

Statistical Physics  
and  
Random Combinatorial  
Optimization

Rémi Monasson

Ecole Normale Supérieure, Paris

<http://www.lpt.ens.fr/~monasson>

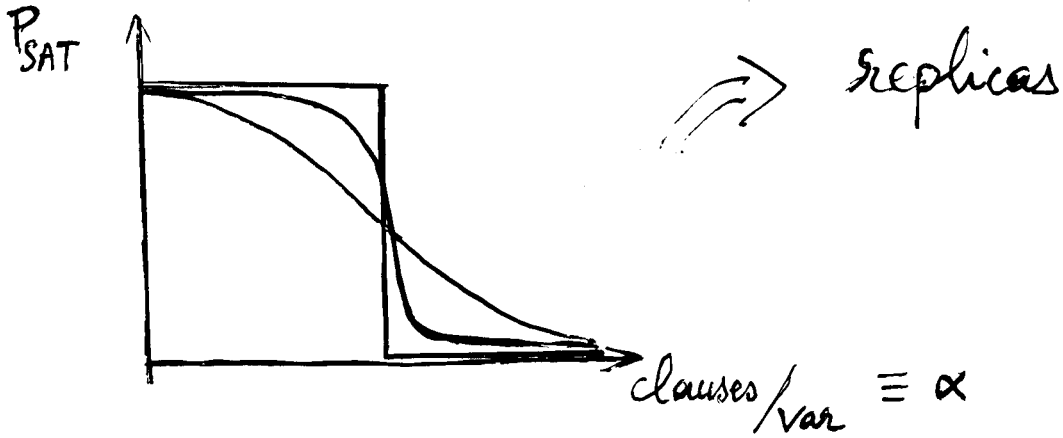
IFAM meeting on

"Phase transitions and Algorithmic Complexity"

June 3 - June 5, 2002.

# Introduction

"Phase transitions ...



from 1984 :

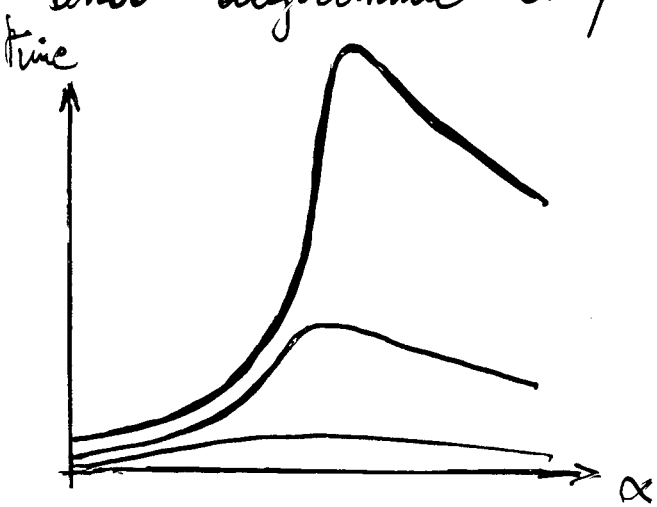
Mézard, Parisi, Vannimenus, Orland  
 Mézard, Parisi, Krauth  
 Fu, Anderson, De Dominicis,  
 ...

TSP  
 Matching  
 Graph partitioning  
 ...

Mertens, Fontanari  
 Weigt, Hartmann  
 R.M., Zecchina, Kirkpatrick, Selman

NPP  
 Vertex cover  
 K-SAT

and algorithmic complexity "



analysis of algorithms  
 = induced dynamics  
 ≠ usual physical dynamics

out-of-equilibrium  
 statistical physics

# Random 3-XORSAT

S. Cecco  
O. Dubois  
J. Mandler

$N$  Boolean variables  $x_i = 0, 1$

$M$  clauses:  $\begin{cases} i_m < j_m < k_m & (m=1, \dots, M) \\ v_m = 0, 1 & \text{prob } 1/2, 1/2 \end{cases}$

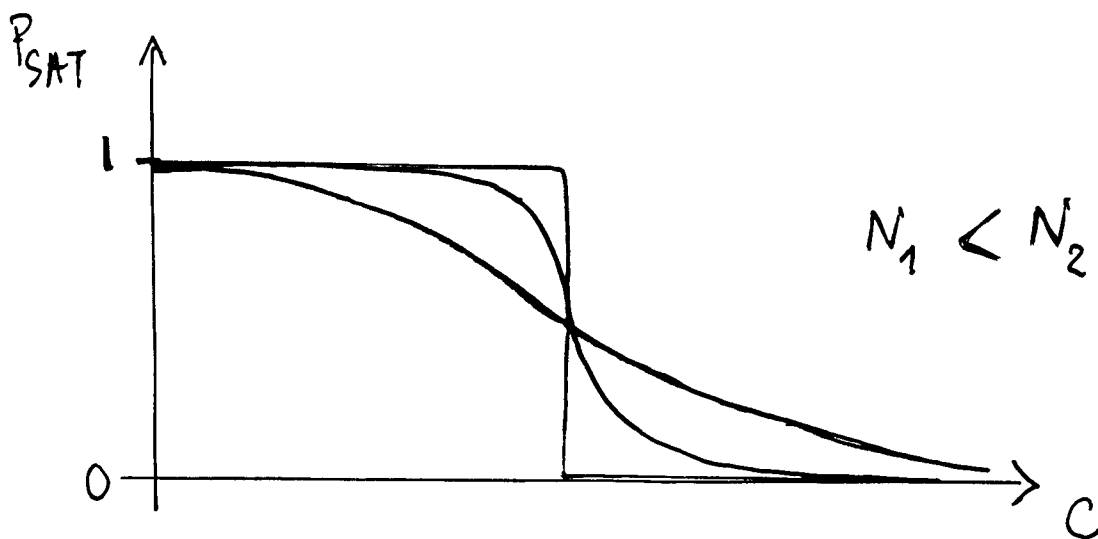
$$x_{i_m} + x_{j_m} + x_{k_m} = v_m \quad (\forall m)$$

- Computationally easy (P)

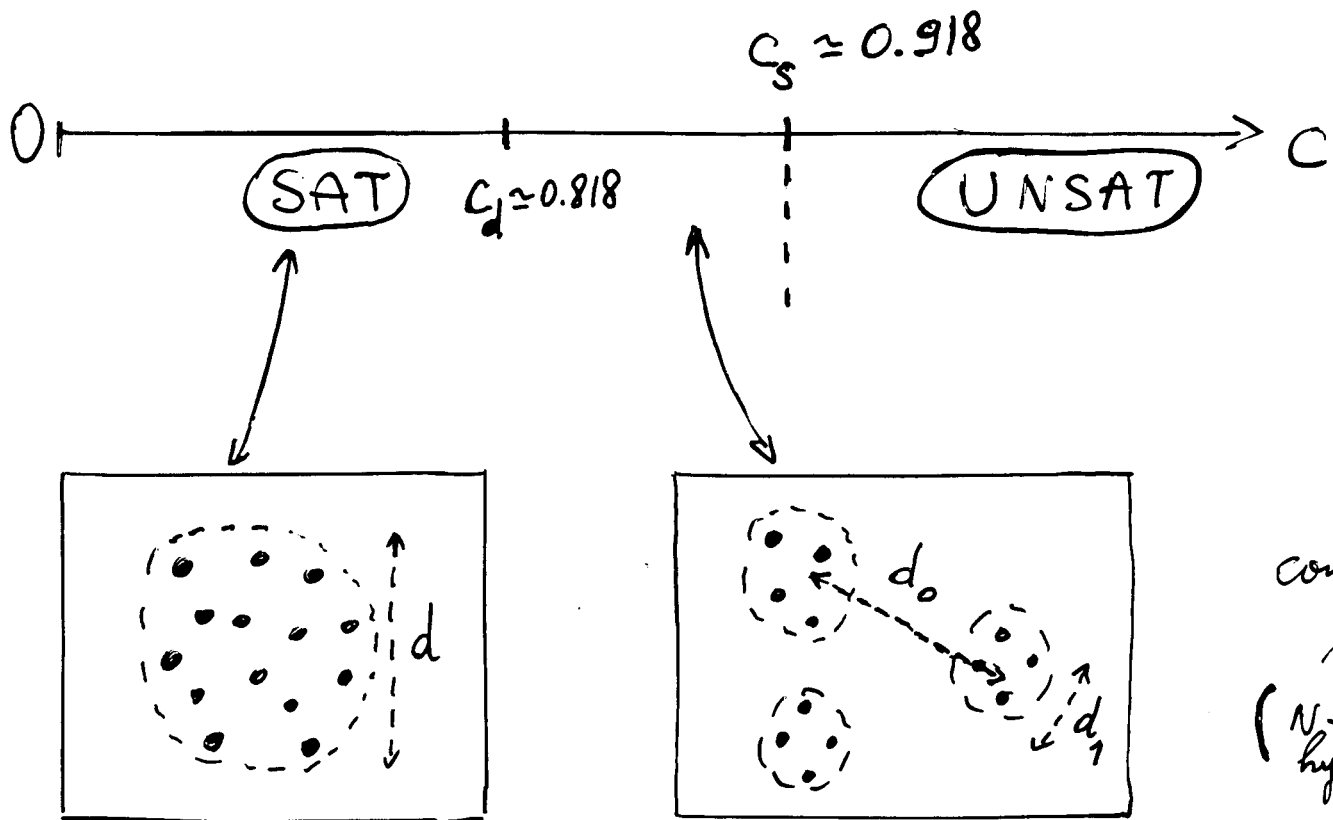
- SAT vs. UNSAT ?

→ same phenomenology as Random 3-SAT

$$c = \frac{M}{N}$$



# Random 3-XORSAT: Results



$2^{Ns}$  solutions

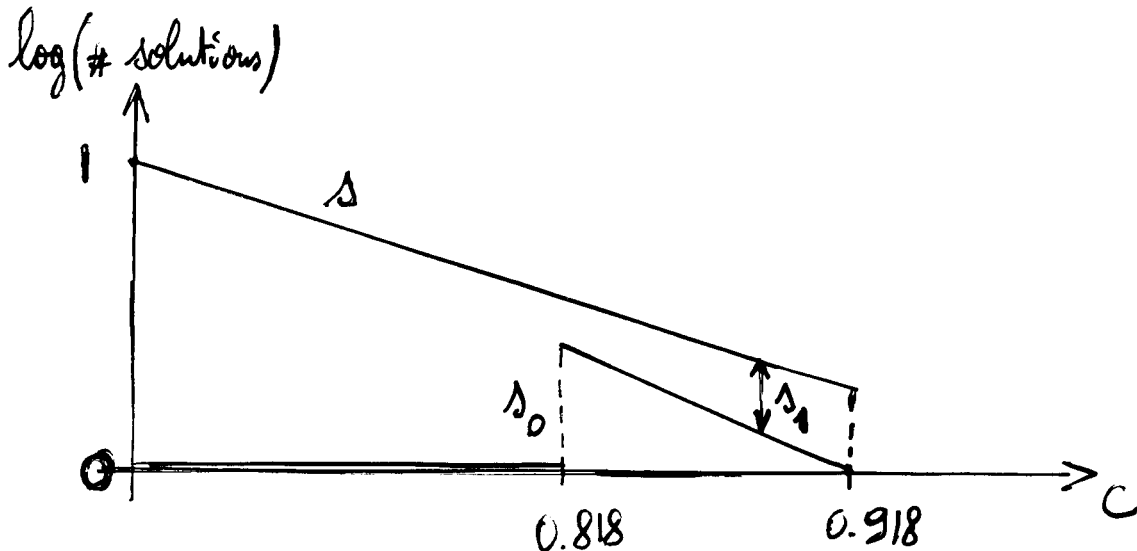
$$s = 1 - c$$

$$d = \frac{1}{2}$$

$2^{Ns_0}$  clusters with  
 $2^{Ns_1}$  solutions each

$$s_0 + s_1 = 1 - c$$

$$d_0 = \frac{1}{2}, \quad d_1 \ll \frac{1}{2}$$



# Replica approach (I)

$$\mathcal{N} = \sum_{\{x_i=0,1\}} \prod_{l=1}^M \mathbb{1}_{x_{il} + x_{jl} + x_{kl} = v_l}$$

$\uparrow$   
 # solutions

$\underbrace{\hspace{10em}}_{\text{instance}}$

Compute moments of  $\mathcal{N}$  ....

$$\bullet E(\mathcal{N}) = \sum_{\{x_i=0,1\}} E \left( \prod_{l=1}^M \mathbb{1}_{x_{il} + x_{jl} + x_{kl} = v_l} \right)$$

$$\underbrace{\hspace{15em}}_{\prod_{l=1}^M E \left( \mathbb{1}_{x_{il} + x_{jl} + x_{kl} = v_l} \right)}$$

$$\left[ E \left( \mathbb{1}_{x_i + x_j + x_k = v} \right) \right]^M$$

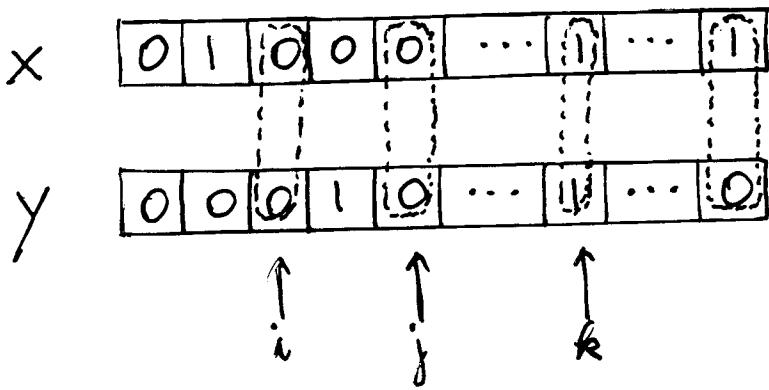
$$= \sum_{\{x_i=0,1\}} \left[ \underbrace{\frac{1}{\binom{N}{3}} \sum_{i < j < k} \frac{1}{2} \sum_{v=0,1} \mathbb{1}_{x_i + x_j + x_k = v}}_{\frac{1}{2}} \right]^M$$

$$= 2^N \cdot \left( \frac{1}{2} \right)^M = 2^{N(1-c)}$$

$c_i = 1$  (upper bound)

# Replica approach (II)

$$\begin{aligned}
 E(\mathcal{N}^2) &= E \left( \left[ \sum_{\{x_i=0,1\}} \prod_{\ell=1}^M \mathbb{1}_{x_{i\ell} + x_{j\ell} + x_{k\ell} = v_\ell} \right]^2 \right) \\
 &= E \left( \sum_{\{x_i=0,1\}} \sum_{\{y_i=0,1\}} \prod_{\ell=1}^M \mathbb{1}_{x_{i\ell} + x_{j\ell} + x_{k\ell} = v_\ell} \prod_{\ell=1}^M \mathbb{1}_{y_{i\ell} + y_{j\ell} + y_{k\ell} = v_\ell} \right) \\
 &= \sum_{\{x_i=0,1\}} \sum_{\{y_i=0,1\}} \left\{ E \left( \mathbb{1}_{x_i + x_j + x_k = v} \mathbb{1}_{y_i + y_j + y_k = v} \right) \right\}^M \\
 &= \frac{1}{2} E \left( \mathbb{1}_{x_i + x_j + x_k = y_i + y_j + y_k} \right)
 \end{aligned}$$



$\approx$  depends upon  
 Hamming distance  
 $0 \leq d \leq 1$

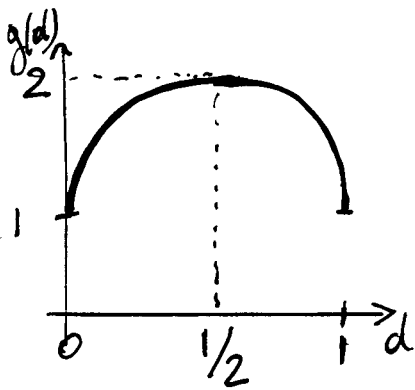
$$\begin{aligned}
 &= \sum_{\{x_i=0,1\}} \sum_{\{y_i=0,1\}} \left\{ \frac{1}{4} \left( 1 - (2d(x,y) - 1)^3 \right) \right\}^M \\
 &= 2^N \sum_{\{y_i=0,1\}} \left[ \frac{1}{4} \left( 1 - (2d(0,y) - 1)^3 \right) \right]^M
 \end{aligned}$$

$$= 2^N \sum_{d=0, \frac{1}{N}, \dots, 1} \left( \frac{1 - (2d-1)^3}{4} \right)^M \mathcal{E}(d)$$

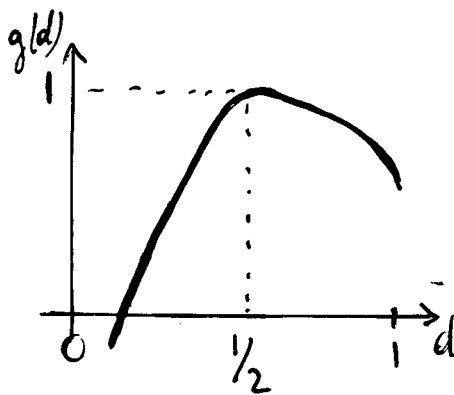
$$\mathcal{E}(d) = \# \text{ configurations at distance } d \text{ from } (0, 0, \dots, 0) = \binom{N}{Nd}$$

$$E(W^2) = \sum_{d=0, \frac{1}{N}, \dots, 1} 2^N g(d)$$

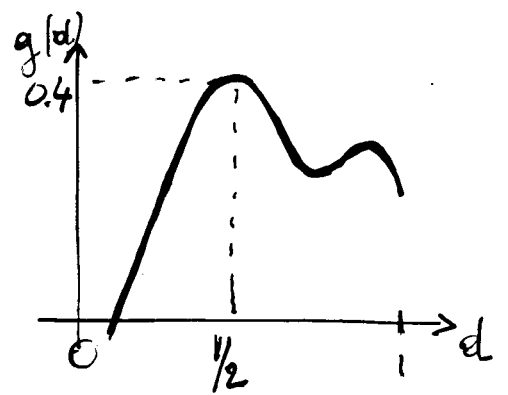
$$g(d) = 1 + c \cdot \log_2 \left( \frac{1 - (2d-1)^3}{4} \right) - (1-d) \log_2 (1-d) - d \log_2 d + o(1)$$



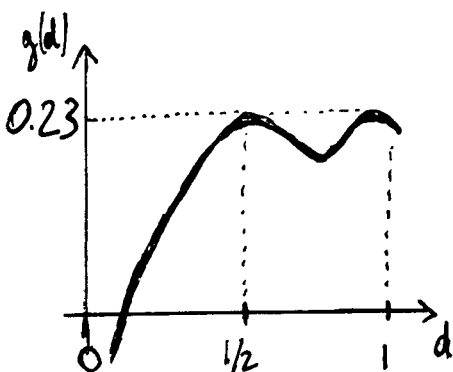
$$c = 0$$



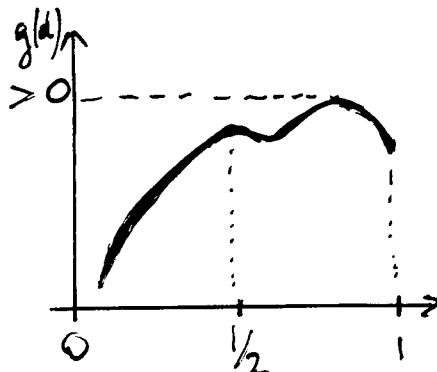
$$c = 1/2$$



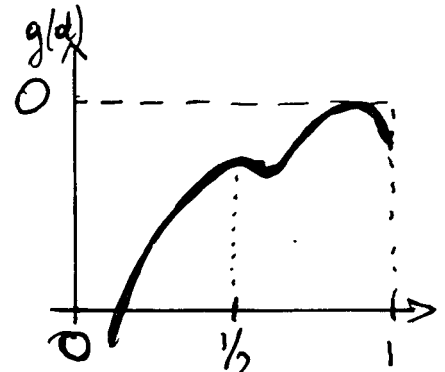
$$c = 0.8$$



$$c = 0.889$$

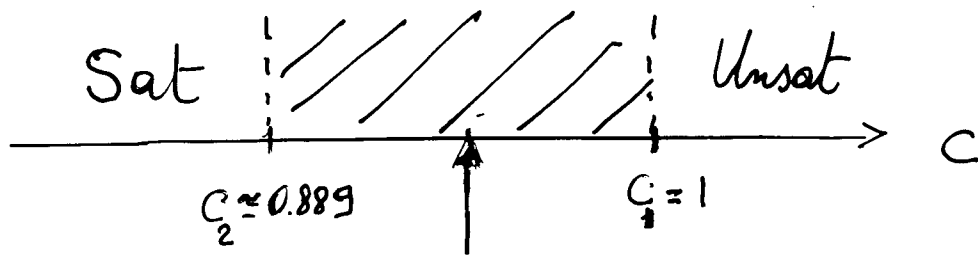


$$c = 0.95$$



$$c = 1.06$$

# 1<sup>st</sup> and 2<sup>nd</sup> moments methods



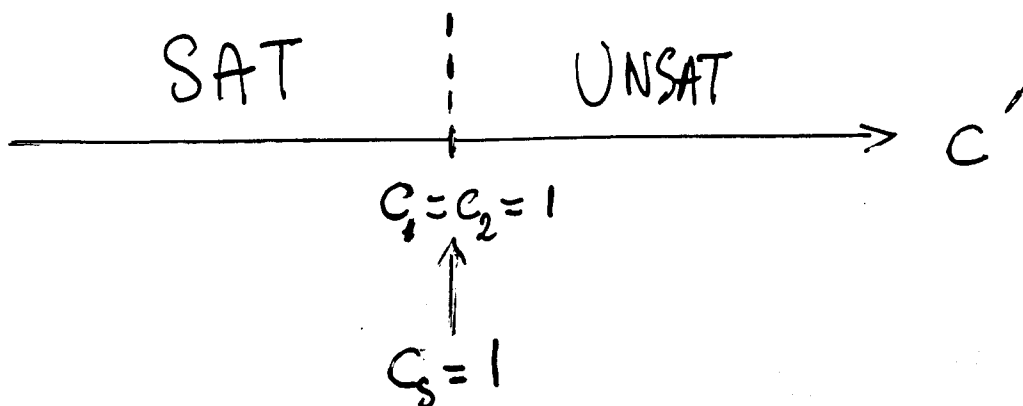
"Random  
3-XORSAT"  
ensemble

Dubois, Mandler  
Cocco, R.M.



pure variable  
algorithm

"Constrained  
Random 3-XORSAT"  
ensemble

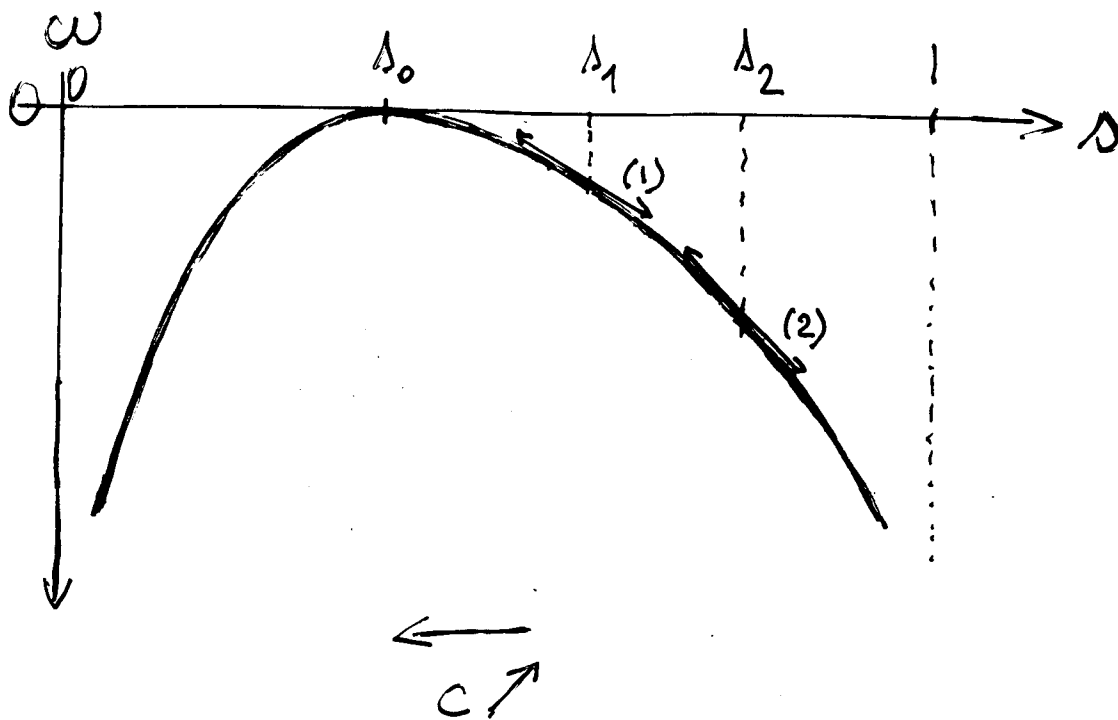




# Replicas and Large deviations

$$\mathcal{N}^q = 2^{N s}$$

$$\mathcal{P}(\mathcal{N}^q) = 2^{N \omega(s)}$$



$$E(\mathcal{N}^q) = \sum_{\mathcal{N}^q=1}^{2^N} \mathcal{P}(\mathcal{N}^q) \mathcal{N}^q$$
$$\sim \int_0^1 ds \, 2^{N(\omega(s) + q s)}$$

Laplace method: maximize:  $\omega(s) + q s (= g(q))$

$$\left. \frac{\partial \omega}{\partial s} \right|_{s^*} = -q$$

Typical case:  $q \rightarrow 0$

# Calculation of $E(W^q)$

•  $E(W^1)$  : immediate

•  $E(W^{p^2})$  :  $\{x^1, x^2\} \rightarrow d(x^1, x^2) = d^{1^2}$

....

•  $E(W^{p^q})$  :  $\{x^1, x^2, \dots, x^q\} \rightarrow \begin{cases} d(x^a, x^b) = d^{ab} \\ d(x^a, x^b, x^c) = d^{abc} \\ d(x^a, x^b, x^c, x^d) = d^{abcd} \\ \dots \end{cases}$

$2^q - q - 1$  order parameters

① maximize  $g[d^{ab}, d^{abc}, d^{abcd}, \dots]$



$$\frac{\partial g}{\partial d^{a_1 \dots a_l}} = 0, \quad 2 \leq l \leq q$$

② get  $g(q)$ , then  $\omega(s) = \min_q [g(q) - qs]$   
and  $s_0 = \left. \frac{dg}{dq} \right|_{q \rightarrow 0}$



\*  $q$  integer-valued, then  $q \rightarrow 0$ .

\*  $E(W^q) \leq (2^N)^q \rightarrow$  moment theorem applies

but here  $N \rightarrow \infty$  first,  $q \rightarrow 0$  next

$\Rightarrow$  No unicity of  $q \rightarrow 0$  continuation.

# Replica Symmetric Theory:

Kac (1967) (← Dyson, 1953)

Edwards - Anderson (1974)

Skerrington - Kirkpatrick (1975)

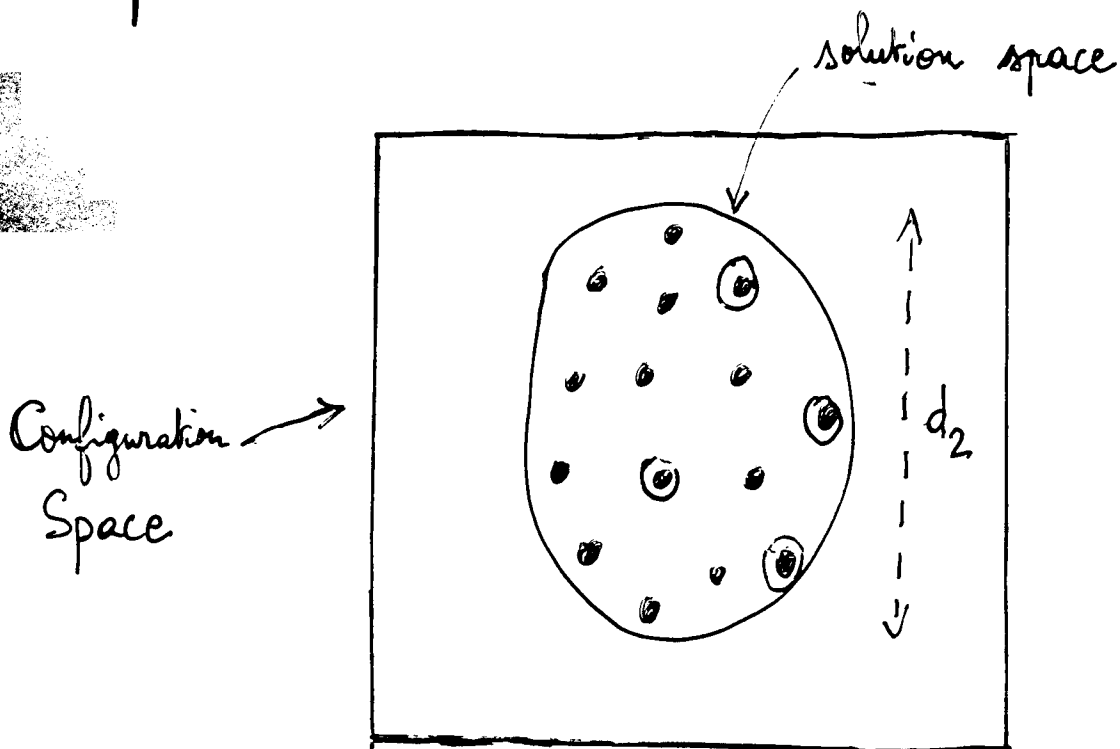
$$\begin{cases} d^{a_1, a_2} = d_2 \\ d^{a_1, a_2, a_3} = d_3 \\ d^{a_1, a_2, a_3, a_4} = d_4 \\ \dots \end{cases}$$

$\forall a_1, a_2, a_3, a_4, \dots$

"replicas cannot be distinguished from each other"

Optimize over  $d_2, d_3, d_4, \dots$   
Then, send  $q \rightarrow 0$ .

Interpretation:



example of  
 $q = 4$   
replicas

# Replica symmetry broken theory

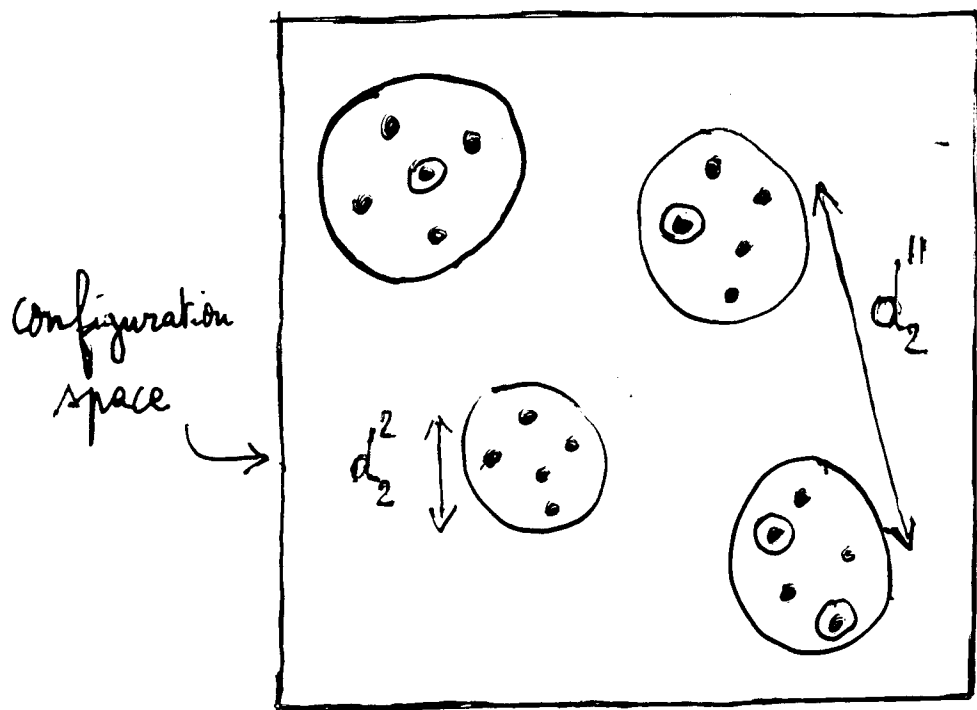
Thouless, Anderson, Palmer 1977

$\Rightarrow$  Parisi 1979, 1980

$$\left\{ \begin{array}{l} d^{a_1, a_2} = d_2^{11}, d_2^2 \\ d^{a_1, a_2, a_3} = d_3^{111}, d_3^{21}, d_3^3 \\ d^{a_1, a_2, a_3, a_4} = d_4^{1111}, d_4^{211}, d_4^{22}, d_4^{31}, d_4^4 \\ \dots \end{array} \right.$$

$\Uparrow \Downarrow d^{a_1, a_2, \dots, a_l}$  has as many values as the number of partitions of  $l$ .

Interpretation:



example of  
 $q = 4$   
 replicas  
 $\binom{d_2^{11}}{4}$

higher levels  
 of symmetry  
 breaking ...

# Replica predictions for 3-XORSAT

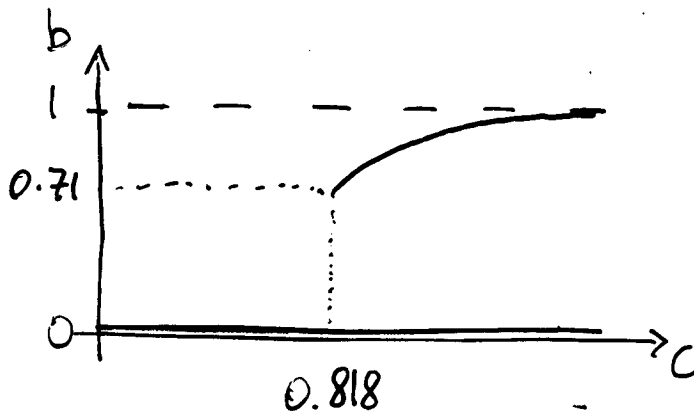
Franz, Ricci, Leone,  
Weigt, Zecchina (2001)

$$\begin{cases} \Delta_0 = b - 3cb^2 + 2cb^3 & (\log \# \text{ clusters}) \\ \Delta_1 = 1 - c - \Delta_0 & (\log \# \text{ solutions in each cluster}) \end{cases}$$

with:

$$b = 1 - e^{-3cb^2}$$

local backbone (in a cluster)



$$\rightarrow \begin{cases} d_2' = \frac{1-b}{2} \\ d_2'' = \frac{1}{2} \end{cases}$$

Hand-waving argument

variable  $x$   $\begin{cases} x + \dots + \dots = \dots \\ x + \dots + \dots = \dots \\ x + \dots + \dots = \dots \end{cases}$

$$1-b = \sum_{l=0}^{\infty} e^{-3c} \frac{(3c)^l}{l!} (1-b^2)^l$$

↑  
proba( $x$  free)

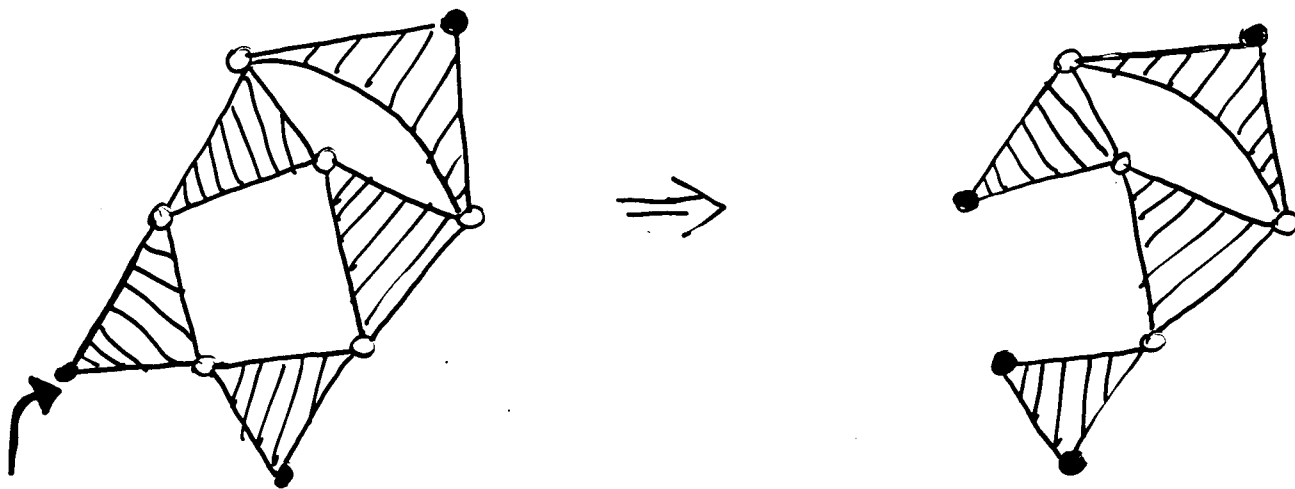
# "Pure Variable" algorithm

Broder et al. 1983

Franco 1980's

Pittel, Spencer, Wormald 1996

= 2-core percolation on hypergraphs



after  $T$  steps (removals) :

- $N_\ell(T) = \#$  variables with  $\ell$  occurrences
- $M(T) = M - T = \#$  clauses

$$E(N_\ell(T+1) - N_\ell(T) | \mathcal{H}) = -\mathbb{1}_{\ell,1} + \mathbb{1}_{\ell,0} + 2p_{\ell+1} - 2p_\ell$$

$$p_j = \frac{j E(N_j(T))}{3M(T)}$$

# Analysis of the algorithm

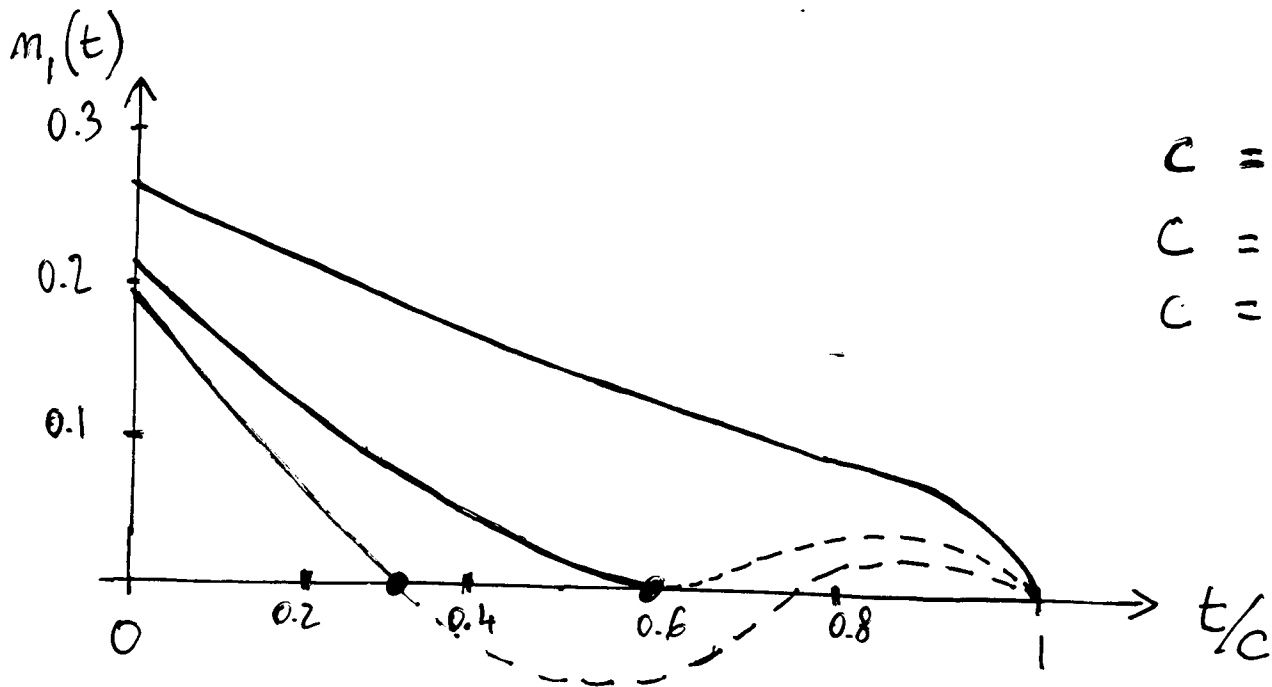
$$N_e(T) \rightarrow N. n_e(t = \frac{T}{N})$$

$$\begin{cases} \frac{dn_e}{dt} = \frac{2}{3(c-t)} \left( (l+1)n_{l+1} - l n_l \right) - \mathbb{1}_{l,1} + \mathbb{1}_{l,0} \\ n_e(0) = e^{-3c} \frac{(3c)^e}{e!} \end{cases}$$

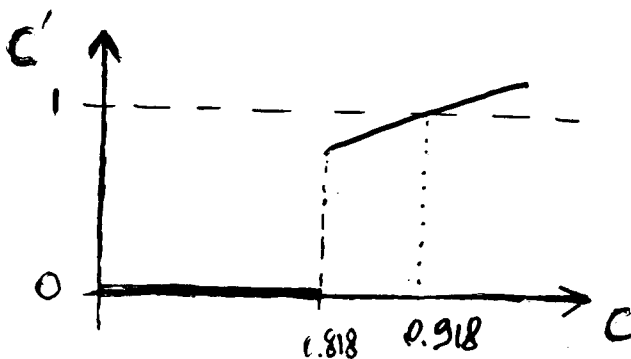
Solution:

$$\begin{cases} n_1(t) = 3cb(t)^2 \left( e^{-3cb(t)^2} + b(t) - 1 \right) \\ n_l(t) = e^{-3cb(t)^2} \frac{(3cb(t)^2)^l}{l!} \quad (l \geq 2) \end{cases}$$

where  $b(t) = \left(1 - \frac{t}{c}\right)^{1/3}$



$$\begin{aligned} c &= 0.7 \\ c &= 0.818 \\ c &= 0.9 \end{aligned}$$



# Constrained random 3-XORSAT

$$\mathcal{F} \longrightarrow \mathcal{F}' \subset \mathcal{F}$$

↑  
each variable appears at least twice.

$$c' = \frac{M'}{N'}$$

- $\overline{\mathcal{N}^0} = 2^{N'(1-c')}$

$$\Rightarrow c'_s \leq 1$$

- $\overline{\mathcal{N}^2}$  more complicated but can be done (Dubois, Mandler 2002)

$$\frac{\overline{\mathcal{N}^0}}{\overline{\mathcal{N}^2}} > 0 \text{ if } c < 1 \Rightarrow c'_s \geq 1$$

$$c'_s = 1$$

- solutions of  $\mathcal{F}'$ :

$$d_0 = \frac{1}{2}$$

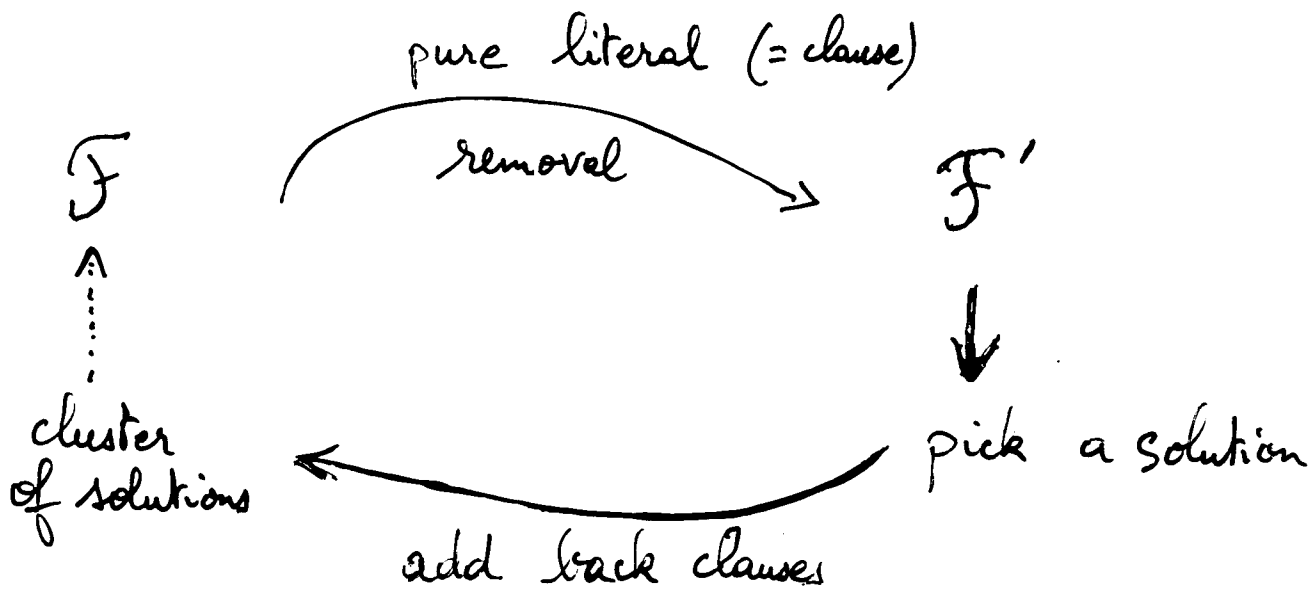
$$\begin{aligned} \lambda_0 &= \log_2 \overline{\mathcal{N}^0} = 1 - c' \\ &= b - 2cb^2 + 3cb^3 \end{aligned}$$



clusters!



# Reconstructing solutions



solution of  $F'$  + clause  $(x + y + z)$

pure literal

A dashed arrow points from the text "solution of  $F'$  + clause  $(x + y + z)$ " to the clause  $(x + y + z)$ . Another dashed arrow points from the clause  $(x + y + z)$  to the label "pure literal".

$$d_1 = 2 \int_0^{t_{\text{stop}}} dz p_1(z) + e^{-3c}$$

variables that never appear

The equation shows the relationship between  $d_1$ , an integral of  $p_1(z)$  from 0 to  $t_{\text{stop}}$ , and an exponential term  $e^{-3c}$ . A dashed arrow points from the exponential term to the text "variables that never appear".

1 solution of  $F'$  + frozen var. + free var.

seed of the cluster

backbone  $b$

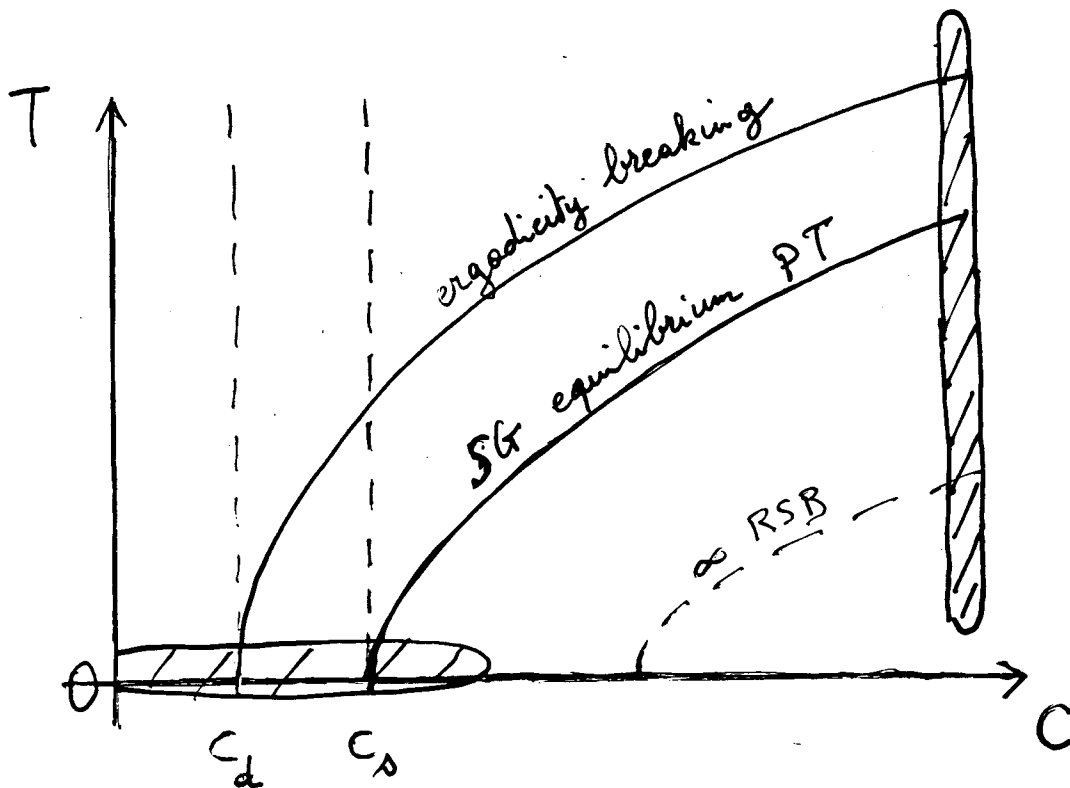
$d_1 = \frac{1-b}{2}$

The text describes the components of the solution: a "seed of the cluster" (1 solution of  $F'$  + frozen var.) and "free var." (free var.). A bracket groups these as the "backbone  $b$ ". An arrow points from this backbone to the equation  $d_1 = \frac{1-b}{2}$ .

# Finite temperature

$\mathcal{F}$   $\longrightarrow$   $\mathcal{F}$   
 + clause with pure literal

$$Z = \Omega^{K-1} (e^{-\beta} + e^{\beta}) \cdot Z'$$



- easy to generalize to larger  $K \geq 4$
- case  $K = 2$ .

