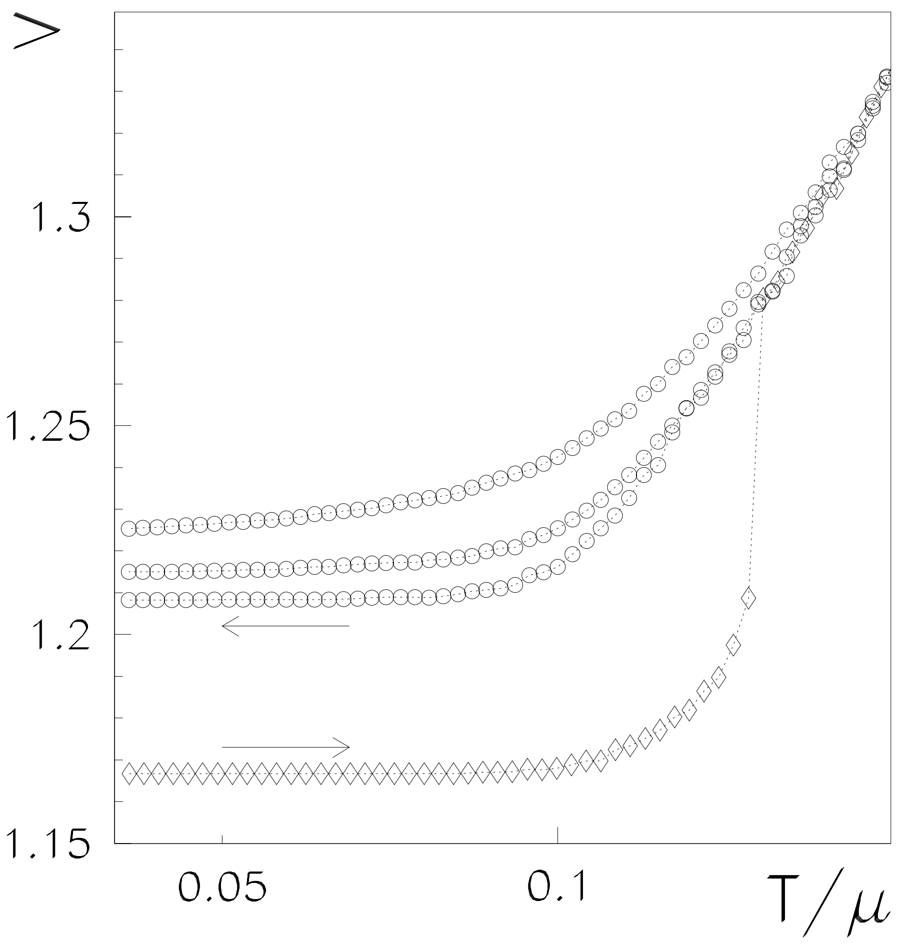
$b = \max[0,$

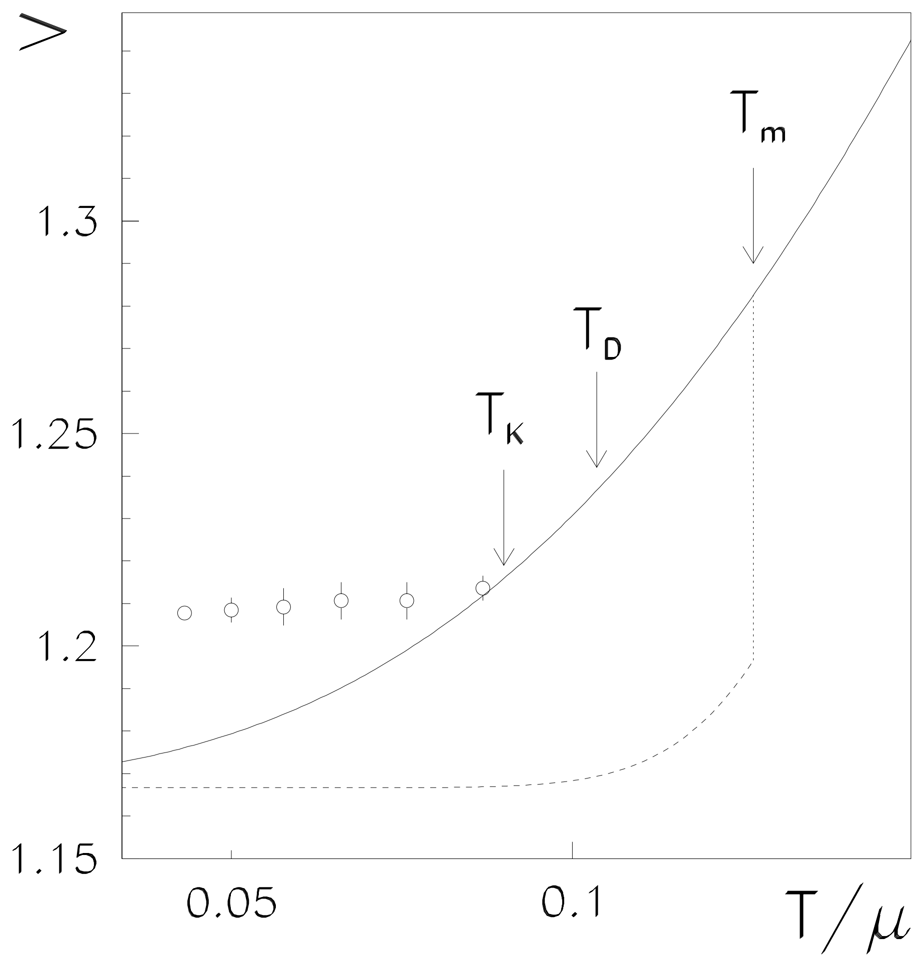
$h = (a, b) \in$

$P^{(m)}(h) = p$ $= \lim_{\mu\to\infty} m\mu$

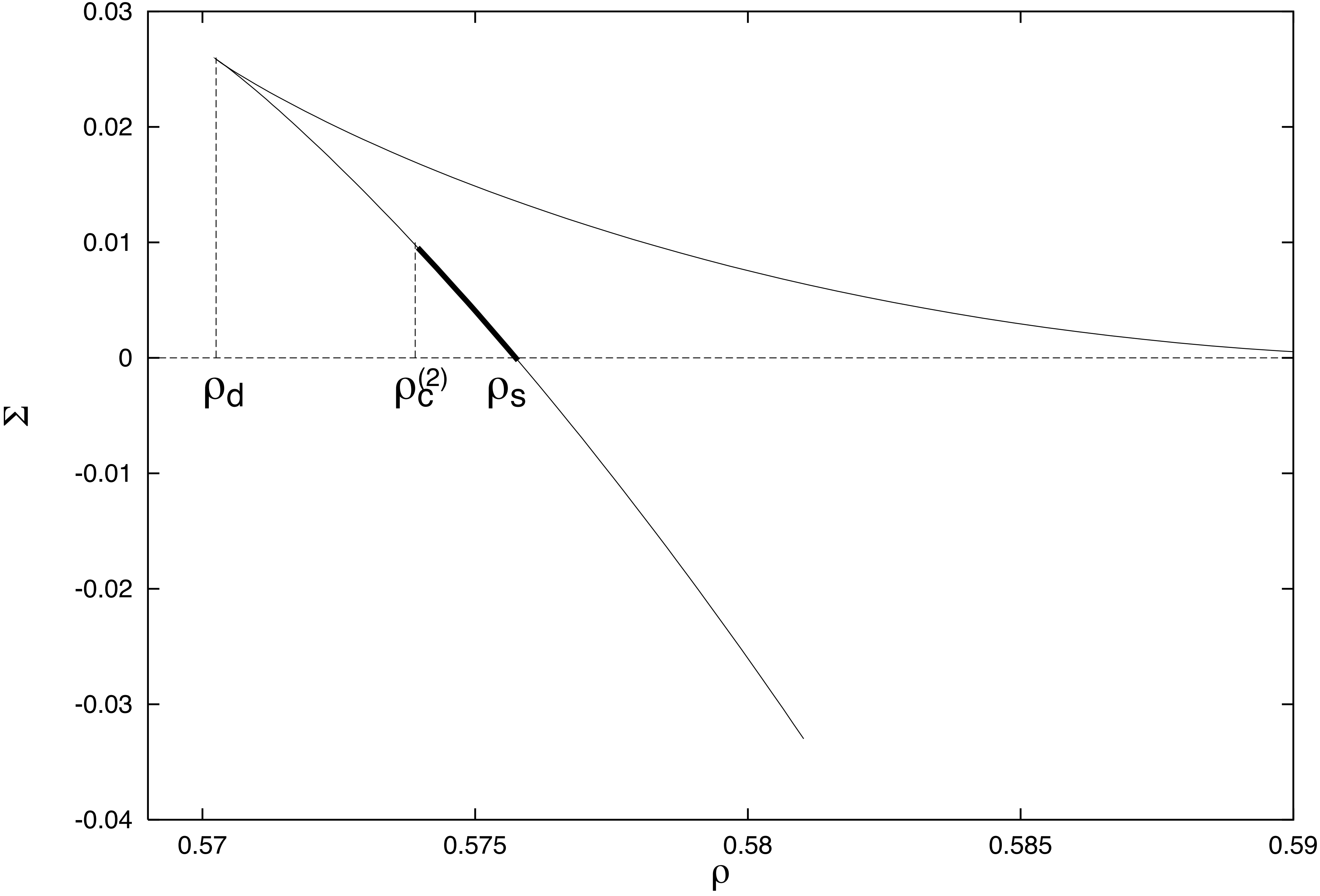
$$p_u = \frac{1}{\mathcal{Z}} p_e^2 e^y \; ; \quad p_s = \frac{1}{\mathcal{Z}} 2 p_u p_e e^y \; ; \quad p_e = \frac{1}{\mathcal{Z}} \left[1 - p_e^2 - 2 p_u p_e\right]$$

# Lattice glass: numerical results



# Lattice glass: numerical results



# Hard computational problems

Discrete optimization (combinatorial)

- Configurations: $N$ discrete variables (e.g. binary)
- Energy (cost) $E(C)$ computable in $O(N^r)$ operations
- Is there a configuration $C$ with energy $E(C) < A$ ?

Examples: Spin Glasses, Lattice Glasses, Electron Glasses,..., Travelling salesman, Matching, Eulerian circuit, Hamiltonian Path, Satisfiability, Protein Folding, Error correcting Codes, Learning in Neural Networks...

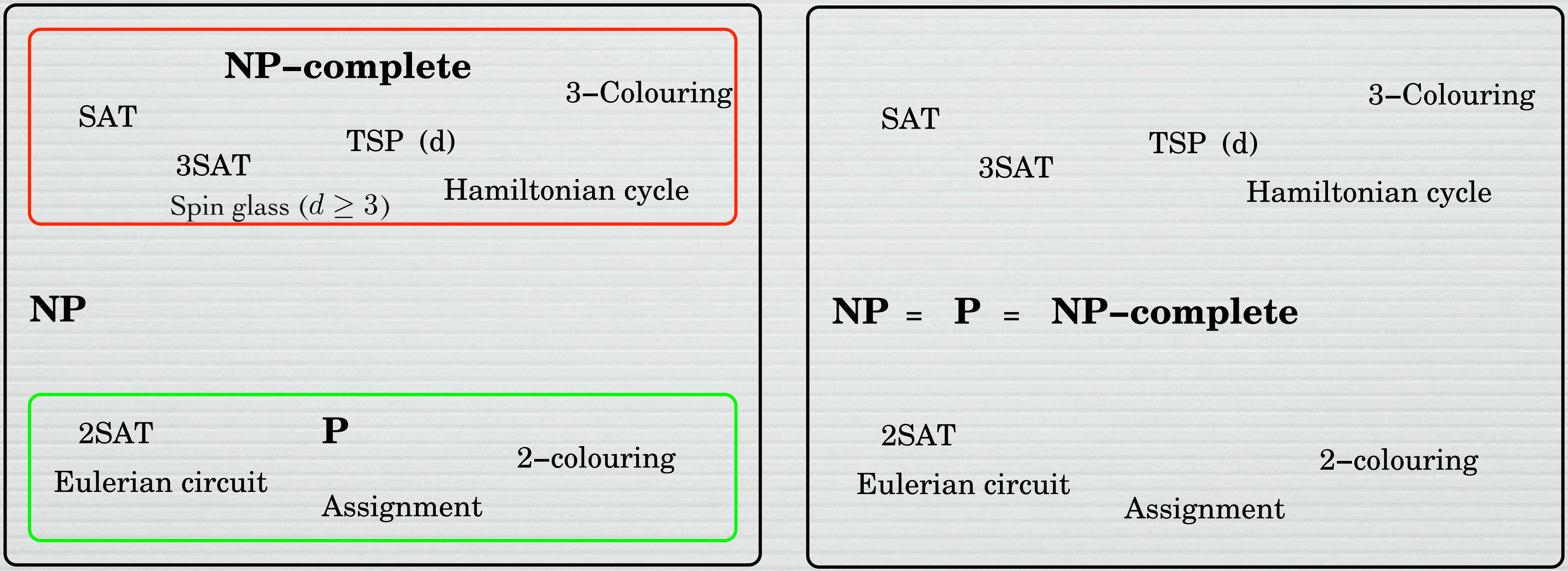
# Hard computational problems

A main achievement from computer science: classification into complexity classes

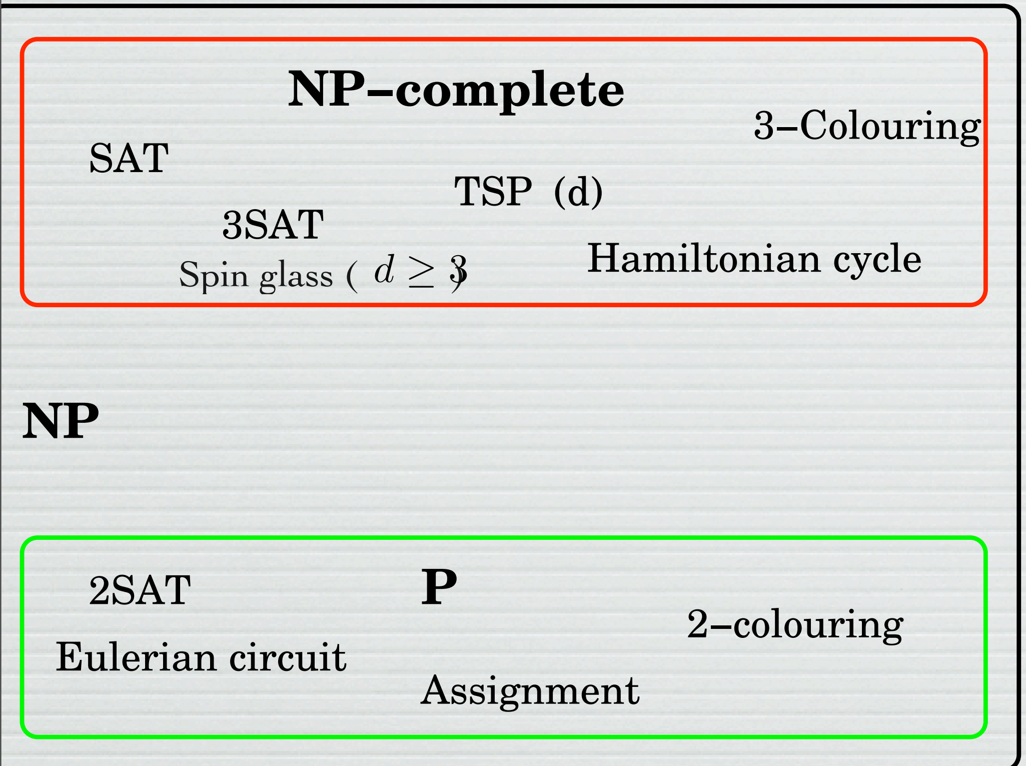
- Class P: finds a configuration $C$ with $E(C) < A$, or shows that it does not exist, in a time $O(N^s)$
- Class NP: all the problems for which the energy can be computed in a time $O(N^r)$
- Class NP complete: the hardest of all NP problems. Problem A is NPC if all the problems in NP can be transformed to A in polynomial time

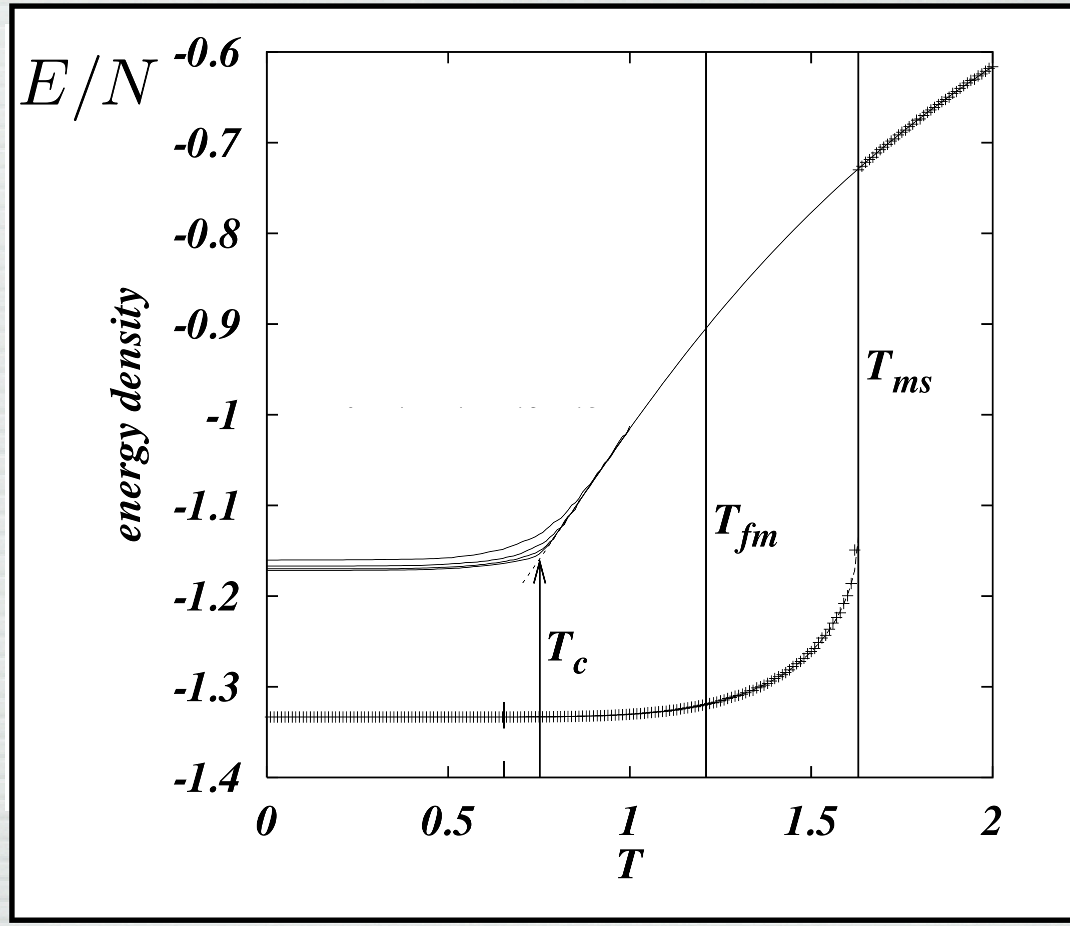
Theorem (Cook 71): Satisfiability is NP-complete

# P≠NP ?



NP–complete
SAT
3SAT
TSP (d)
3–Colouring
Hamiltonian cycle
Spin glass ($d \geq 3$)
NP
2SAT
Eulerian circuit
P
Assignment
2–colouring
SAT
3SAT
TSP (d)
3–Colouring
Hamiltonian cycle
NP = P = NP–complete
2SAT
Eulerian circuit
Assignment
2–colouring




Q: is there any relation between the computational hardness and the slow relaxation in glassy systems?

Q: is there any relation between the computational hardness and the slow relaxation in glassy systems?

A few initial remarks:

- Physical dynamics = constrained (detailed balance).
- Complexity classes = worst case analysis. Physics= typical case

It may be that difficult instances are very rare, "exceptional" ones, or it may be that they are typical (Instance= sample).

- No general relation between worst-case NP-completeness and typical-case, detailed-balance physical behaviour.
- But physics can help to develop some understanding of "typical case" complexity:

Structural properties of typical instances.

Examples: (glasses), satisfiability, error correcting codes.

# Satisfiability

*"..a theatrical director feels obligated to cast either his ingénue, Actress Alvarez, or his nephew, Actor Cohen, in a production. But Miss Alvarez won't be in a play with Cohen (her former lover), and she demands that the cast include her new flame, Actor Davenport. The producer, with her own favors to repay, insists that Actor Branislavsky have a part. But Branislavsky won't be in any play with Miss Alvarez or Davenport. Is it possible to satisfy the tangled web of conflicting demands?"*

(from G. Johnson, The New York Times 1999).

$$A, B, C, D \in \{0, 1\}$$

Constraints = clauses, e.g.: $A \vee C$

# Satisfiability

$N$ Binary variables $x_i \in \{0,1\}$

$M$ Constraints = clauses, e.g.: $x_1 \vee \overline{x}_2 \vee x_3$

Is there a configuration of the $\{x_i\}$ which satisfies all the constraints?

The grandfather of NP-complete problems (Cook 71)

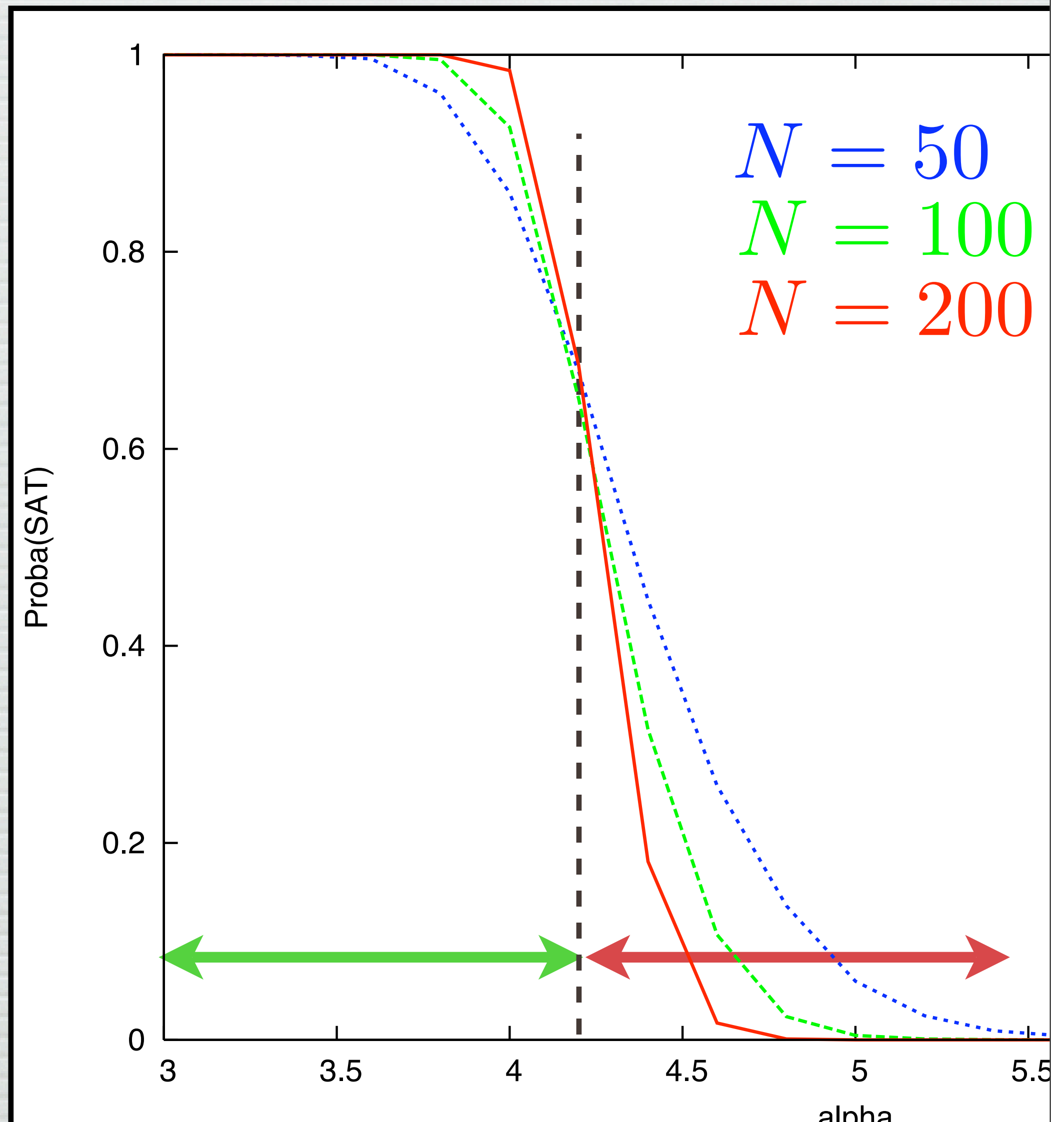
3-SAT (clauses of length 3) is also NP-complete

Typically hard instances: random 3-SAT: Generate each clause with three randomly chosen variables in $\{x_i, \overline{x}_i\}$

# Typical satisfiability and phase transition

Random 3-SAT: N variables, M clauses. 3 variables in each clause, randomly chosen, randomly negated:

Large N limit: $\alpha = M/N$
=density of constraints




SAT for $\alpha < \alpha_c$

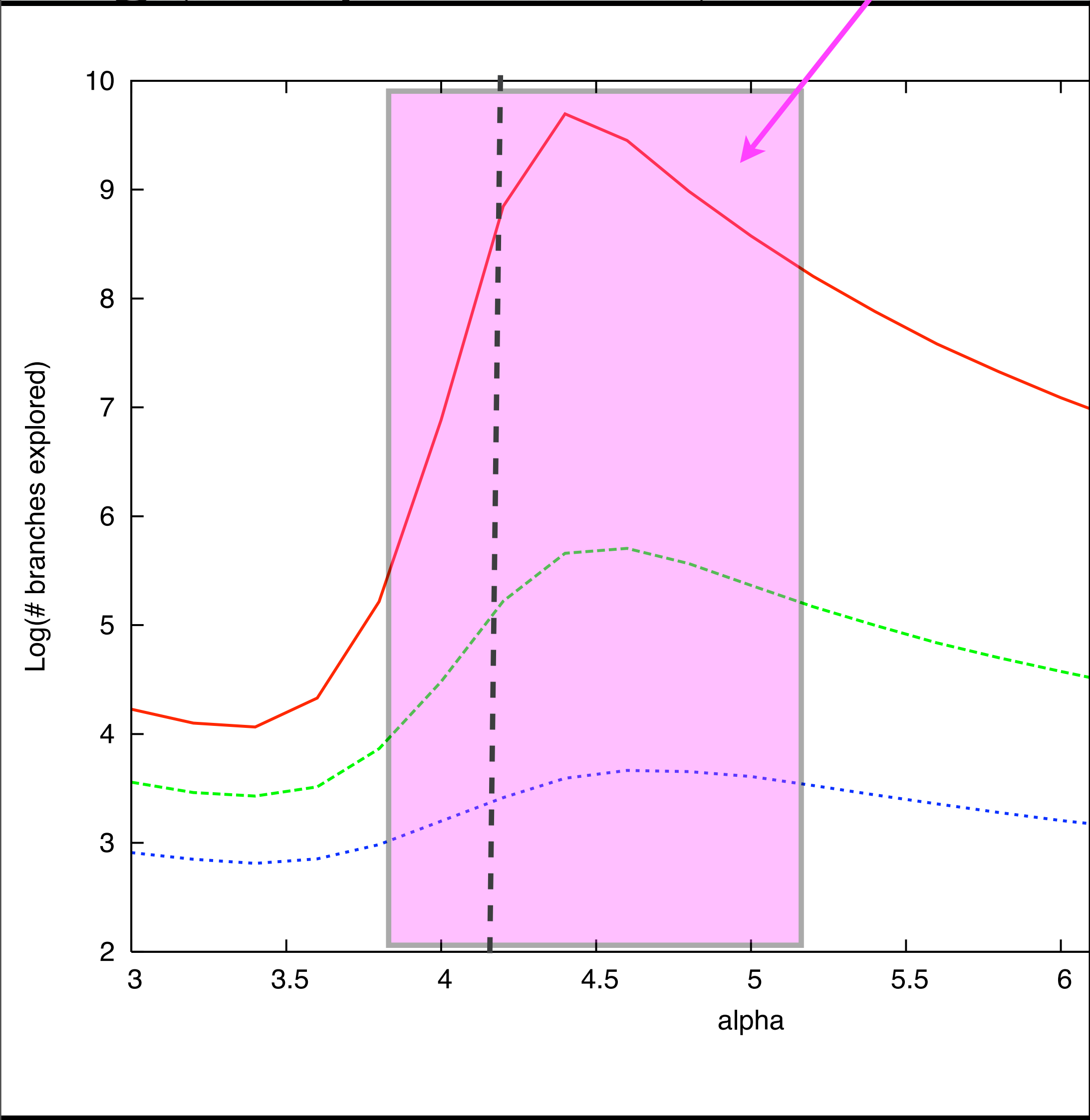
UNSAT for $\alpha > \alpha_c$

"Phase transition"

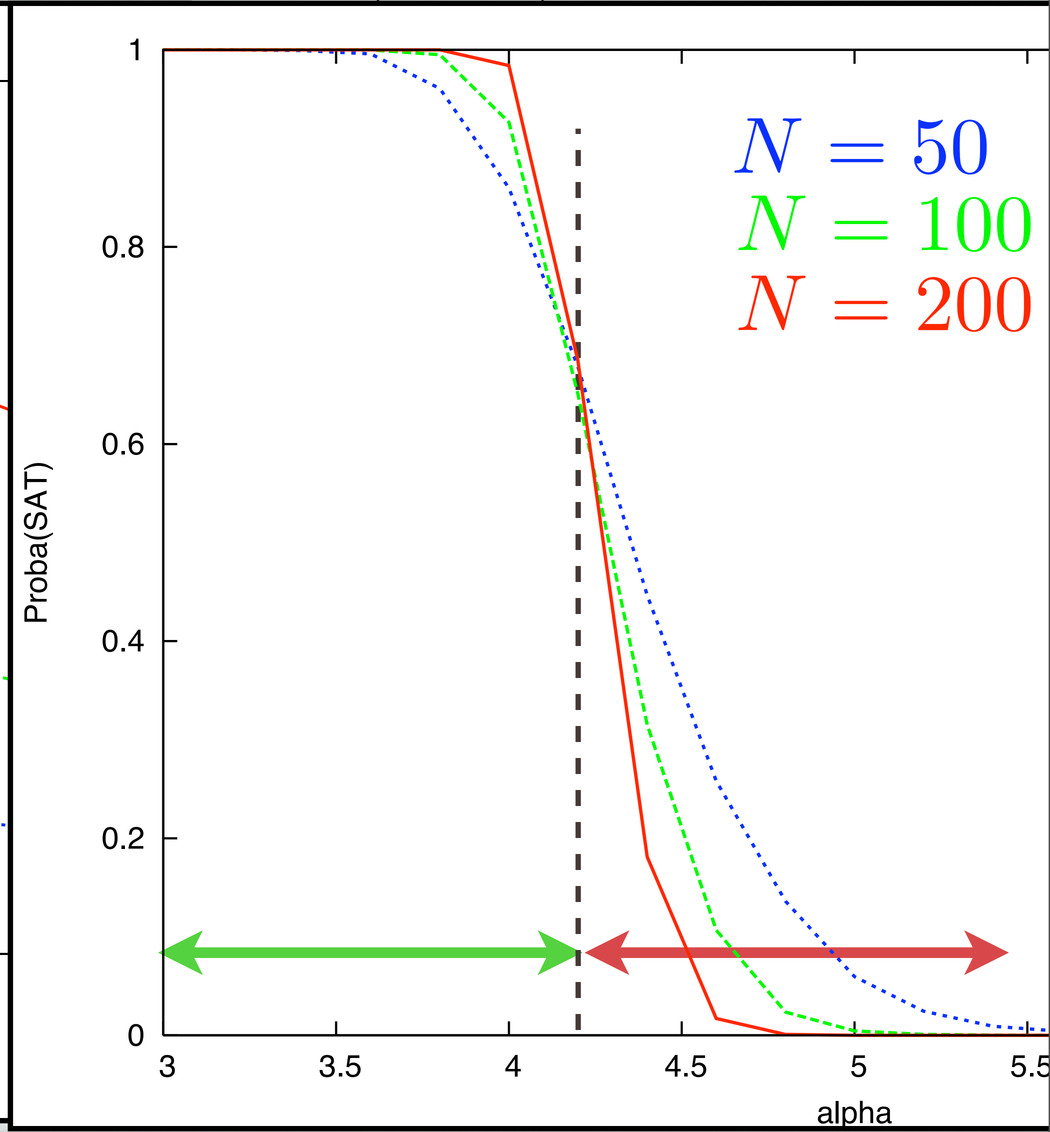
Selman, Kirkpatrick,...

# Hardest problems: close to the phase transition

Log(computer time)

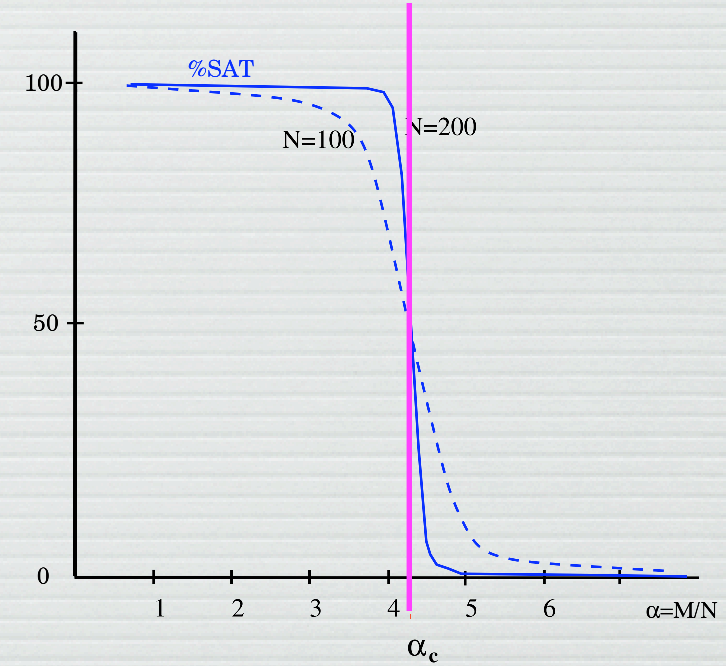



Proba(SAT)

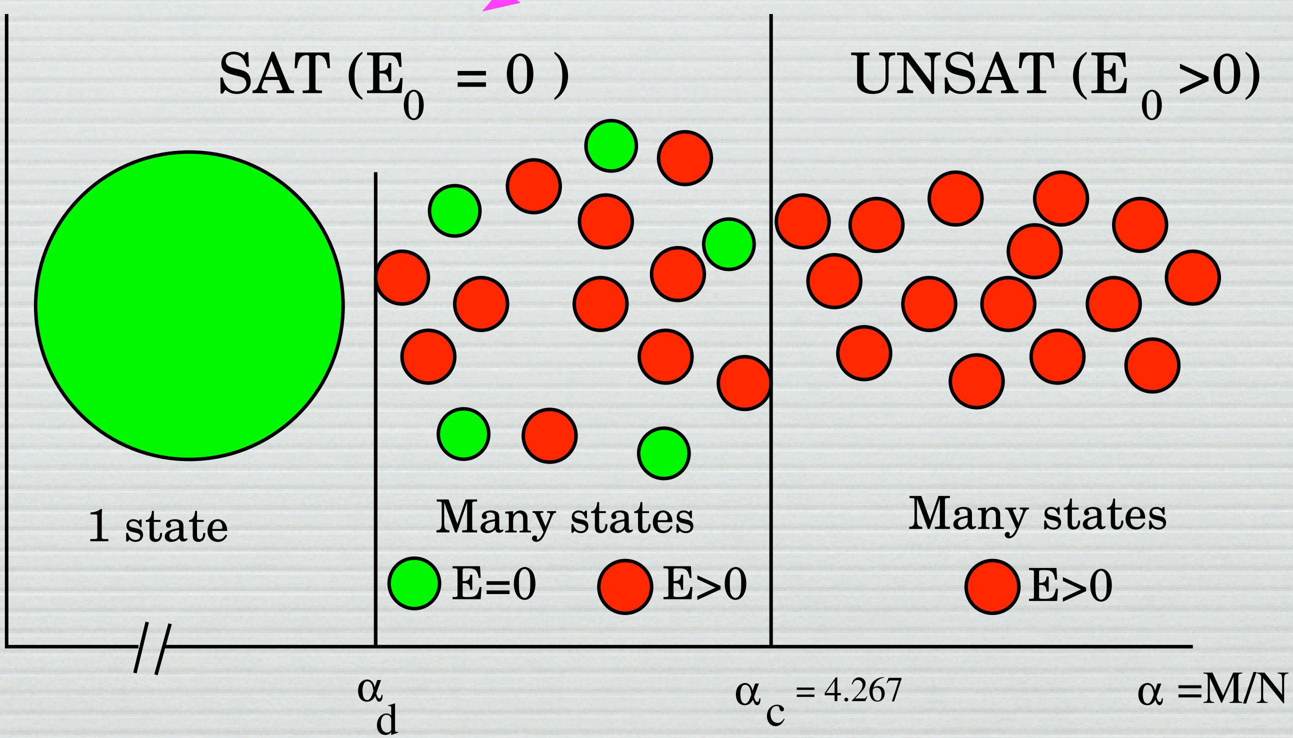


# Physical analysis

- SAT-UNSAT transition at the critical constraint density $\boxed{\alpha_c = 4.2667..}$



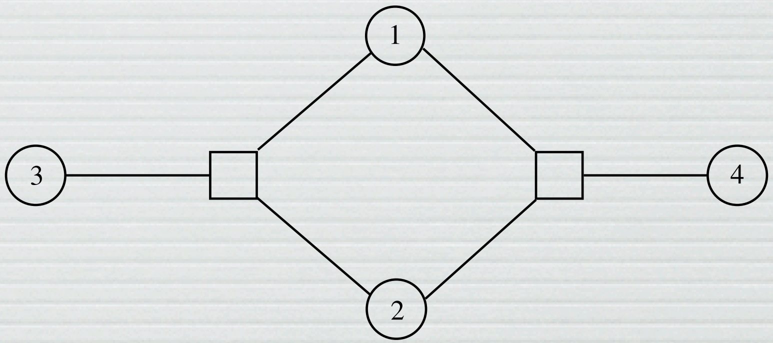

- Intermediate glass phase: $\alpha_D < \alpha < \alpha_c$



# Factor graph representation

Graphical representation of a satisfiability problem

One circle per variable,
one square per constraint:




$$(x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_4)$$

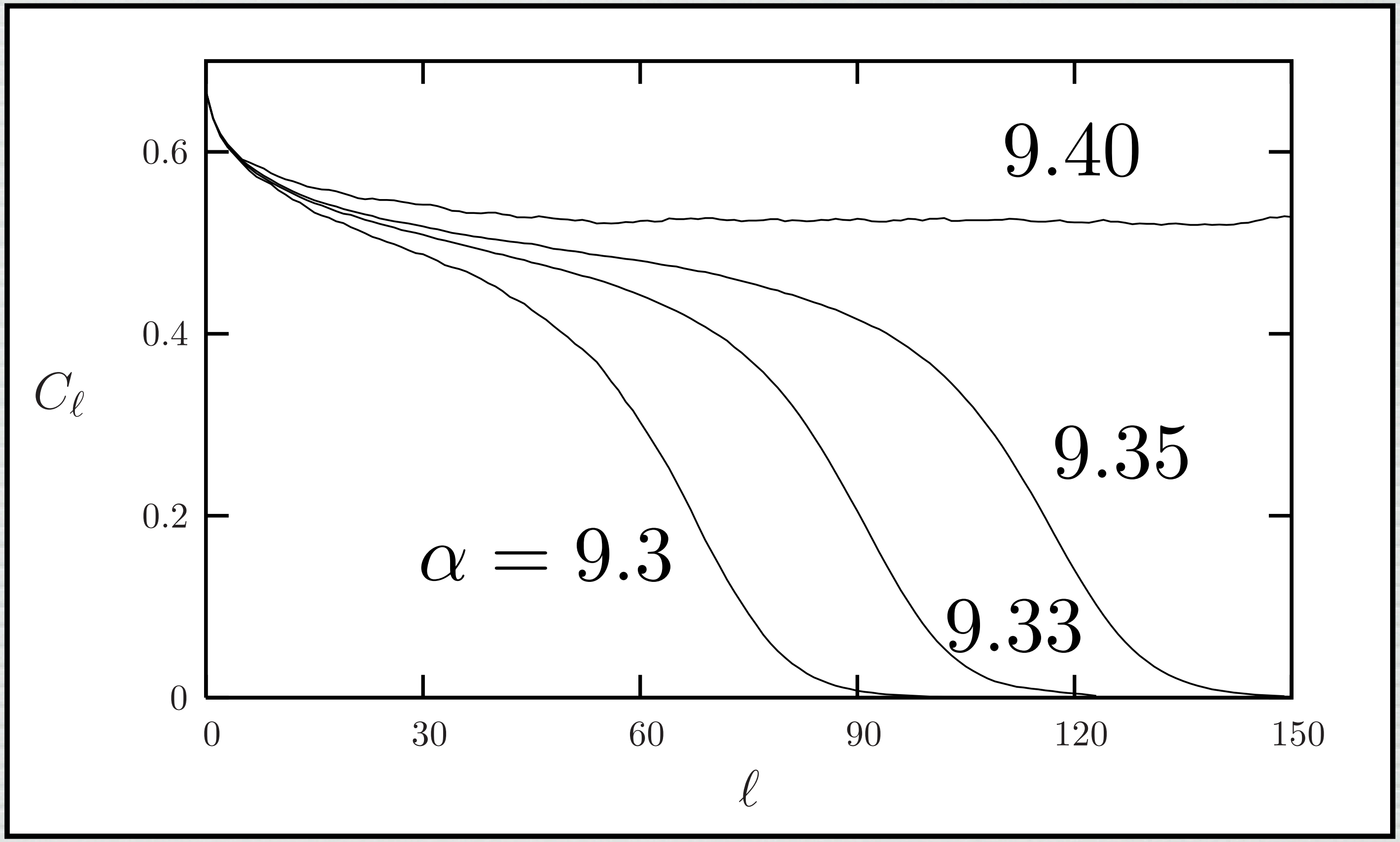
Encodes some distance
properties of the variables:

$d(i, j)$ = length of shortest path between $i$ and $j$

# Point-to-set correlations in 4-satisfiability

$\alpha_d = 9.38$

Clustered phase=onset of long range point-to-set correlations



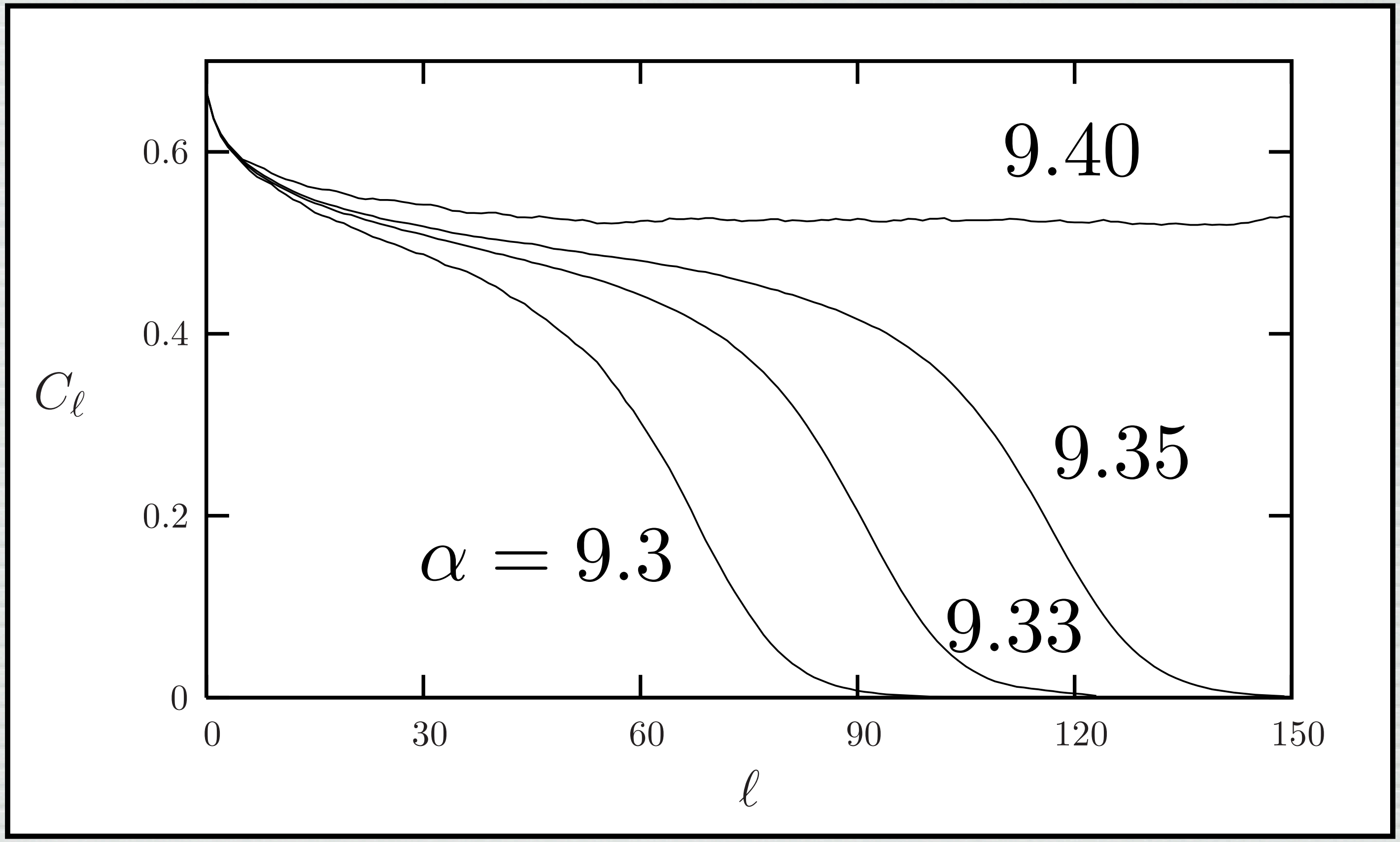

$\langle \sigma_i \rangle_B$ =average of $\sigma_i$ given a fixed configuration of variables at distance $\ell$

$$C_\ell = \sum_B P(B) \langle \sigma_i \rangle_B^2 - \left( \sum_B P(B) \langle \sigma_i \rangle_B \right)^2$$

# Point-to-set correlations in 4-satisfiability

$\alpha_d = 9.38$

Clustered phase=onset of long range point-to-set correlations




Biroli, Bouchaud (structural glasses); Mézard, Montanari (reconstruction); Montanari, Ricci-Tersenghi, Semerjian (4-SAT); Cavagna, Grigera, Verrochio;...

## Clustered SAT phase: properties of the uniform measure over all solutions. 4-SAT:

Clusters appear at $\alpha_d \simeq 9.38$ : dynamical transition

Condensation at $\alpha_{cond} \simeq 9.55$ : Kauzmann transition

SAT-UNSAT: $\alpha_c \simeq 9.93$

Algorithms:

- Monte Carlo
- Focused random walk
- Message Passing

# Technique: Cavity Method (Mean Field) = Message Passing algorithms Applications to many problems: graphical models

$$P(x_1, ..., x_N) = C \prod_{a=1}^{M} \psi_a(X_a)$$

$$X_a = \{x_{i_1(a)}, \cdots, x_{i_K(a)}\}$$

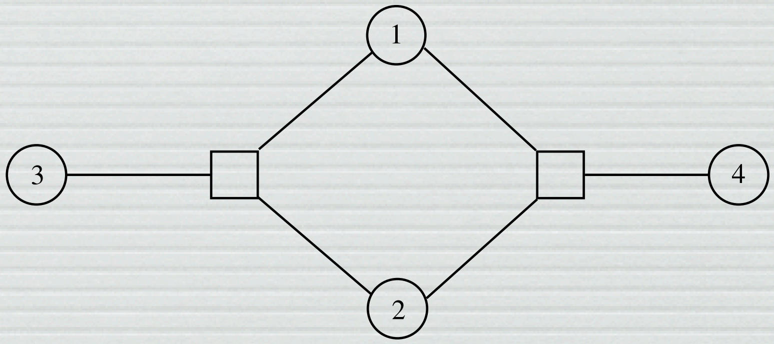
- Satisfiability of Boolean formulas
- Graph coloring
- Decoding in error correcting codes
- Group testing
- Spin glasses
- Learning in neural networks
- ....

# Message passing algorithms

$$P(x_1, ..., x_N) = C \prod_{a=1}^{M} \psi_a(X_a)$$

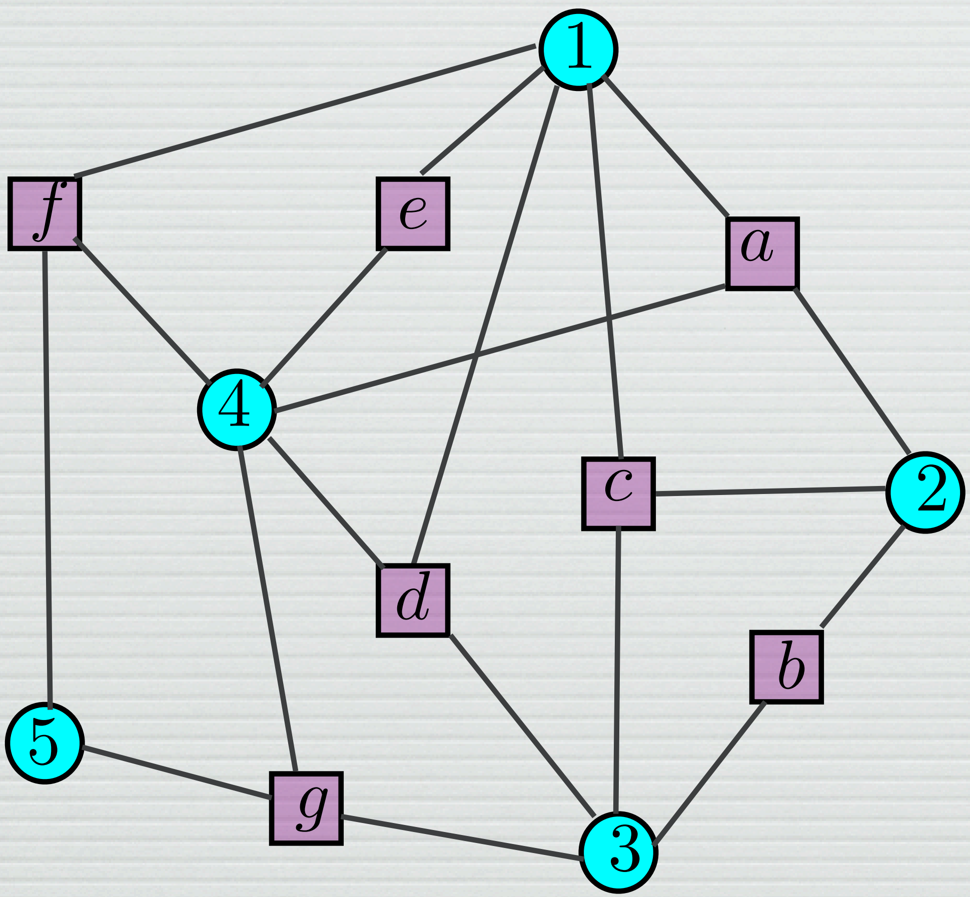
One circle per variable, one square per constraint:

Exchange probabilistic messages along the edges of the 'factor graph':



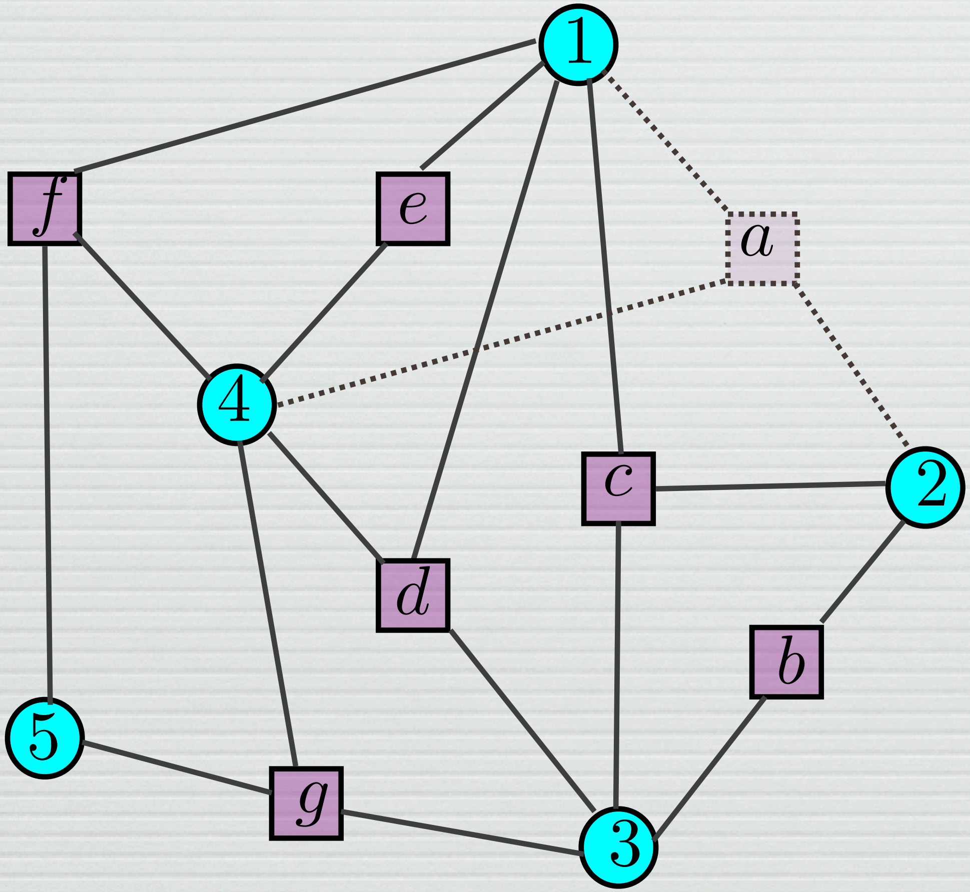

$$(x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_4)$$

# Belief Propagation




$$P(x_1, \cdots, x_5) = \psi_a(x_1, x_2, x_4)\psi_b(x_2, x_3)\cdots$$

# Belief Propagation (cavity equations)

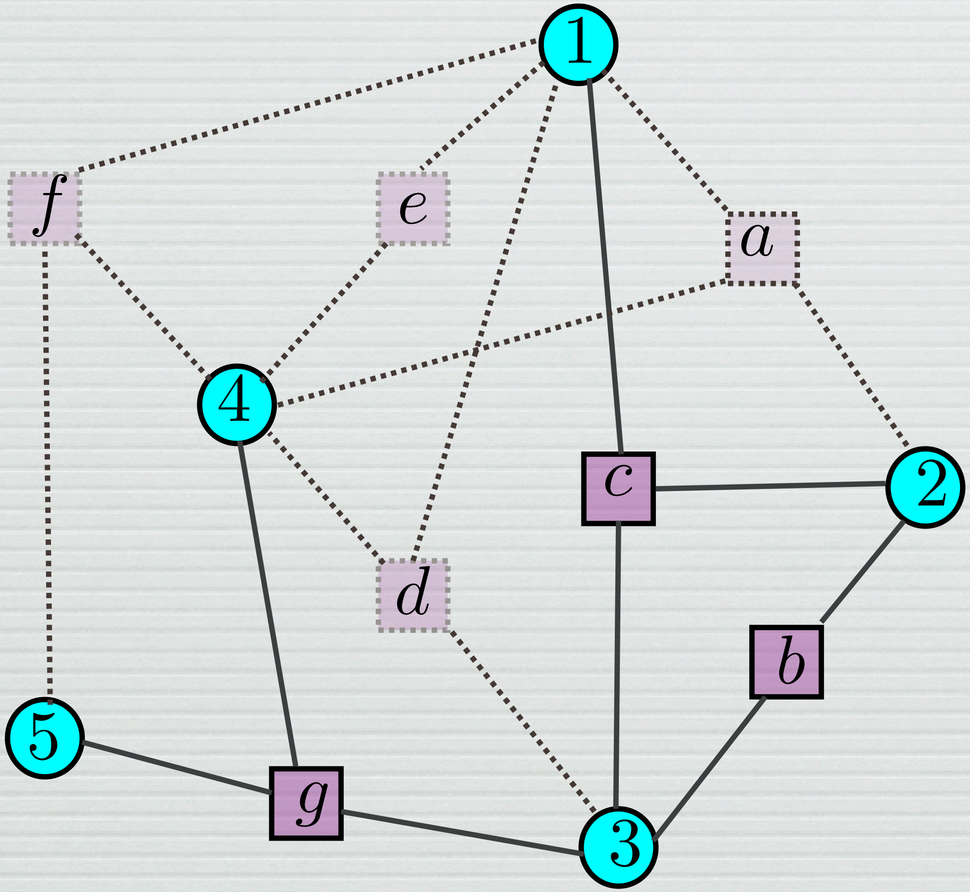



Messages:

Probability of $x_1$ in the absence of a:

$$m_{1\to a}(x_1)$$

# Belief Propagation (cavity equations)

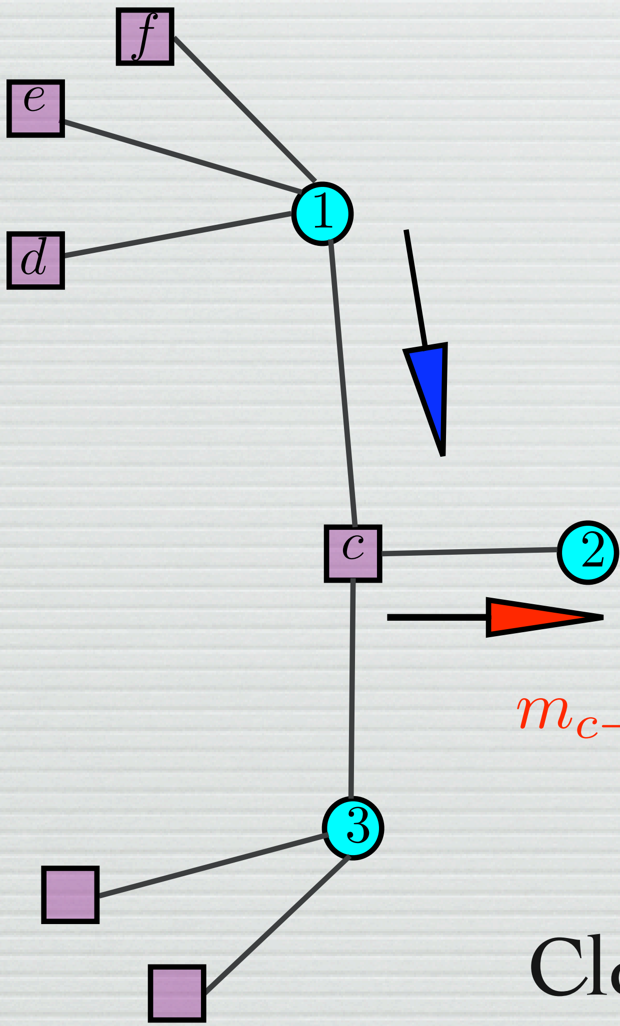



Messages:

Probability of $x_1$ when it is connected only to $c$ :

$$m_{c\to 1}(x_1)$$

# Belief Propagation (Bethe-Peierls, Gallager, Pearl, cavity equations)



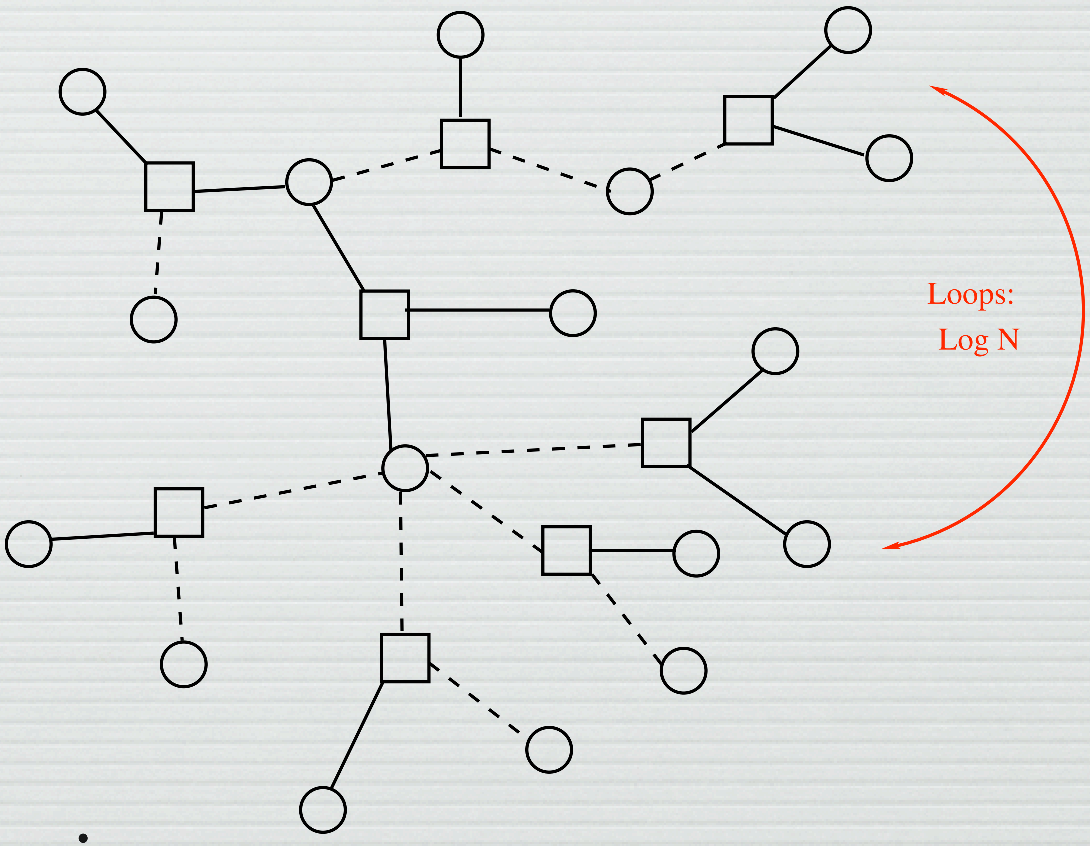

$$m_{1\to c}(x_1) = C m_{d\to 1}(x_1) m_{e\to 1}(x_1) m_{f\to 1}(x_1)$$

$$m_{c\to 2}(x_2) = \sum_{x_1,x_3} \psi_c(x_1,x_2,x_3) m_{1\to c}(x_1) m_{3\to c}(x_3)$$

Closed set of equations: two messages "propagate" on each edge of the factor graph.

# Belief Propagation validity

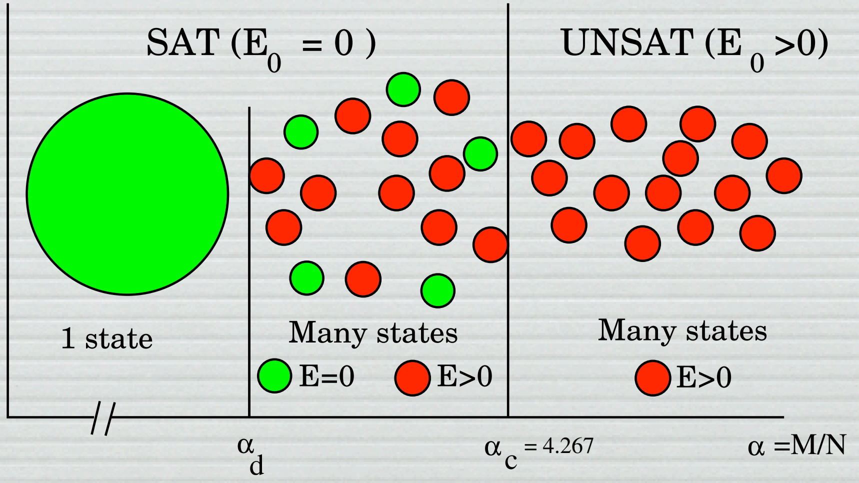
Factor graph of random 3-SAT: not a tree, but "locally tree-like"



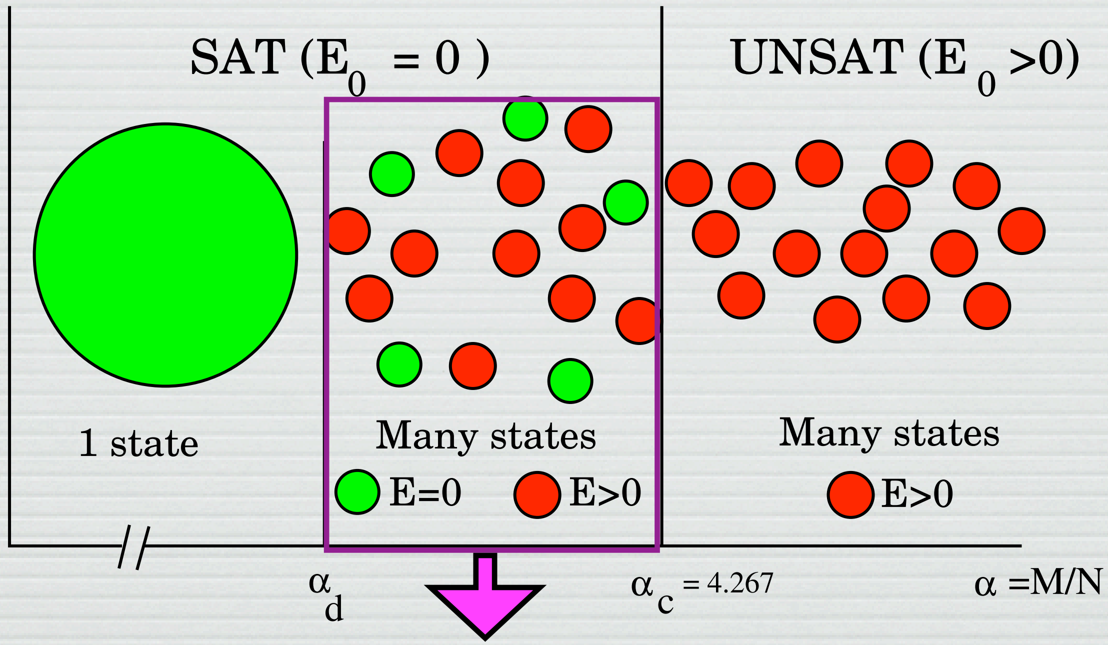

BP is valid if the correlation between two variables decay at large distance. OK in the "easy-SAT" phase

BP: unique solution when

$M/N < \alpha_d$



# Hard-SAT phase: Survey Propagation




Glass phase: many clusters.

Each cluster $\mu$ $\longleftrightarrow$ one solution of the BP equations

$$m^{\mu}_{c\to 2}(x_2) = \sum_{x_1,x_3} \psi_c(x_1,x_2,x_3) m^{\mu}_{1\to c}(x_1) m^{\mu}_{3\to c}(x_3)$$

# Survey Propagation =(Belief Propagation)$^2$

Glass phase: many clusters.

Each cluster $\mu \longleftrightarrow$ one solution of the BP equations

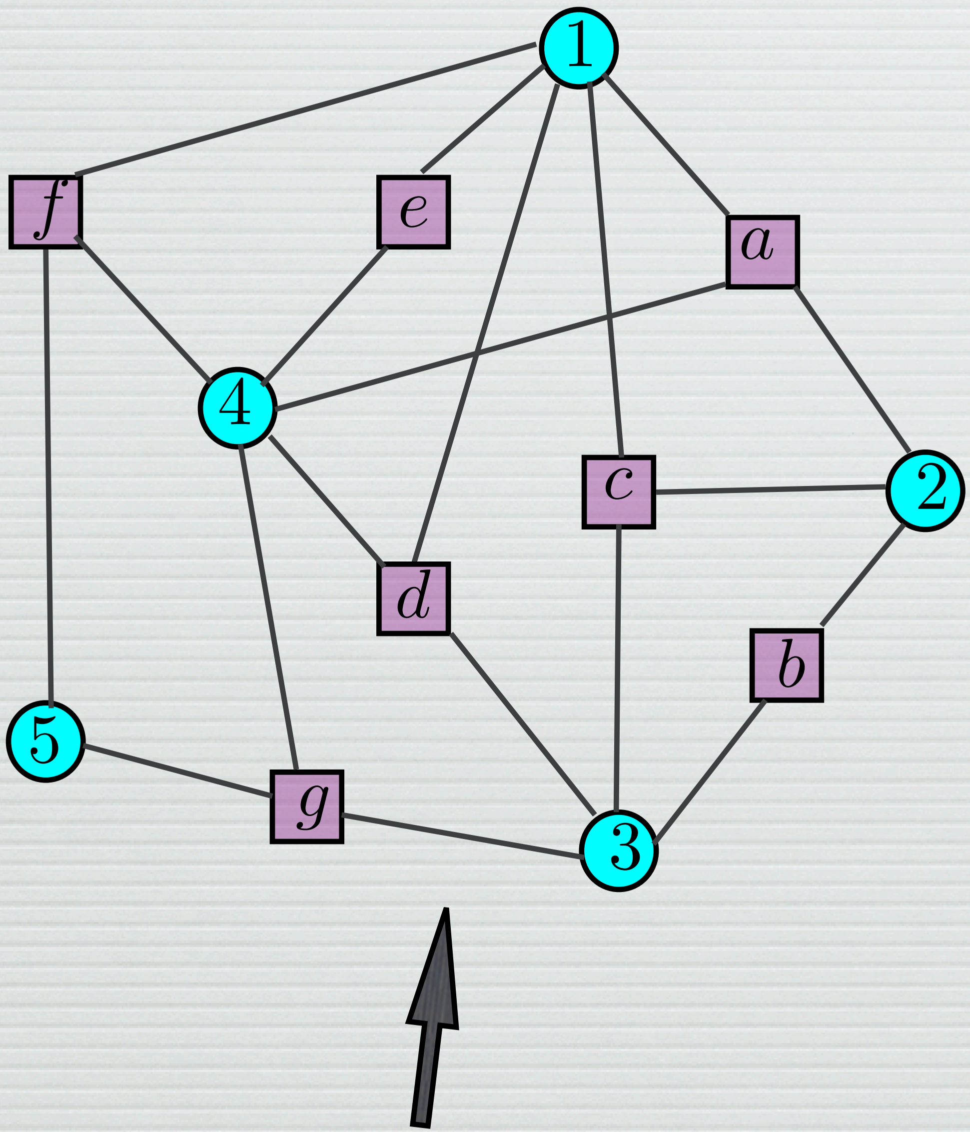
$$m^{\mu}_{c\to 2}(x_2) = \sum_{x_1,x_3} \psi_c(x_1,x_2,x_3) m^{\mu}_{1\to c}(x_1) m^{\mu}_{3\to c}(x_3)$$

Statistical physics over the clusters, i.e. the solutions of BP equations

$$P(\{m_{a\to i}\}\{m_{j\to b}\}) = \frac{1}{Z} \prod_{ai} \mathbb{I}(m_{a\to i} = f(\{m_{j\to a}\}) \prod_{jb} \mathbb{I}(m_{j\to b} = f(\{m_{c\to j}\})$$

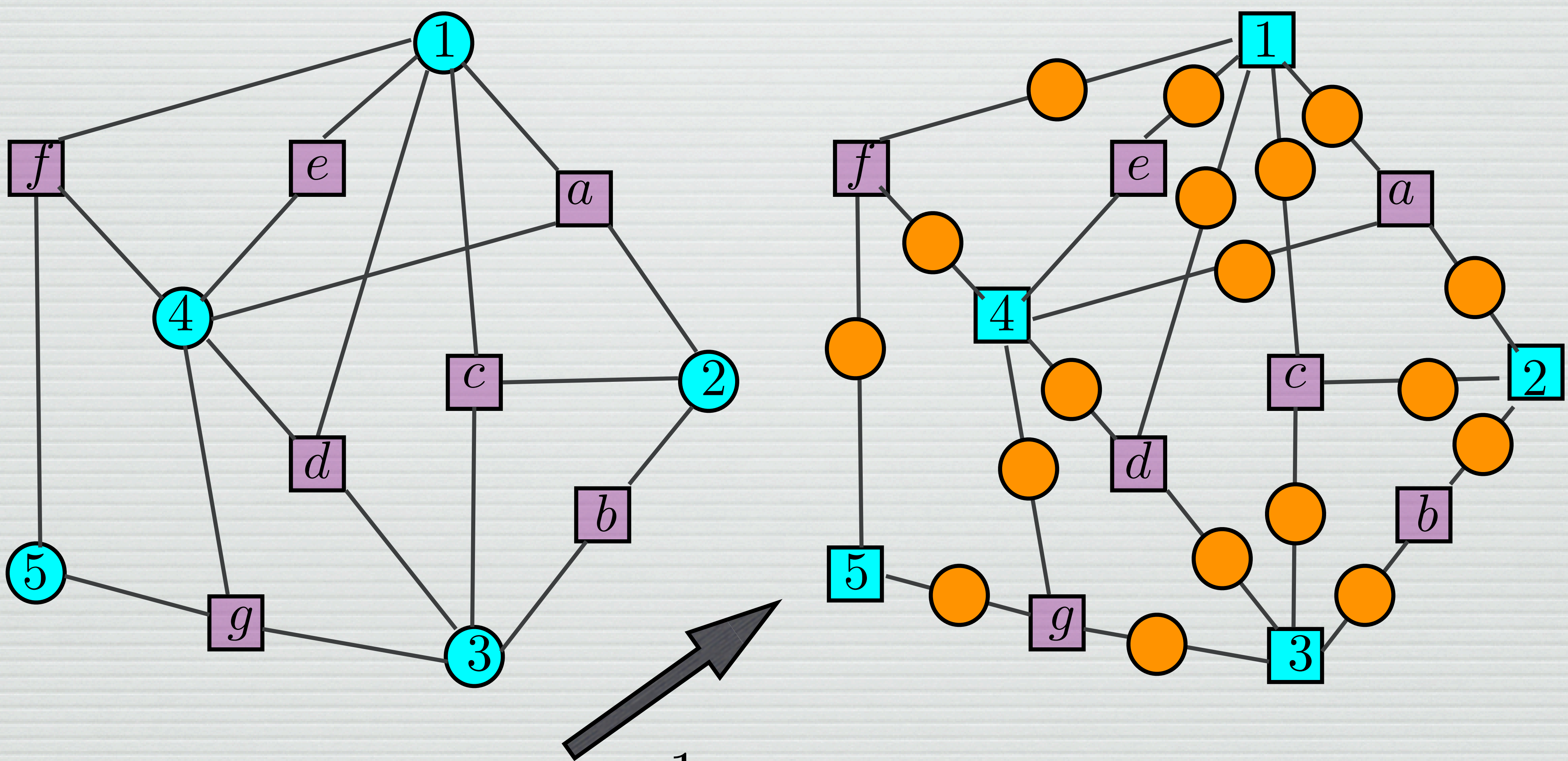
New graphical model, with local factors! Use BP on it (use BP to count the number of solutions of BP eqns (=1 step RSB cavity method = survey propagation)).

SP=BP $^2$




$$P(x_1, \cdots, x_5) = \psi_a(x_1, x_2, x_4)\psi_b(x_2, x_3)\cdots$$

# SP=BP$^2$



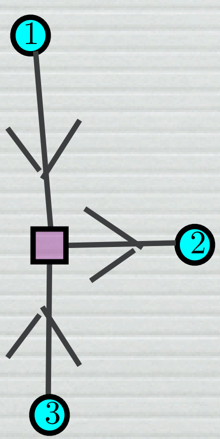

$$P(\{m_{a\to i}\}\{m_{j\to b}\}) = \frac{1}{Z}\prod_{ai}\mathbb{I}(m_{a\to i} = f(\{m_{j\to a}\})$$

$$\prod_{jb}\mathbb{I}(m_{j\to b} = f(\{m_{c\to j}\})$$

# Survey Propagation results

Statistical analysis of SP messages ➡ Phase diagram (SAT-UNSAT threshold)

SP can be used as an algorithm, with decimation: find the most polarized variable (on average over all clusters of solutions), fix it, reduce the problem, iterate... Best algorithm for finding SAT assignments in the hard SAT phase: solves problems with $N = 10^7$ at $\alpha = M/N = 4.25$



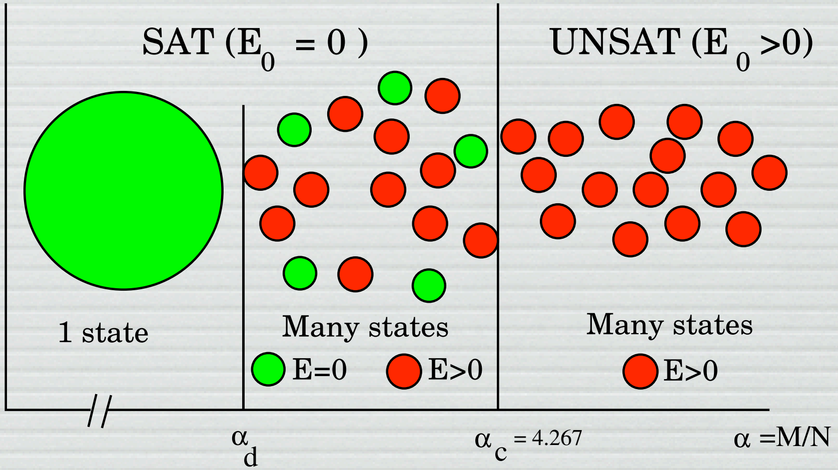

Local, simple update equations: Each message is updated using information from incoming messages on the same node. Distributed, solves hard global pb

# Survey Propagation results

Statistical analysis of SP messages ➡ Phase diagram (SAT-UNSAT threshold)

SP can be used as an algorithm in the hard-SAT phase

Existence of two SAT phases:



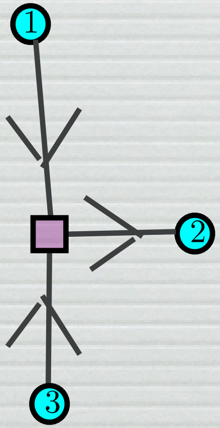

Mathematical status of phase diagram and threshold computation?... "Educated conjecture" +:

1) SP works   2) Existence of clustered phase proven
3)solvable cases where it can be checked (XORSAT)

# Power of message passing algorithms

Approximate solution of very hard, and very large constraint satisfaction problems, ...FAST! (typically linear time)

- BP: Best decoders for LDPC error correcting codes
- SP: Best solver of random Satisfiability problems
- BP: Best algorithm for learning patterns in neural networks (e.g. binary perceptron)
- Data clustering, graph coloring, Steiner trees, etc...




Local, simple update equations: Each message is updated using information from incoming messages on the same node. Distributed, solves hard global pb

# Conclusions

- The core NP-complete problem, satisfiability, displays several phase transitions. Ideal glass transition: clustered phase below the SAT-UNSAT transition
- True in many other problems (error correcting codes, graph colouring, etc...)
- Glass-theory methods and concepts are particularly useful. E.g. message passing algorithms (cavity method): best satisfiability solvers close to the SAT-UNSAT transition

- Very powerful message passing algorithms
- Appealing feature: simple local exchange of information.

# Conclusions

Glasses are everywhere! Even in the software. Unexpected applications of (spin) glass theory

***THE END!***

References available on my web page