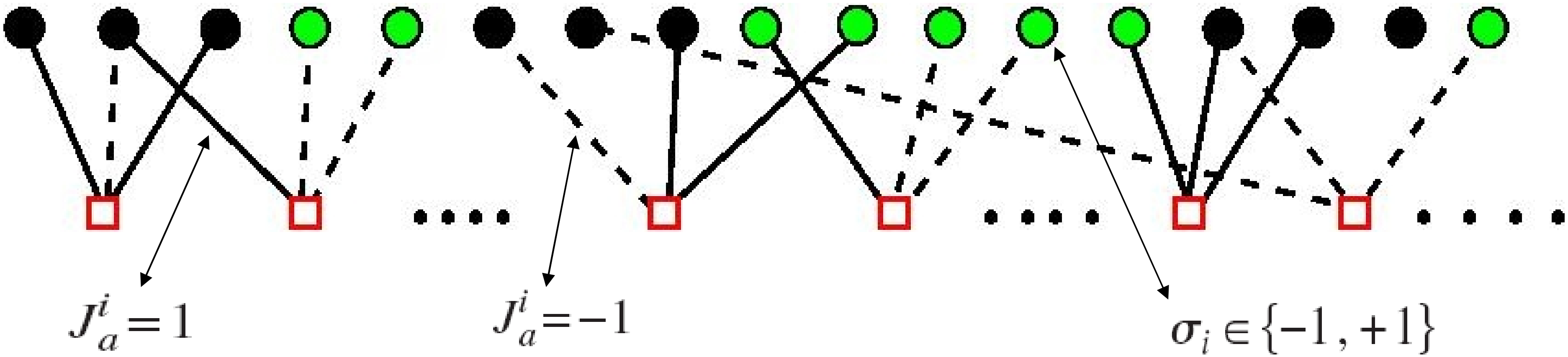
Solution Space Heterogeneity
and
Dynamical Heterogeneity
of
random constraint satisfaction problems

Haijun Zhou
周海军

Institute of Theoretical Physics,
the Chinese Academy of Sciences,
Beijing 100190
中国科学院理论物理研究所

- Background *Random CSPs*, *What are Known*
- Solution Space Heterogeneity *Experiment* & *Theory*
- ☆ Dynamical heterogeneity
- ☆ Search by Random Walking

random constraint satisfaction problems: k-satisfiability



$$E(\sigma_1, \sigma_2, \ldots, \sigma_N) = \sum_{a=1}^{M} \prod_{i \in \partial a} \left(\frac{1 - J_a^i \sigma_i}{2} \right)$$

$\alpha \equiv M/N$

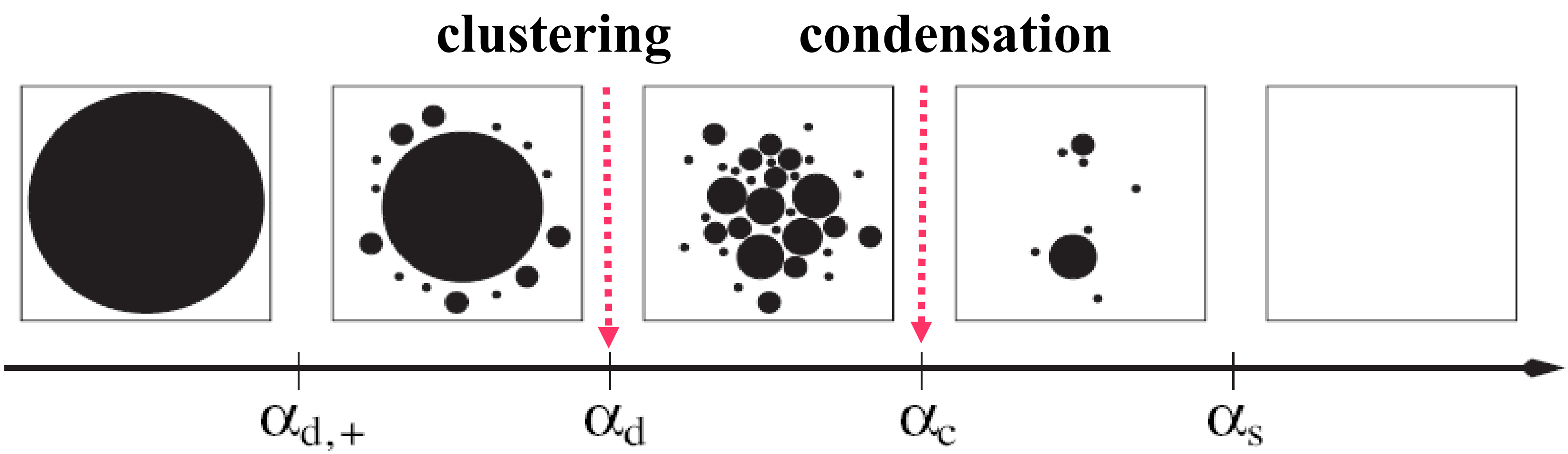
constraint density

K-SAT:
each constraint has K neighbors

K-SAT is the first problem proved to be NP-complete [Cook, 1971]

StatPhys treatment:
Monasson & Zecchina (1996);
Mezard, Parisi, Zecchina (2002)
...
...

solution space phase evolution for random K-SAT



The solution space of a random K-SAT formula contains all the spin configurations of zero total energy

solution clusters have different sizes!

Similar to spin-glasses and structural glasses as function of temperature.

Entropic zero-temperature 1RSB cavity theory

Mezard, Palassini, Rivoire (2005); Krzakala, Montanari, Ricci-Tersenghi, Semerjian, Zdeborova (2007)

Influence to stochastic search:
Krzakala & Kurchan (2007);
Alava, Ardelius, Aurell, Kaski, Krishnamurthy, Orponen, et al. (2008).

Following single Gibbs state with T:
Krzakala & Zdeborova (2009)

random constraint satisfaction problem: K-XORSAT

$$E(\sigma_1, \sigma_2, \ldots, \sigma_N) = \sum_{a=1}^{\alpha N} \frac{1 - J_a \prod_{j \in \partial a} \sigma_j}{2}$$

J_a=+1 or -1 with equal probability

K-XORSAT: each constraint a again has K neighbors

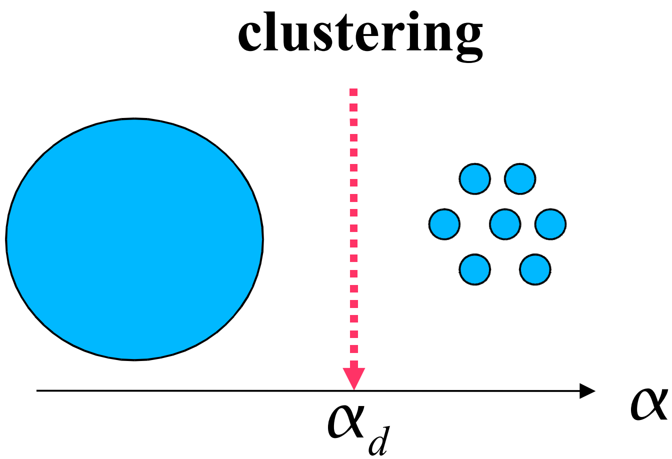
Energy function corresponds to the p-body-interaction spin glass system: → spin glass theory

Deep link to coding systems (e.g., Sourlas code and LDPC codes): → information theory

K-XORSAT as constraint satisfaction is in the class P

StatPhys treatment:
Cocco, Mezard, Monasson, Montanari, Mora, Ricci-Tersenghi, Semerjian, Zecchina, ……

solution space phase evolution for K-XORSAT

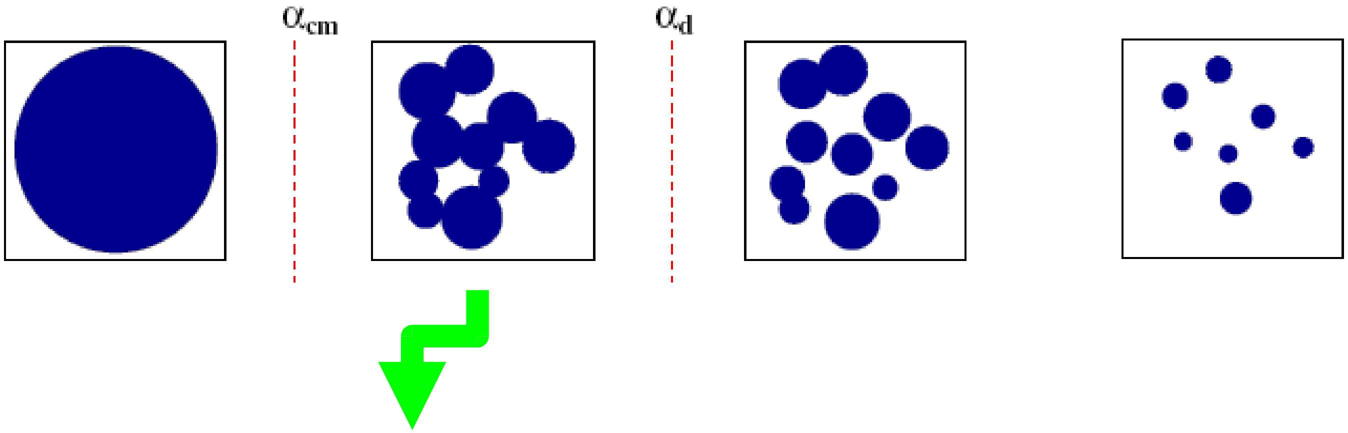


Similarity with K-SAT: there is also a clustering transition

Difference with K-SAT: all solution clusters have the same size

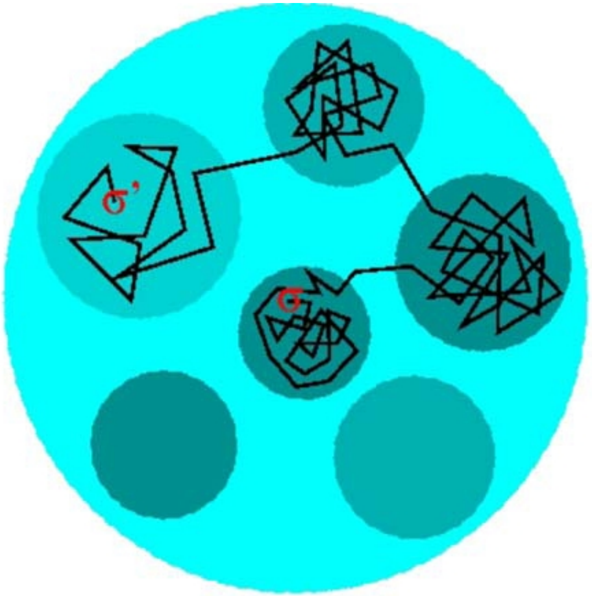
The clustering transition of the solution space at certain critical value of constraint density is a general phenomenon for random CSPs

existence of a heterogeneity transition before clustering



Emergence of many solution communities
in the ergodic solution space

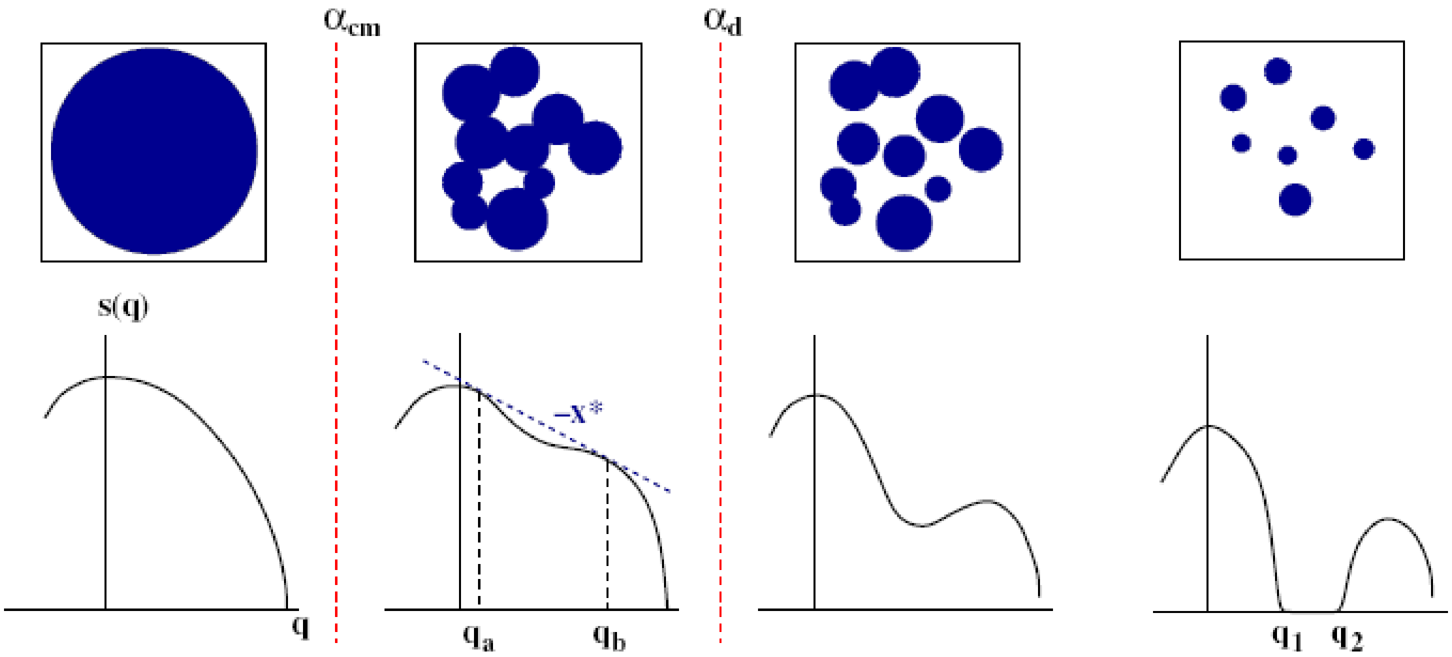
Zhou, Ma (2009), Zhou (2009), Zhou, Wang (2010)



Dynamical consequence:
heterogeneity of diffusion
process at zero-temperature

(Zhou, Wang, 2010)

detecting heterogeneity by measuring solution-pair similarity



$$q(\vec{\sigma}^1, \vec{\sigma}^2) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i^1 \sigma_i^2$$: overlap between two solutions

$\mathcal{N}(q)$: # solution-pairs with overlap value q

$$s(q) = \frac{1}{N} \ln \mathcal{N}(q)$$: entropy density as function of overlap

calculating s(q) by cavity method

partition function $Z(x) = \sum_{\vec{\sigma}^1 \in \mathcal{S}} \sum_{\vec{\sigma}^2 \in \mathcal{S}} \exp\left(x \sum_{i=1}^{N} \sigma_i^1 \sigma_i^2\right)$

$$= \sum_q \exp\left[N\left(s(q) + xq\right)\right]$$

mean overlap $\overline{q}(x) = \arg\ \max_q \left(s(q) + xq\right)$

Non-concavity of s(q) can be detected by
discontinuity of mean overlap q
as a function of field x

when s(q) non-concave, its shape can be obtained by
the 1RSB mean-field cavity method

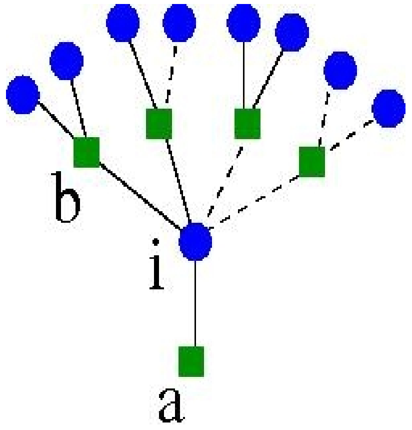
replica symmetric approach

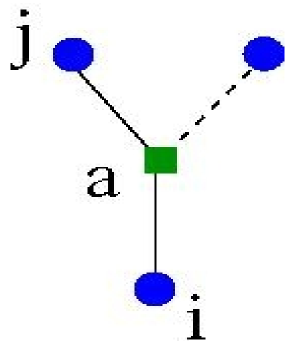
Each variable has a vector state (σ_i, σ_i')

$p_{i\to a}(\sigma_i, \sigma_i')$ Prob.: i takes this state in the absence of a

$\hat{p}_{a\to i}(\sigma_i, \sigma_i')$ Prob.: a being sat in case i takes this state

$$p_{i\to a}(\sigma_i, \sigma_i') = C e^{x\sigma_i\sigma_i'} \prod_{b\in\partial i\setminus a} \hat{p}_{b\to i}(\sigma_i, \sigma_i')$$

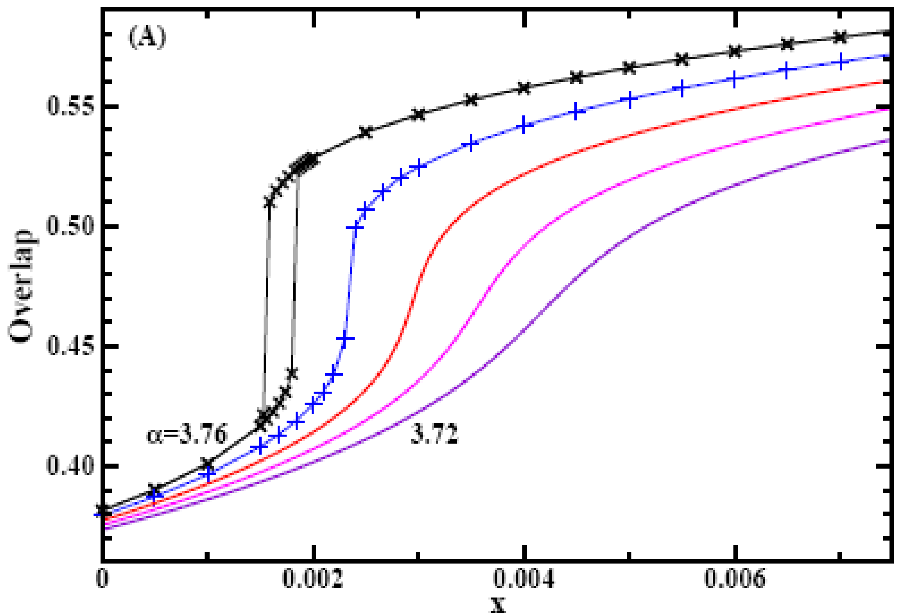




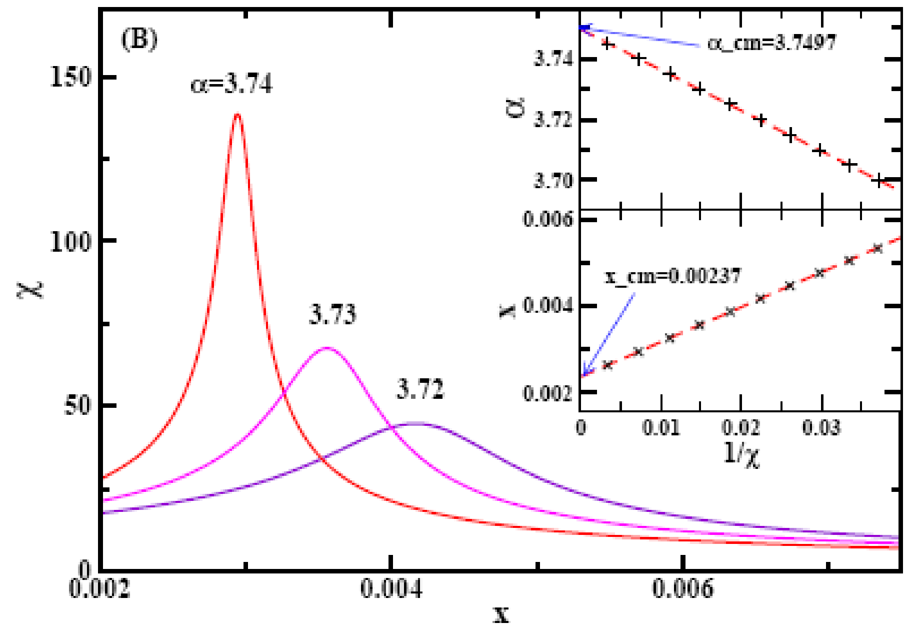
$$\hat{p}_{a\to i}(\sigma_i, \sigma_i') = 1 - \delta_{\sigma_i}^{-J_a^i} \prod_{j\in\partial a\setminus i} \left[\sum_{\sigma} p_{j\to a}(-J_a^j, \sigma)\right] - \delta_{\sigma_i'}^{-J_a^i} \prod_{j\in\partial a\setminus i} \left[\sum_{\sigma} p_{j\to a}(\sigma, -J_a^j)\right] + \delta_{\sigma_i}^{-J_a^i}\delta_{\sigma_i'}^{-J_a^i} \prod_{j\in\partial a\setminus i} p_{j\to a}(-J_a^j, -J_a^j)$$

determine α_{cm}

3-SAT



overlap q(x)



overlap susceptibility χ(x)

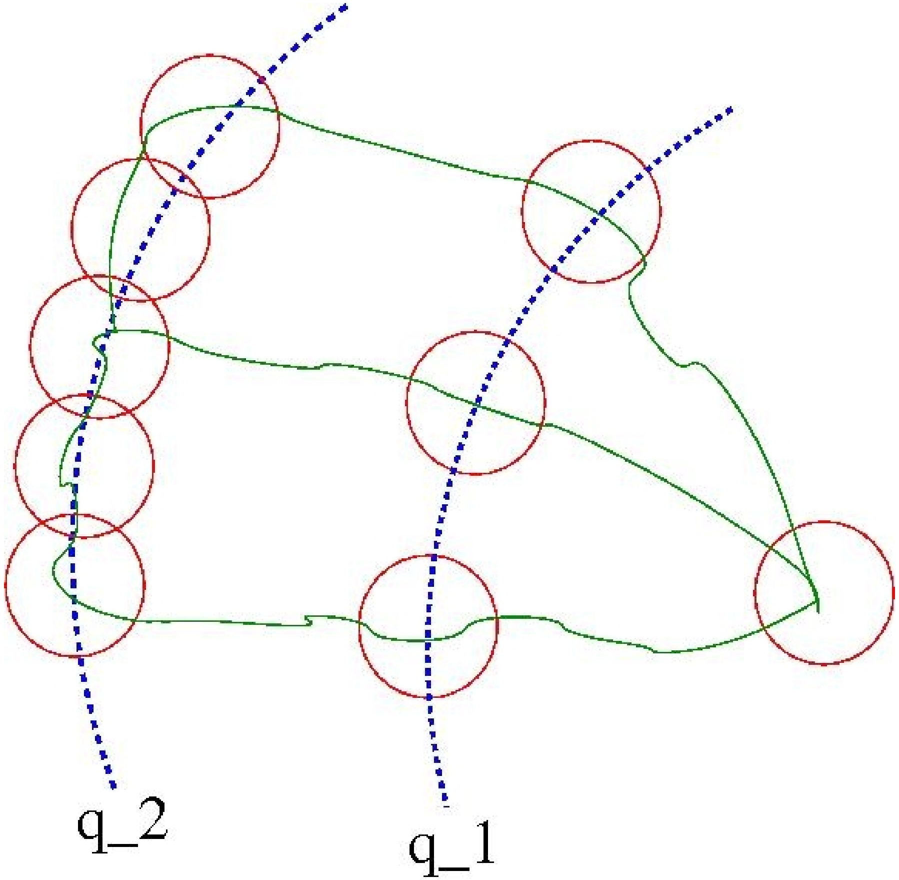
as α approaches 3.75, the peak of χ(x) ⟶∞

s(q) becomes non-concave for α>3.75

For random 4-SAT, the critical value is 8.47

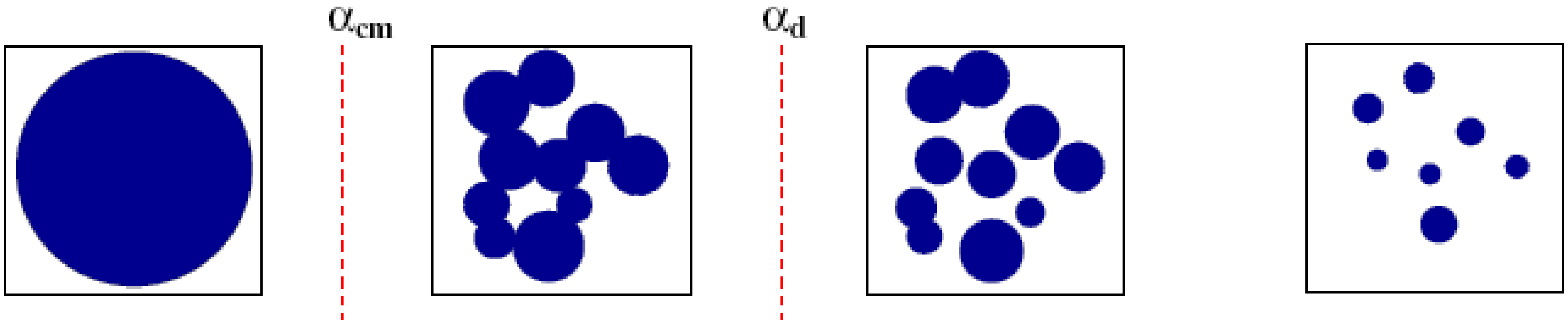
$$\chi(x) = \frac{d\,\bar{q}(x)}{d\,x}$$

inside the heterogeneity regime $\alpha_{cm} < \alpha < \alpha_d$



The solutions on a hyper-surface of fixed overlap q to a typical reference solution is divided into exponentially many clusters within this hyper-surface, when q is intermediate

Replica-symmetry-breaking cavity method needed to describe the solution space heterogeneity



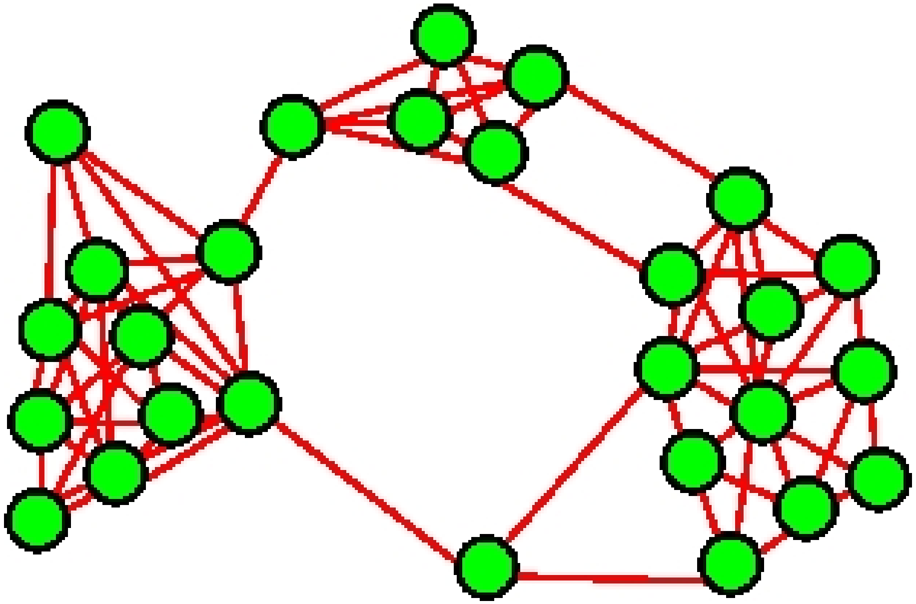
for $\alpha_{cm}<\alpha<\alpha_d$, solution space ergodic but heterogeneous. many solution communities formed, each contains a group of relatively similar solutions

solution communities are precursors of solution clusters at $\alpha>\alpha_d$

α_{cm}=3.75 for random 3-SAT, α_d =3.87

α_{cm}=8.47 for random 4-SAT, α_d=9.38

Glauber dynamics by single-spin flips



Represent the solution space as a complex graph:

node → solution
edge → single-spin flip

configuration at time t: $\vec{\sigma} = (\sigma_1, \ldots, \sigma_i, \ldots, \sigma_N)$

$\vec{\sigma}' = (\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N)$

randomly choose a spin i to flip

configuration at t+δt:

if σ' not a solution: $\vec{\sigma}(t+\delta t) = \vec{\sigma}(t)$

otherwise $\vec{\sigma}(t+\delta t) = \vec{\sigma}(t)$ prob. 1/2 $\vec{\sigma}(t+\delta t) = \vec{\sigma}'$ prob. 1/2

overlap and dynamical susceptibility

overlap of configurations at time interval τ:

$$q = \frac{1}{N} \sum_{i=1}^{N} \sigma_i(t)\sigma_i(t+\tau)$$

different overlap values at different starting time t.

overlap variance:

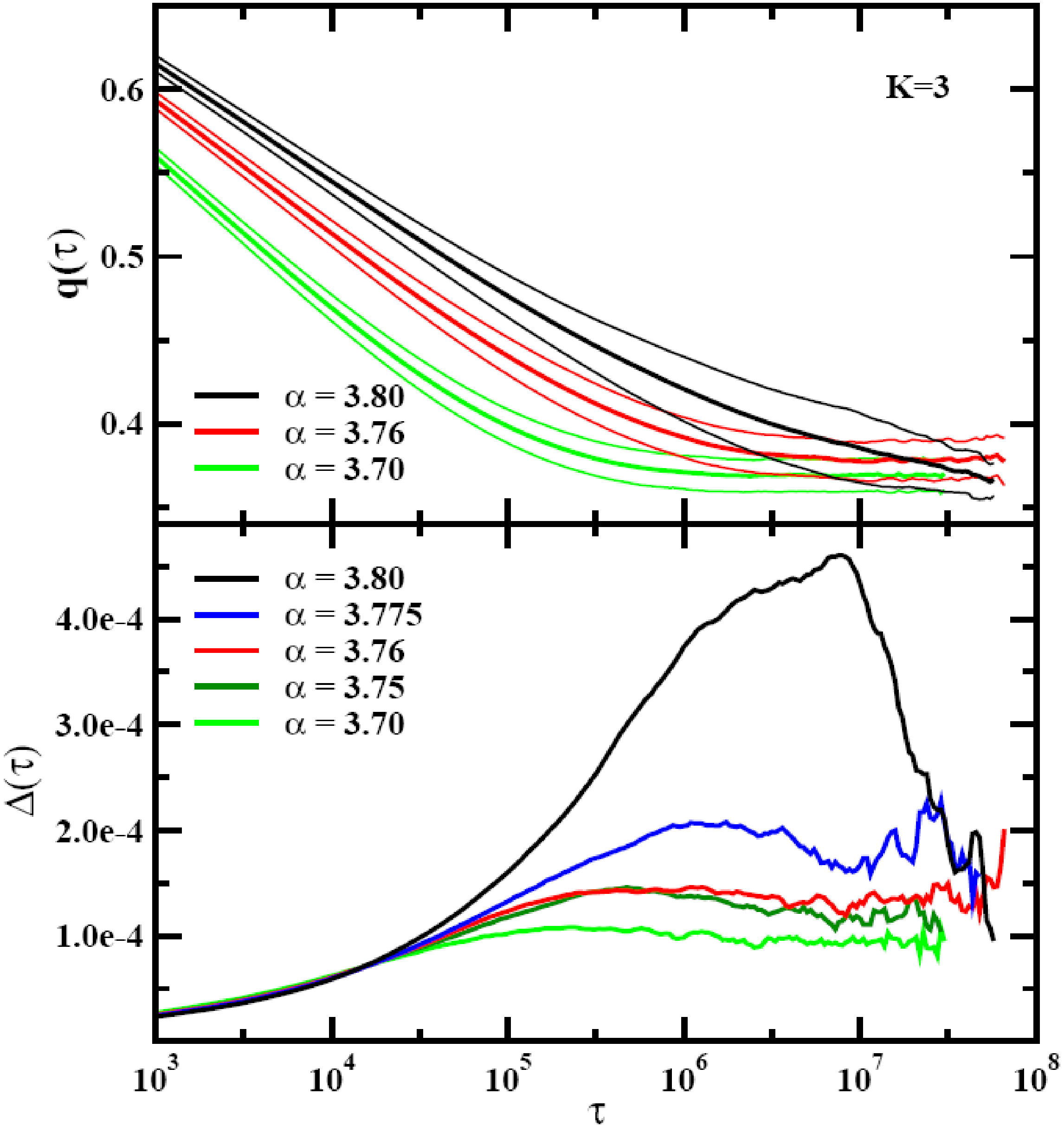
$$\Delta(\tau) = \langle q^2 \rangle - \langle q \rangle^2$$

$$\frac{1}{N^2} \sum_{i,j=1}^{N} \left\{ \langle \sigma_i(t)\sigma_i(t+\tau)\sigma_j(t)\sigma_j(t+\tau) \rangle - \langle \sigma_i(t)\sigma_i(t+\tau) \rangle \langle \sigma_j(t)\sigma_j(t+\tau) \rangle \right\}$$

Relation to dynamical susceptibility χ(τ):

$$\chi(\tau) = N\,\Delta(\tau)$$

simulation results for random 3-SAT



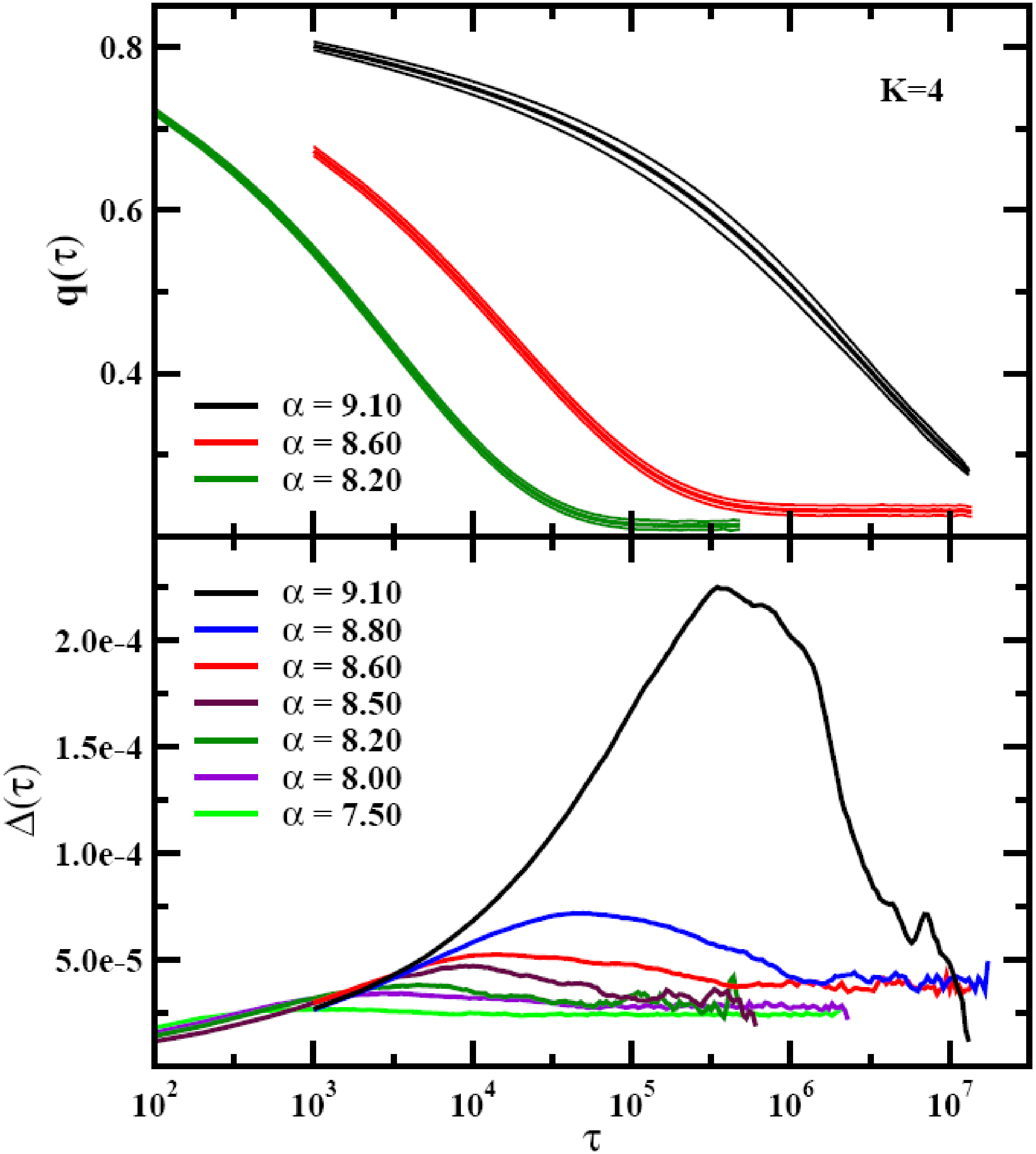
N=100,000

As α exceeds α_{cm}=3.75, dynamical heterogeneity evident in diffusion process

→ typical time scale of escaping solution communities

→ peak of dynamical susceptibility

simulation results for random 4-SAT



N=100,000

As α exceeds α_{cm}=8.47, dynamical heterogeneity evident in diffusion process

→ typical time scale of escaping solution communities

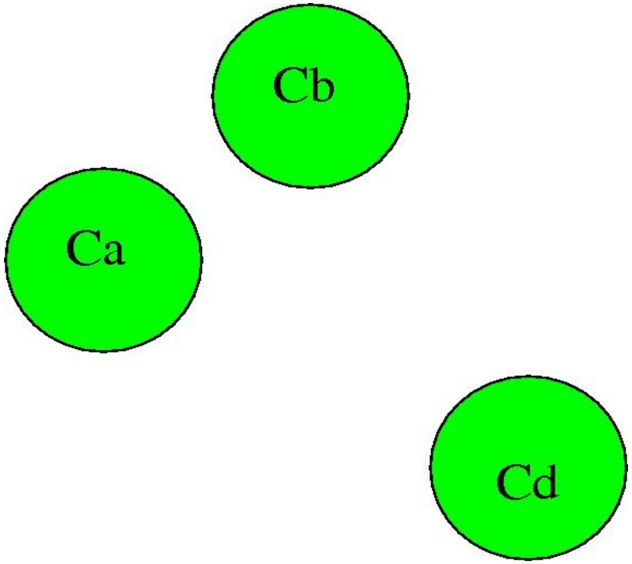
→ peak of dynamical susceptibility

clustering analysis of sampled solutions

Solutions are sampled at equal time interval Δ

Δ controls resolution of structural details.
Δ≈105 (large-scale structure)**

Jain & Dubes, Algorithms for Clustering Data (1988);
Barthel & Hartmann (2004).



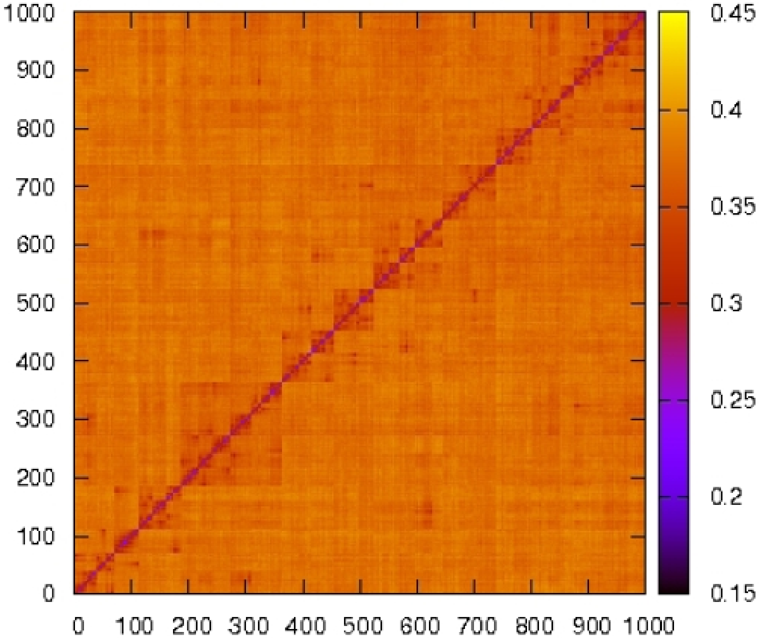
$$d(C_c, C_d) = \frac{(|C_a| + |C_d|)d(C_a, C_d) + (|C_b| + |C_d|)d(C_b, C_d) - |C_d|d(C_a, C_b)}{|C_c| + |C_d|}$$

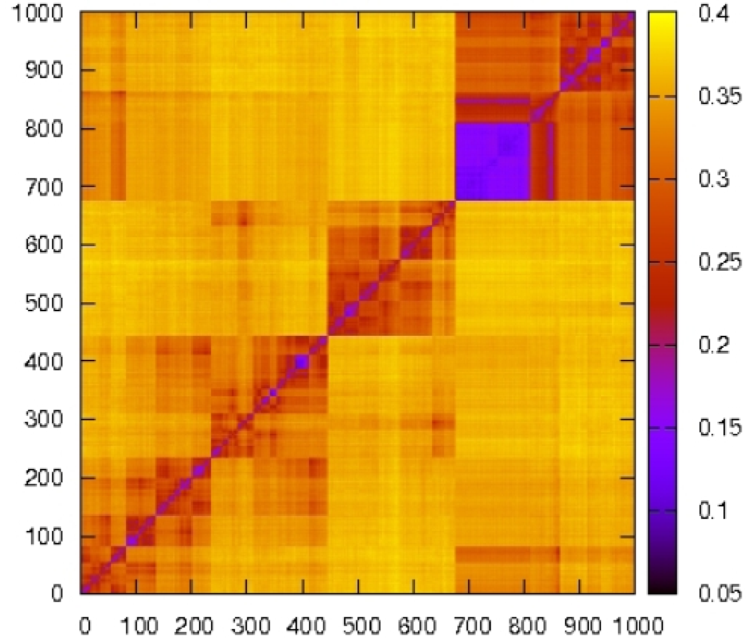
clustering analysis results

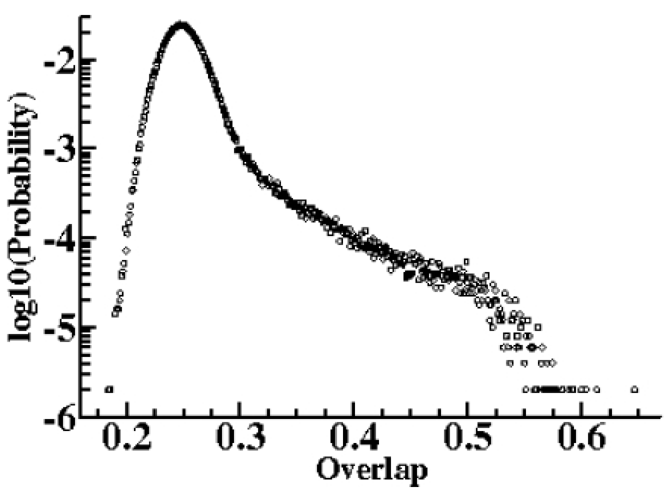
4-SAT, N=20,000

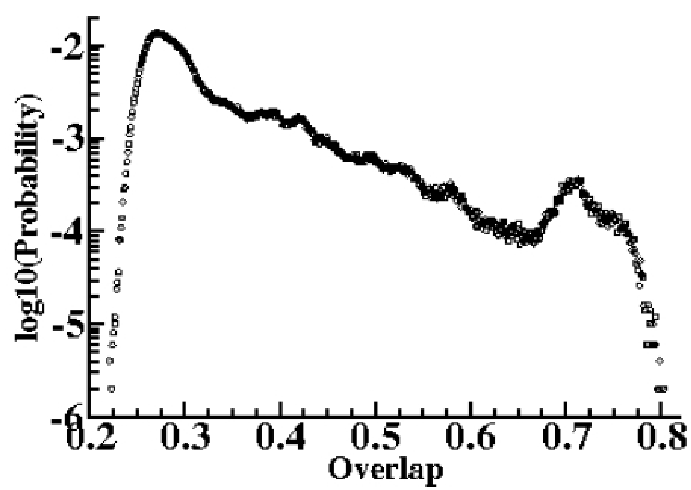
α_{cm}=8.47
α_d=9.38

α=9.10 (left), α=9.22 (right)

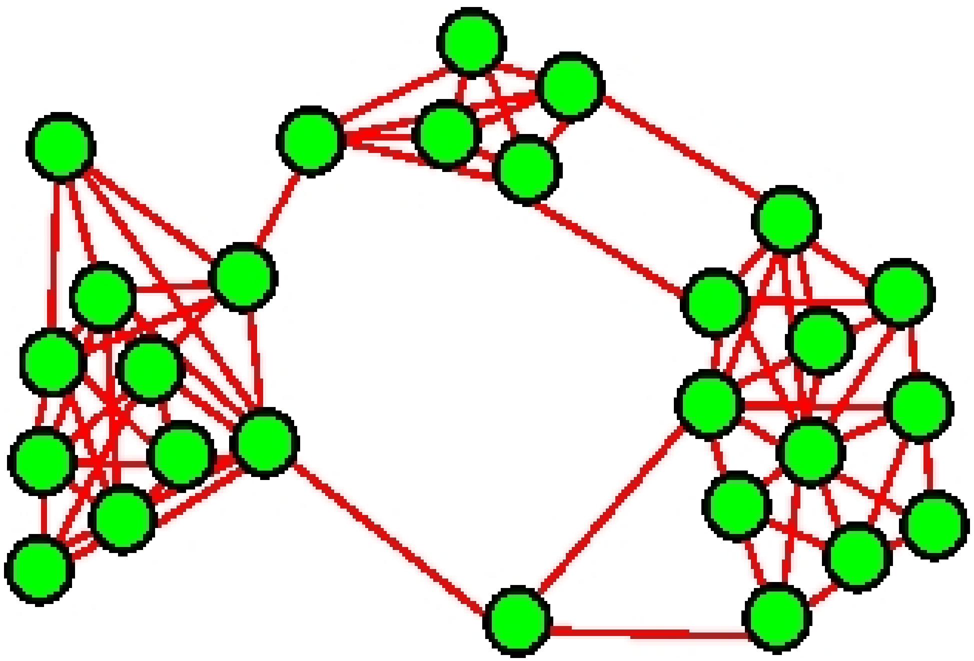








random walk search



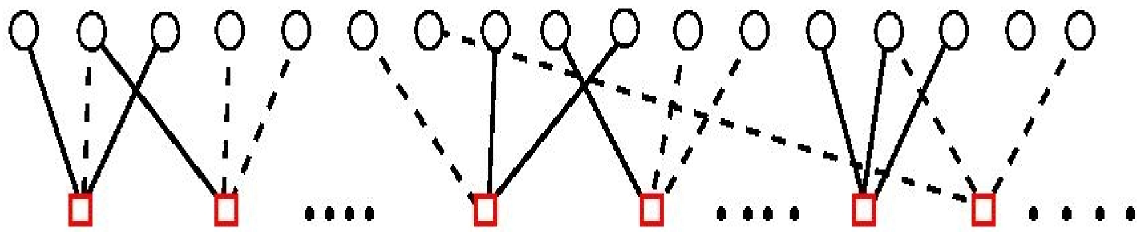
Represent the solution space as a complex graph:

node ←→ solution
edge ←→ single-spin flip

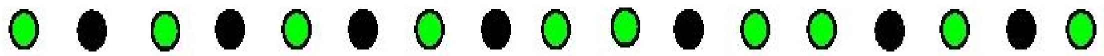
Random walk in solution space:

$$P(\sigma \rightarrow \sigma') = \frac{1}{|\partial\sigma|}$$

node degree

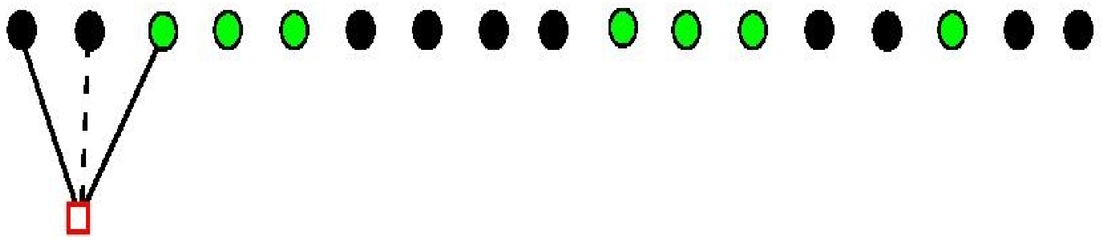


Objective:
input a formula
output a solution

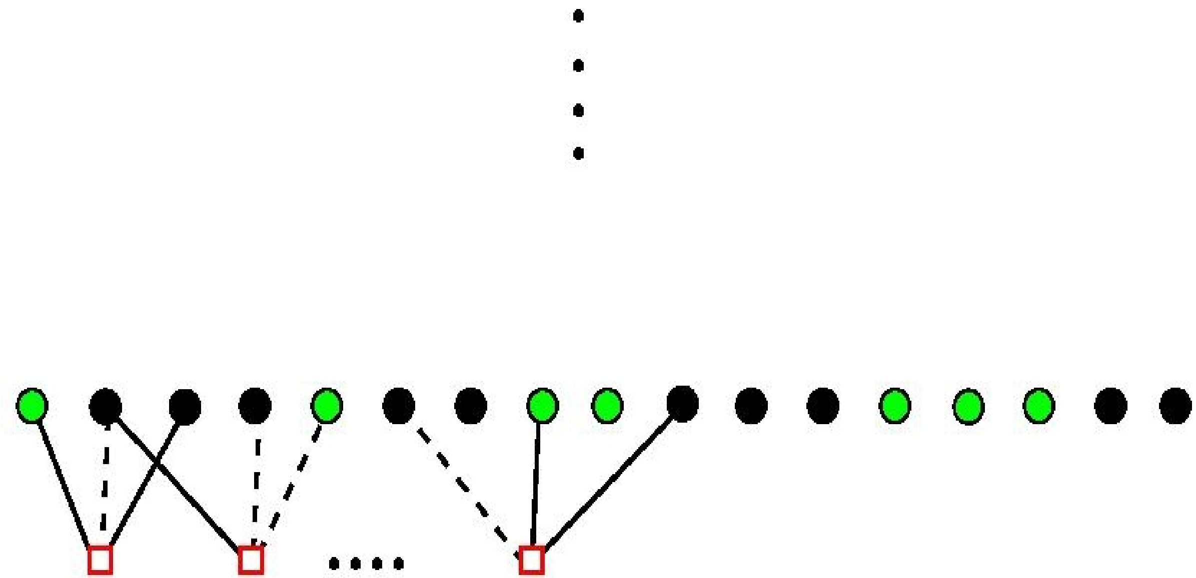


(0) remove all constraints,

create a random initial configuration

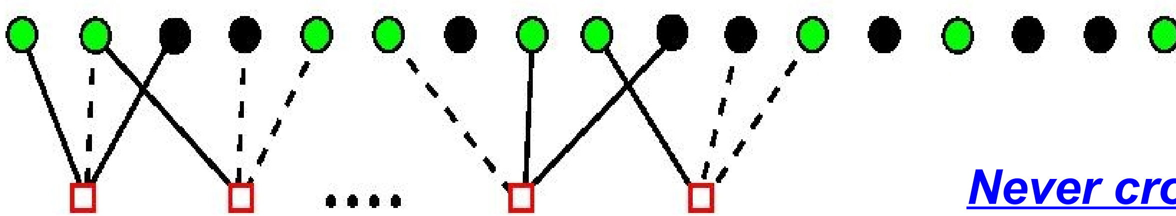


(1) random walking in the solution space until reach a configuration that sat the 1st constraint



(m+1): random walking on the solution cluster of the satisfied sub-formula of m constraints

until reach a configuration that sat the (m+1)-th constraint



Never crosses any energy barrier!

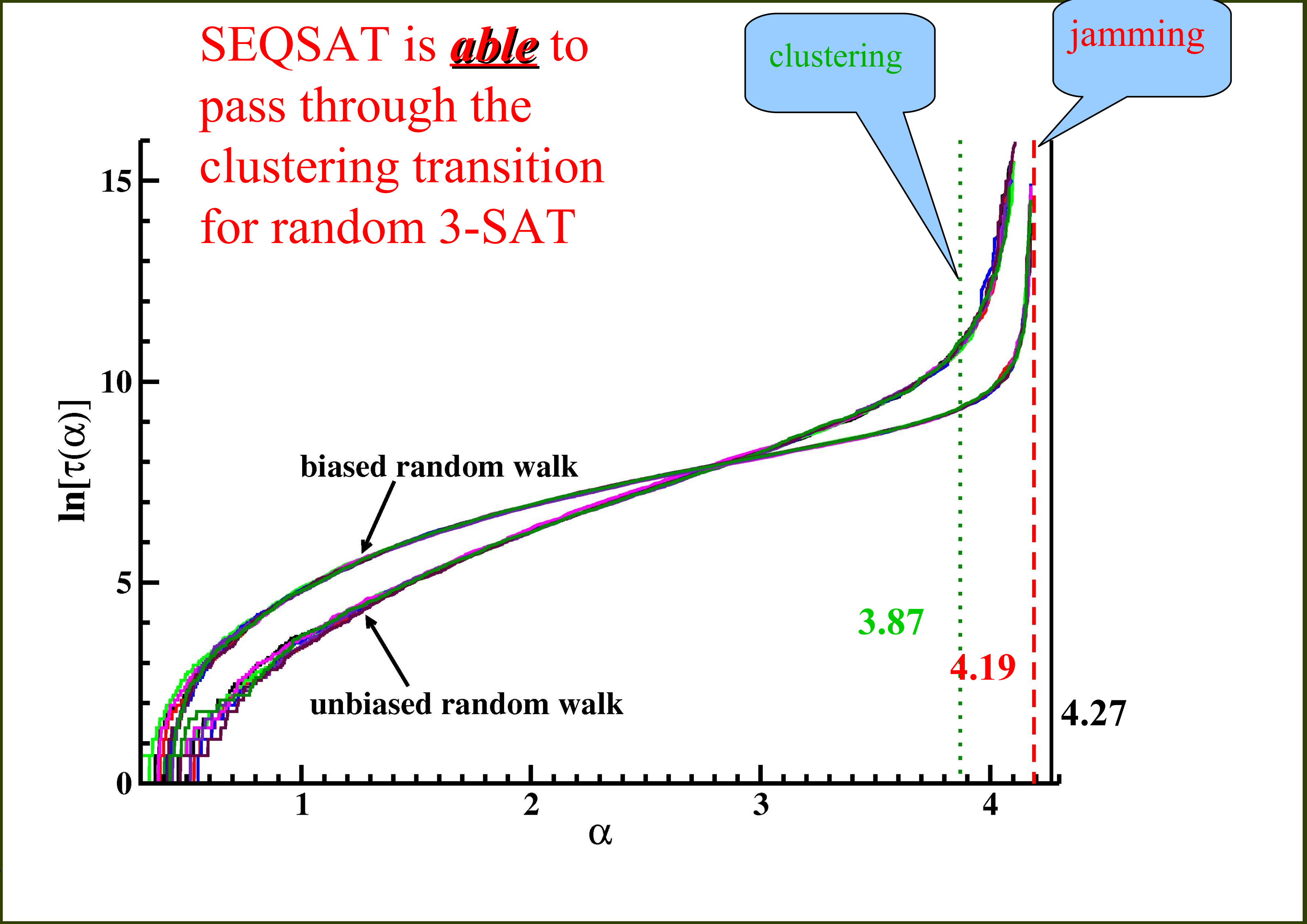
Related other protocols

Krzaka & Kurchan (2007);

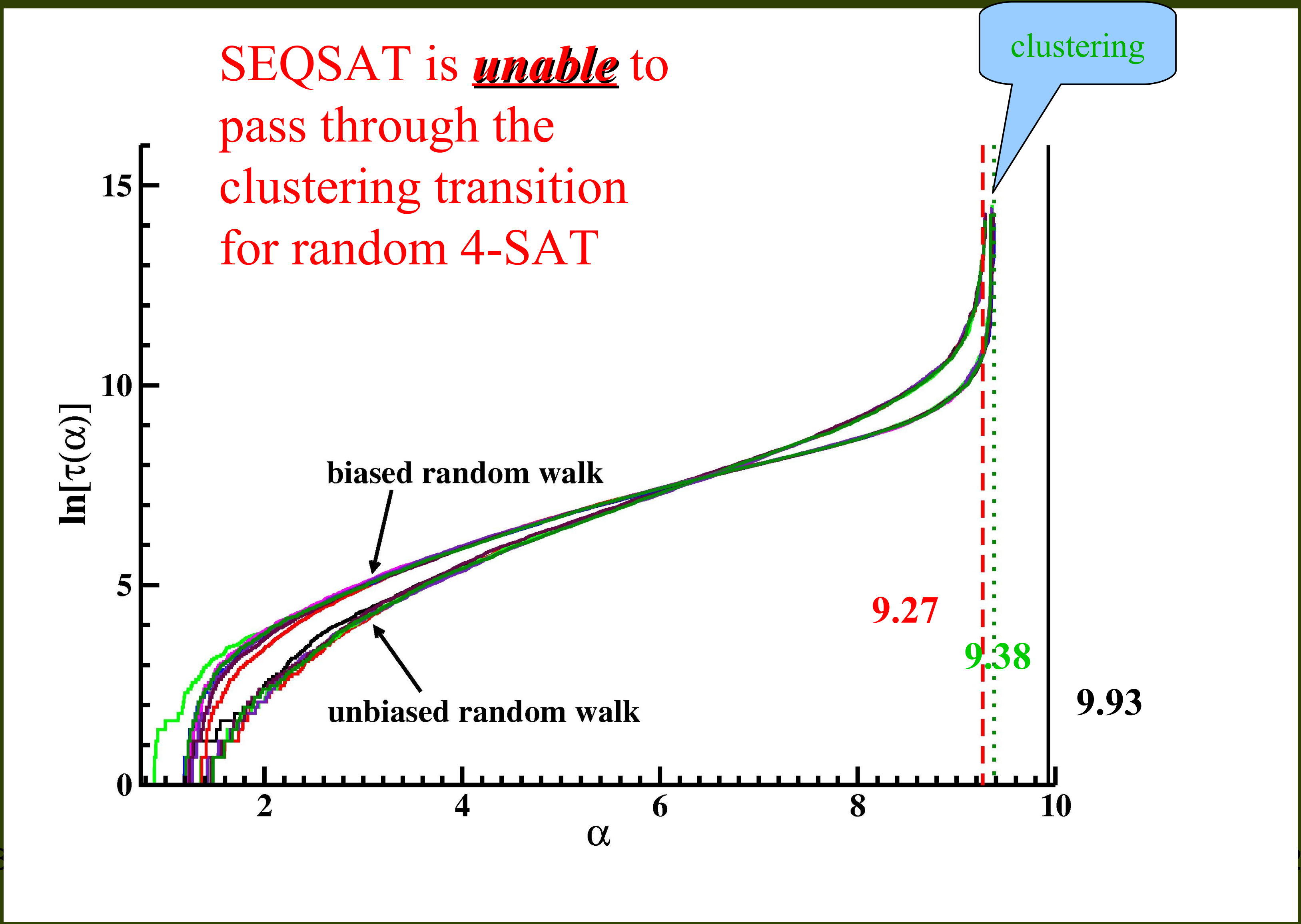
Alava, Ardius, Aurell, et al., (2008)

performance of SEQSAT

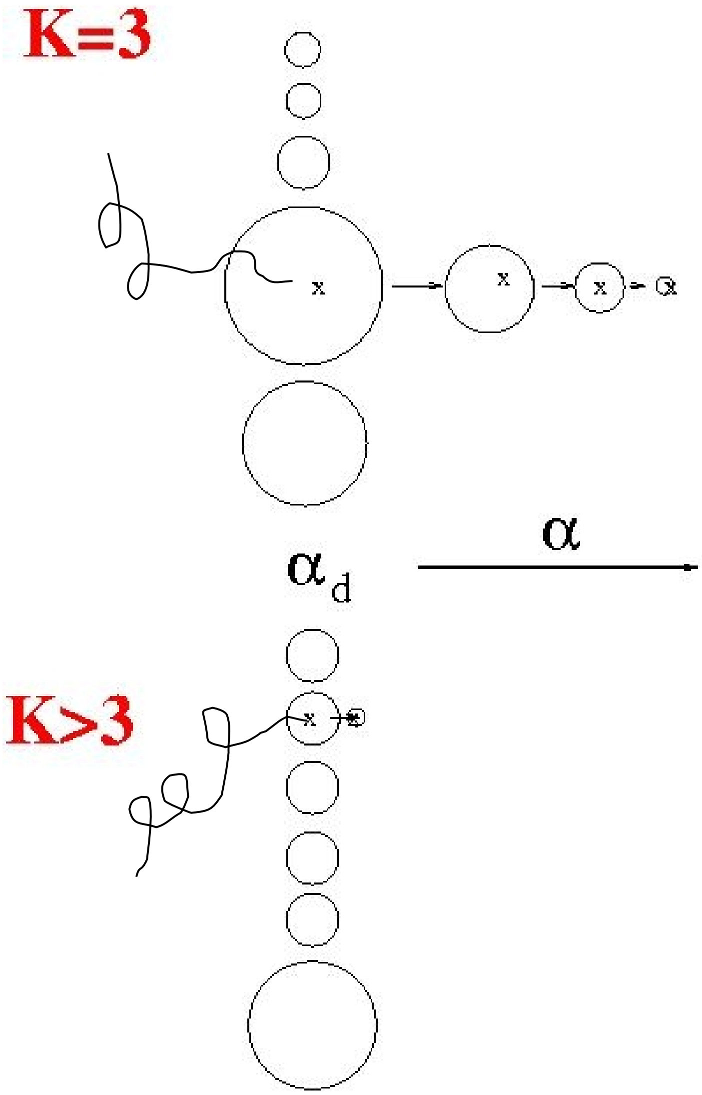
3-SAT, N=100,000



4-SAT, N=100,000

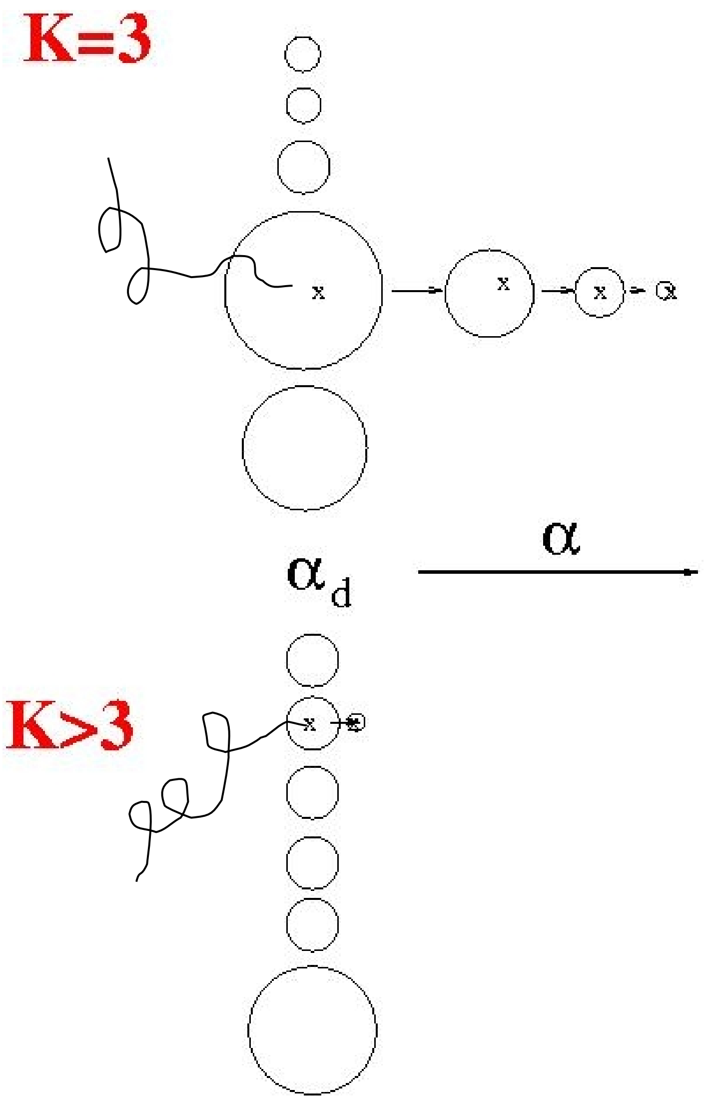


why SEQSAT differs for K=3 and K>4



Random 3-SAT:
solution space dominated by a few largest clusters at clustering transition

Random K-SAT (K>3):
solution space dominated by an exponential number of median-sized clusters at clustering transition



how to reach the largest solution cluster?

Discussion

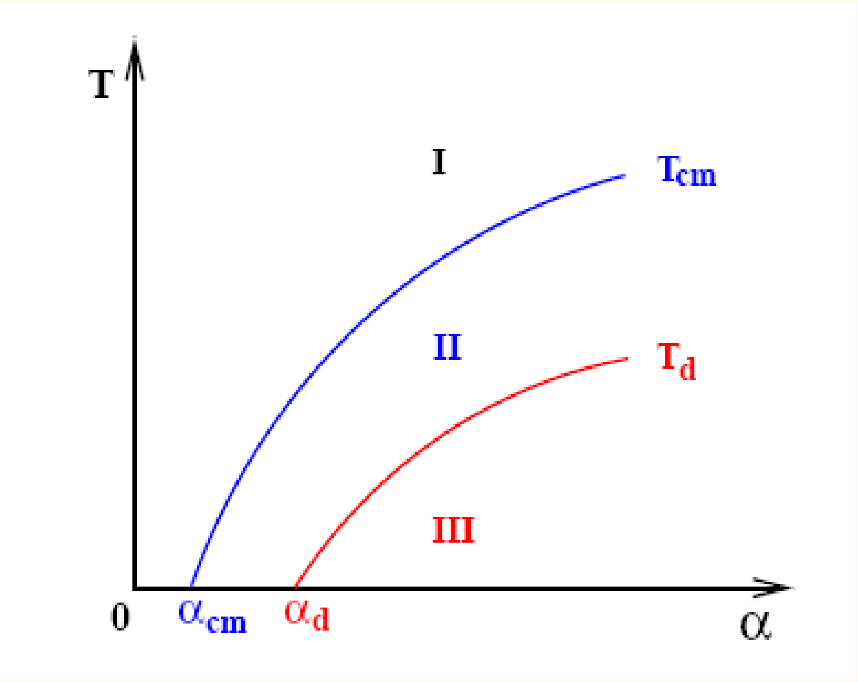
As number of constraints increases, the solution space of the random K-SAT formula first becomes heterogeneous and then breaks ergodicity.

This phenomena is not specific to the random K-SAT problem but appears to be rather general.

We have studied the random K-XORSAT problem and found the same behaviour.

Discussion (continued)

When the constraint density α is fixed but temperature T is finite, a heterogeneity transition should also occur to the configuration space before the dynamical (clustering) transition.



Related earlier work:

For the completely-connected p-body spherical spin-glass model, the existence of a heterogeneous but ergodic phase in the configuration space was predicted by Franz and Parisi (1995,1997)

Acknowledgement

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