Long time dynamics in mean field glassy systems

Florent Krzakala
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in collaboration with
Lenka Zdeborová
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The energy landscape in mean field glassy systems

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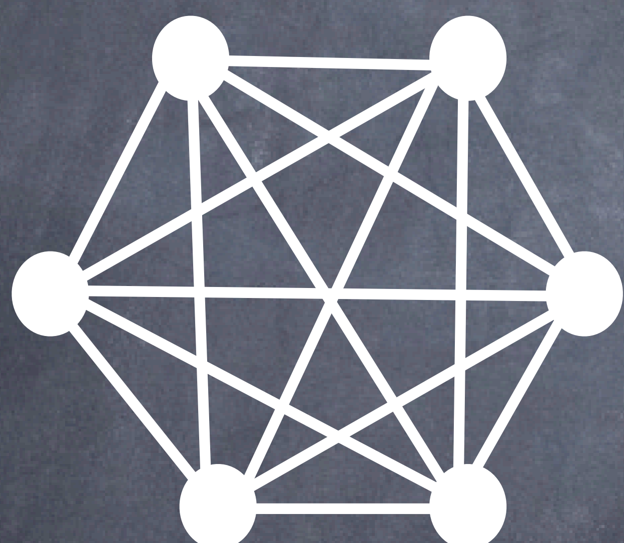
Mean field systems

Fully connected models

(Curie-Weiss, Sherrington-Kirkpatrick, etc....)



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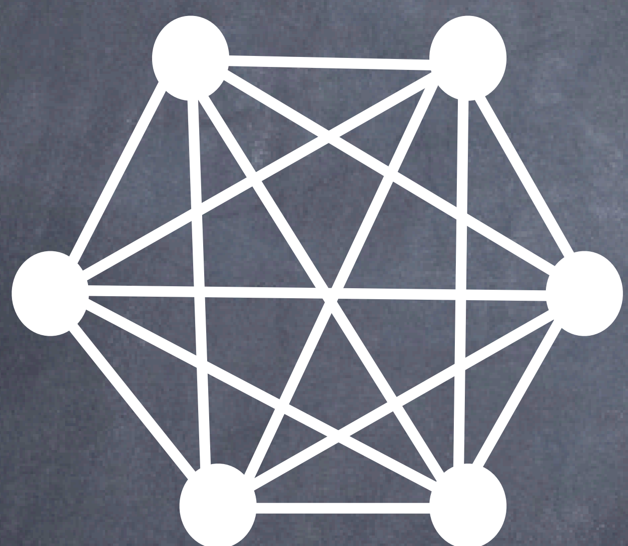
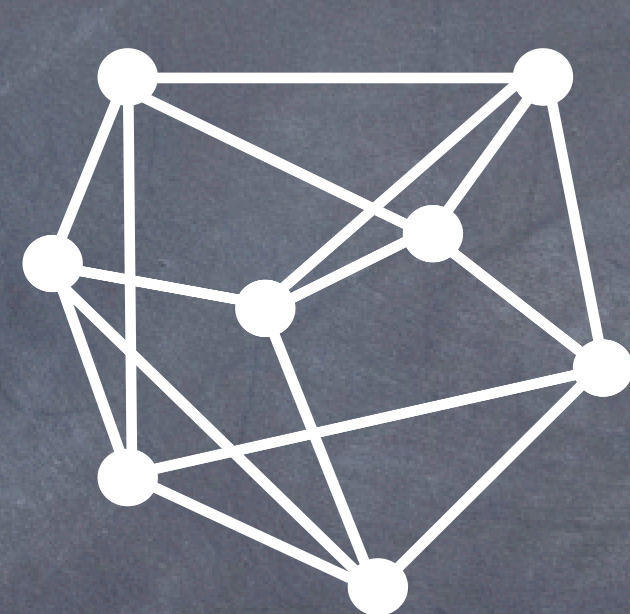


Diluted models

(random graphs, Bethe lattices)



Locally

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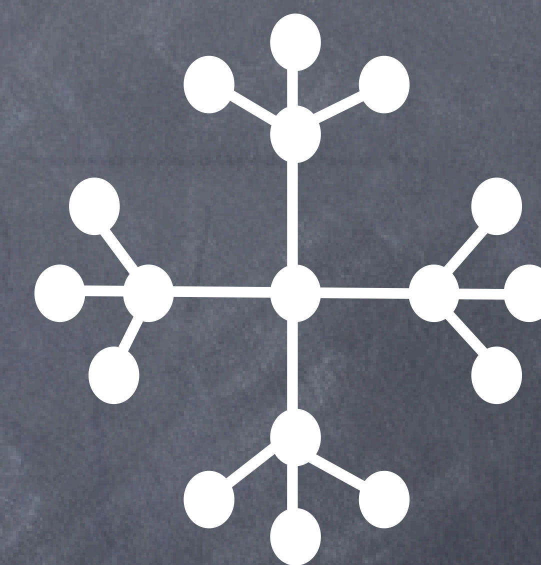

Shortest cycle going trough a typical node has length log(N).

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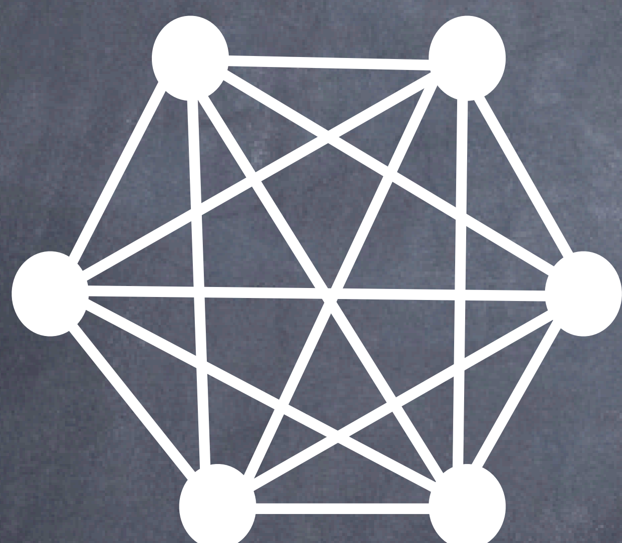

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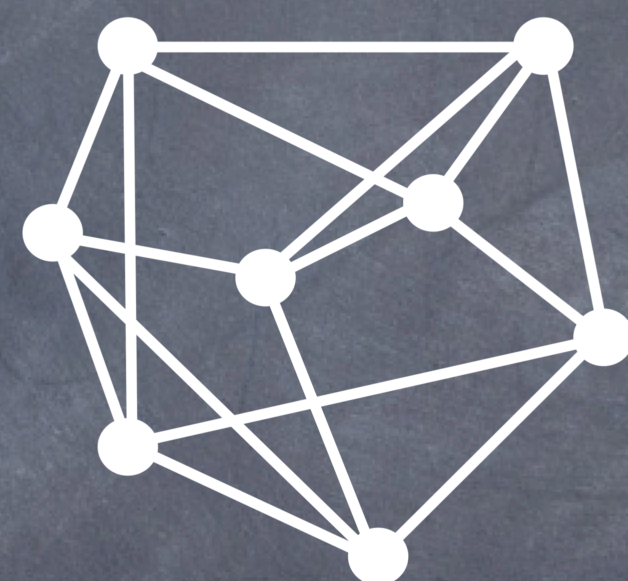

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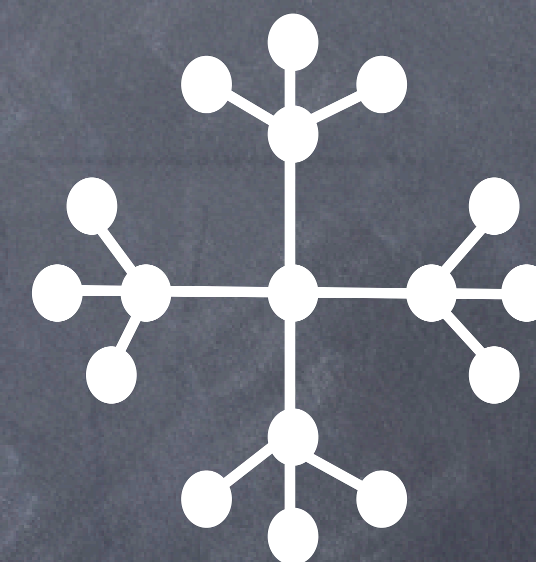

Thermodynamics:
Solvable using the replica or the cavity method (Bethe-Peierls)

Shortest cycle going trough a typical node has length log(N).

Some examples

- Spin glasses: Sherrington-Kirkpatrick, Vianna-Bray (Bethe lattice spin glass),
- Optimization problems: Coloring (Potts antiferromagnet), K-satisfiability, graph partitioning (Ising with fixed magnetization), vertex cover, ...
- Glasses, hard spheres, colloids, ...: p-spin model, Biroli-Mezard lattice glass, lattice model for colloidal glass, mean field models for hard spheres, quantum systems on random lattices, Coulomb glasses...

Examples in this talk

p-spin glass (XOR-satisfiability):

$$H = -\sum_{(ij)} J_{ij} \prod_{i=1}^{p} S_i \qquad S_i \in \{-1, +1\}$$

Potts glass (graph coloring):

$$H = \sum_{(ij)} \delta_{S_i, S_j} \qquad S_i \in \{1, \ldots, q\}$$

Glassy Mean field systems

Several things we know about them

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Dynamical glass transition

- broken ergodicity
- structural entropy appears

Glassy Mean field systems

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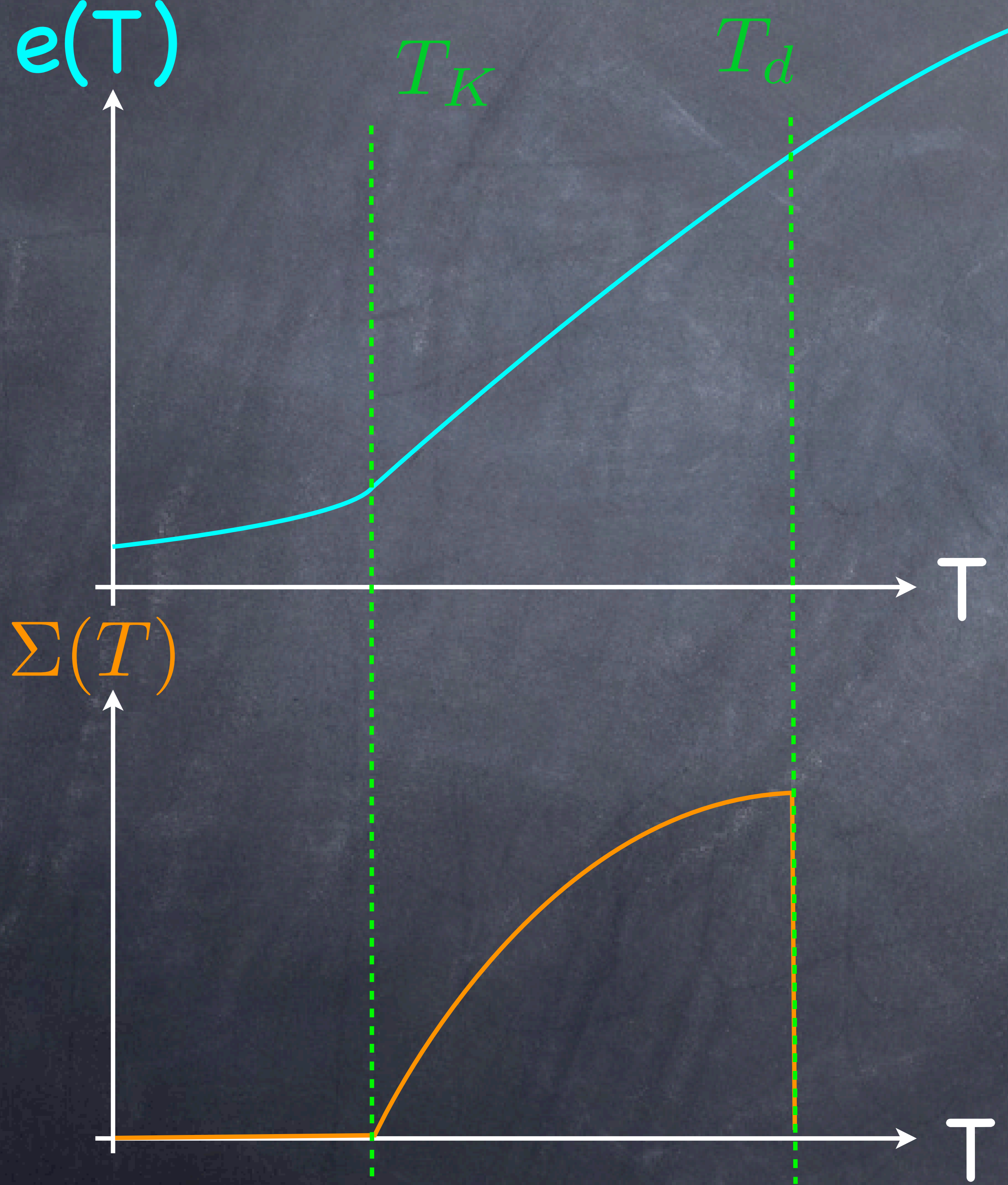

Dynamical glass transition

- broken ergodicity
- structural entropy appears

Static (ideal) glass transition

- non-analyticity in free energy
- structural entropy vanishes

Glassy Mean field systems

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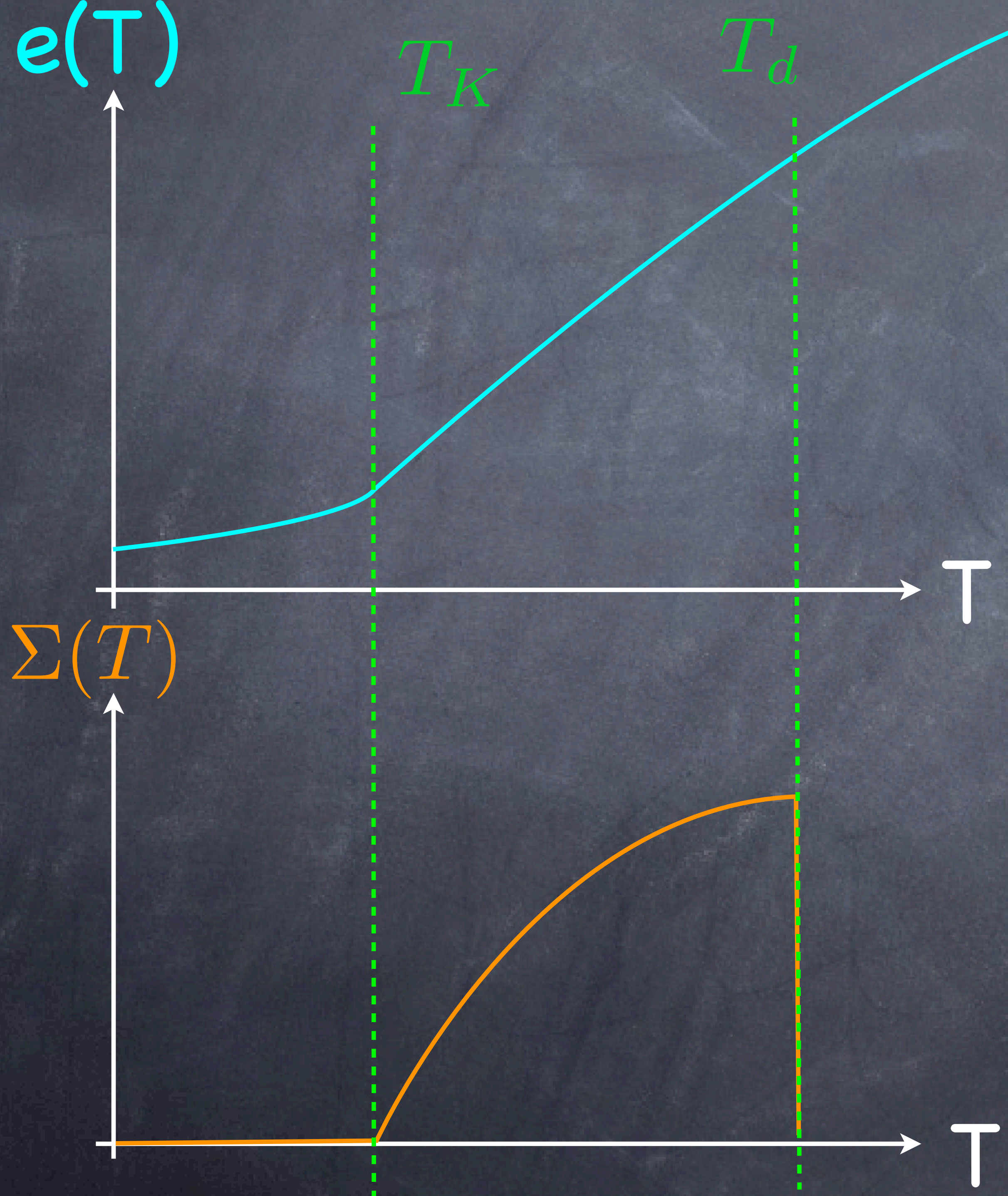

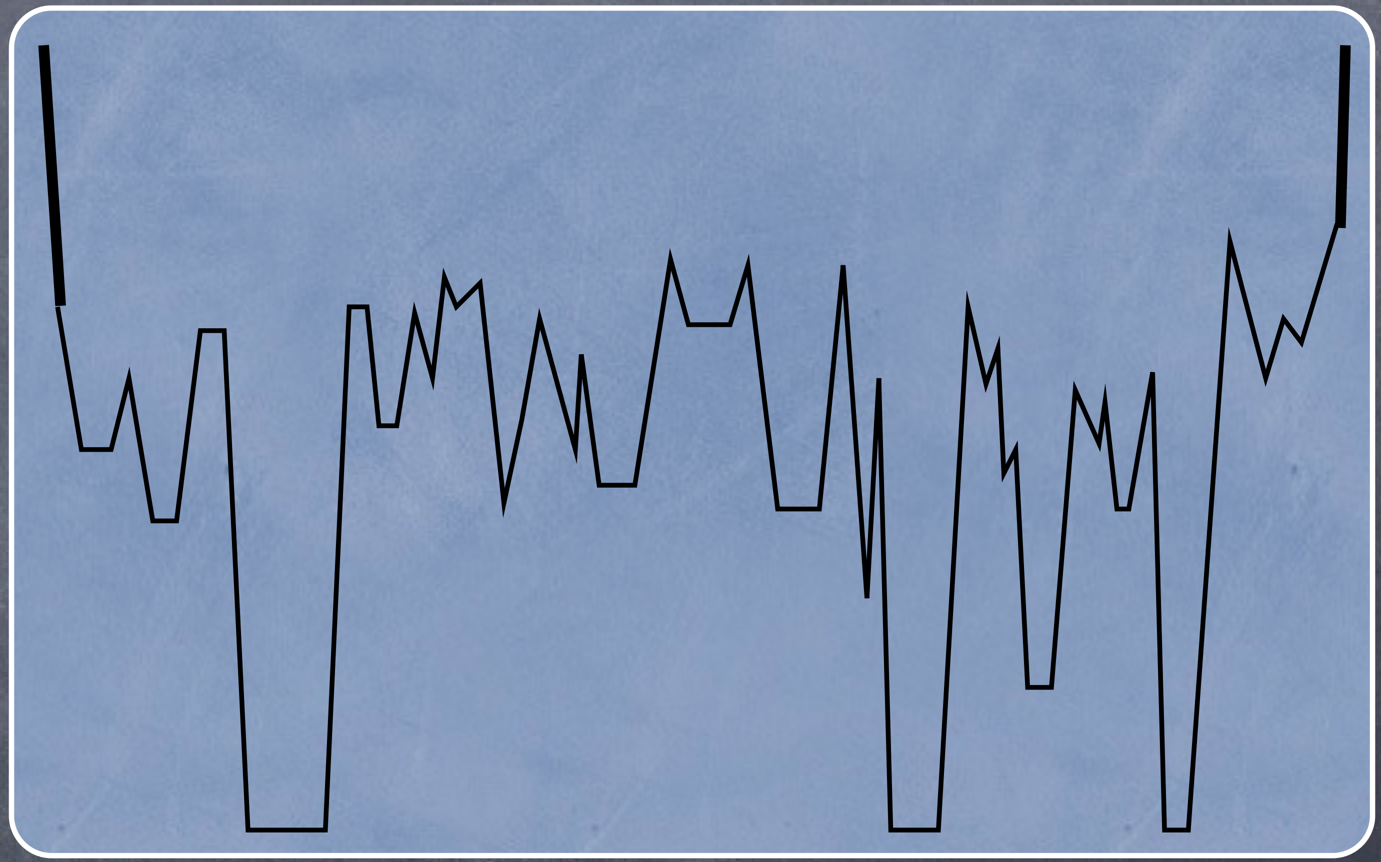

Energy landscape

Glassy Mean field systems

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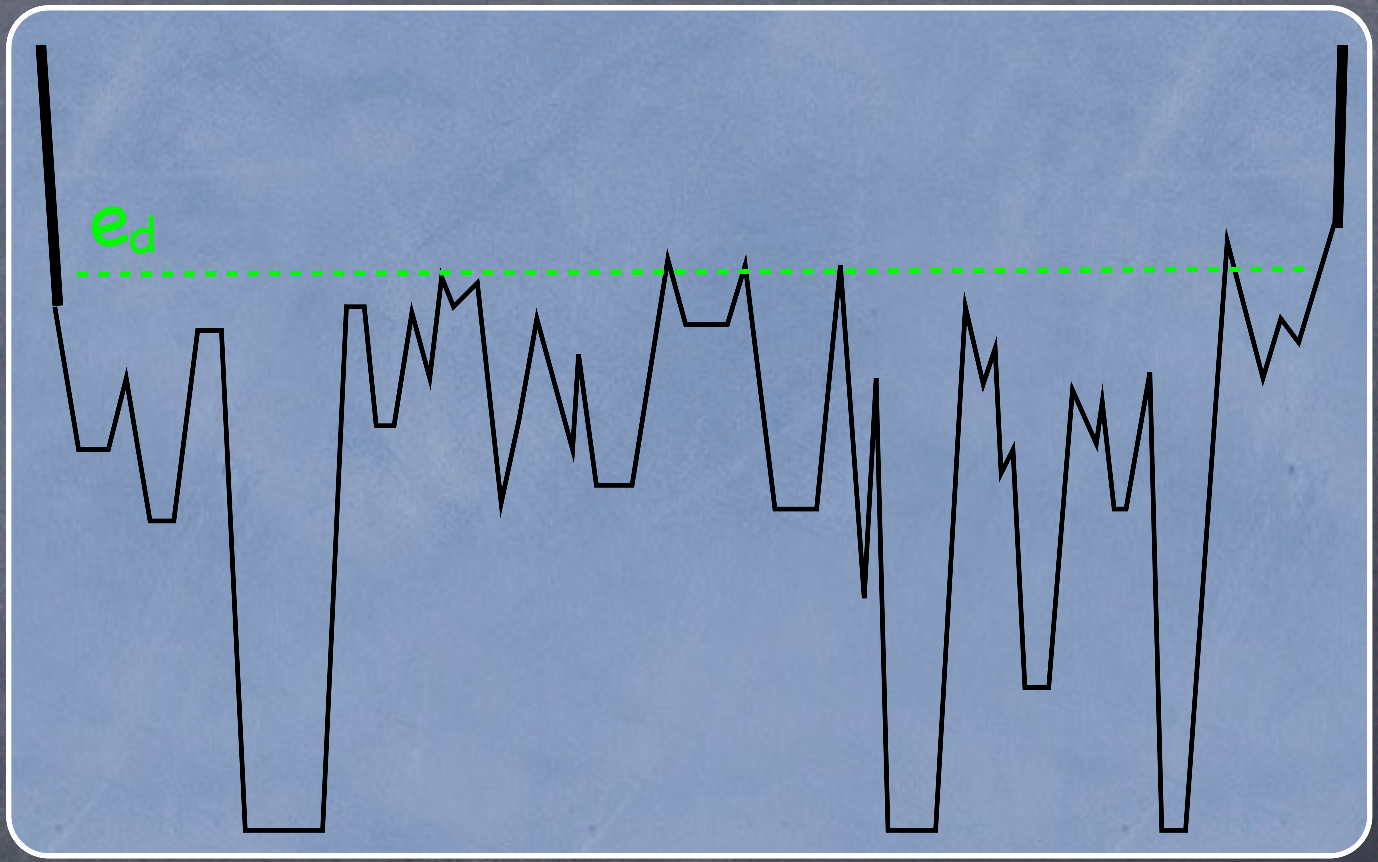

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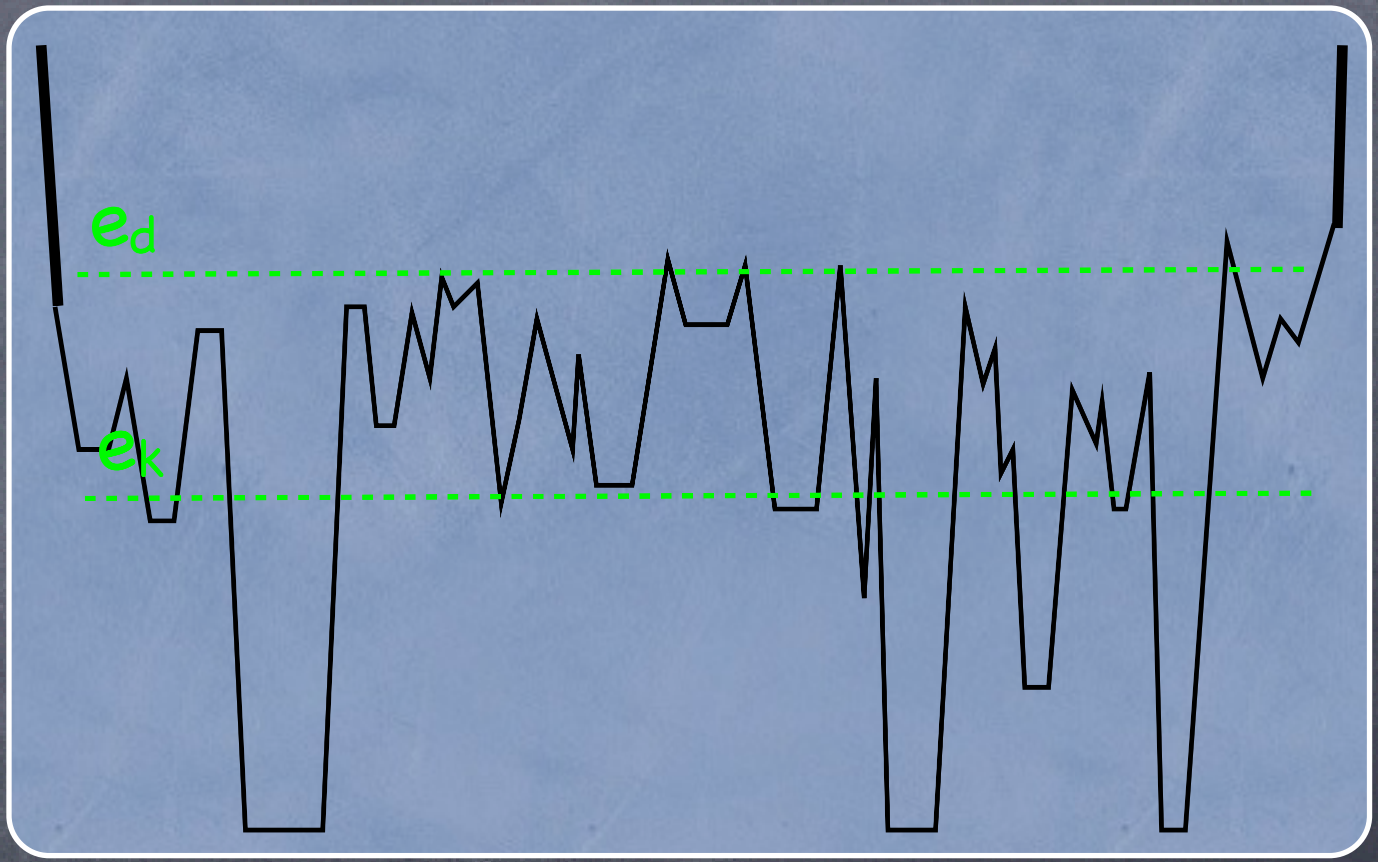


Energy landscape

Replica & Cavity Methods

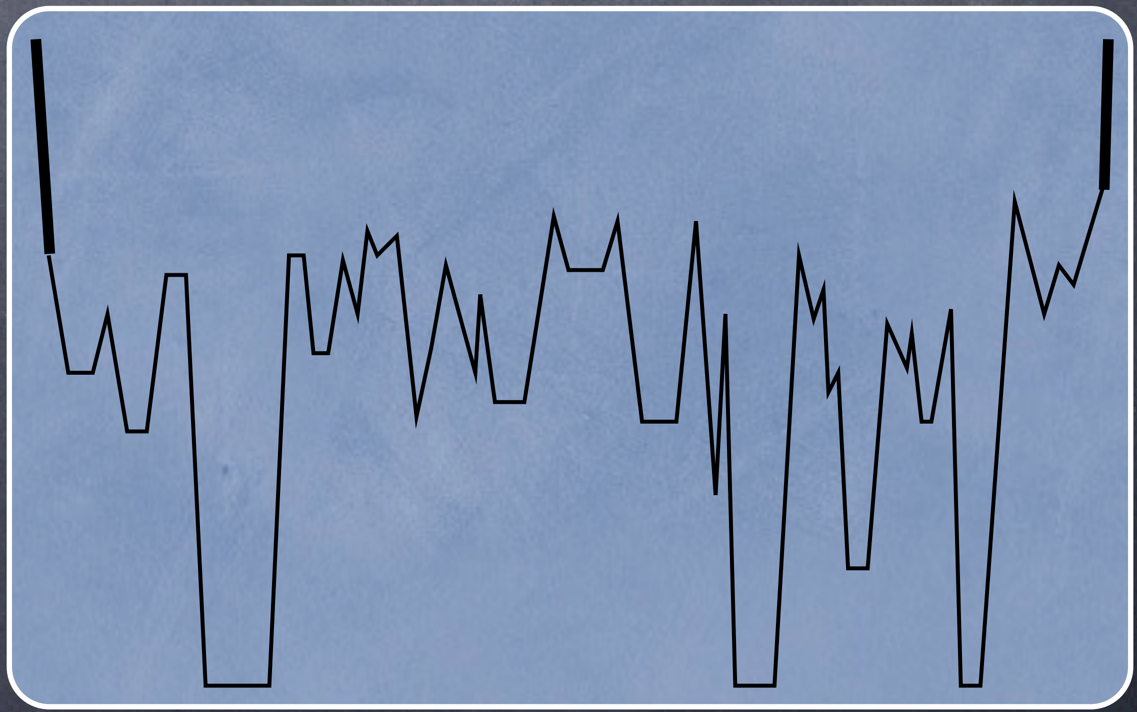
(Parisi'80) (Mezard, Parisi'01)

Computational method giving properties of the energy landscape:

- Total energy, entropy, temperature
- Properties of states/valleys/TAP - their number, size ...

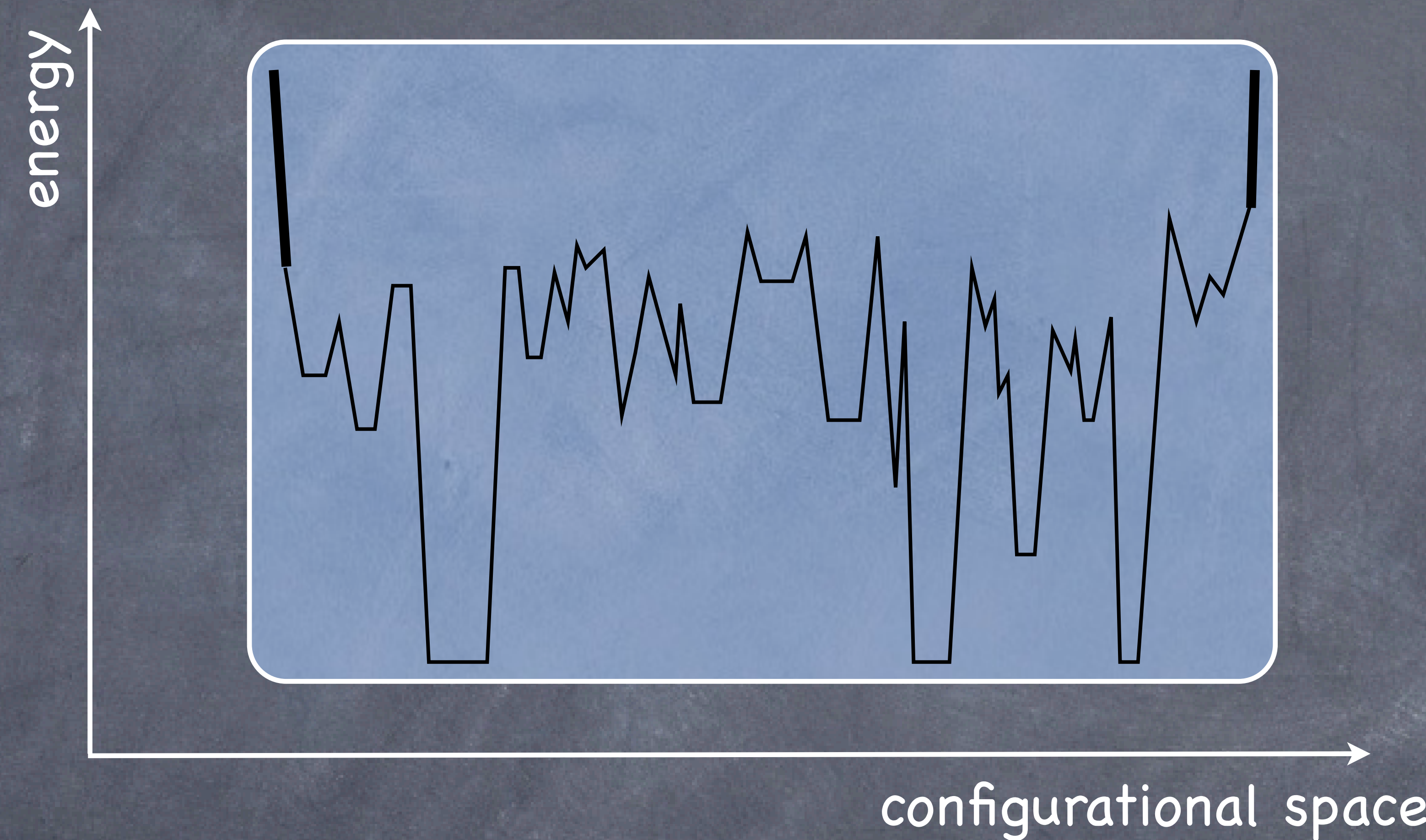
$$\mathcal{N}_{\text{states}} = e^{N\Sigma} \qquad \Sigma(e,s)$$

- Overlaps between and within states etc.



Glassy Mean field systems

Things we DO NOT know about them



Glassy Mean field systems

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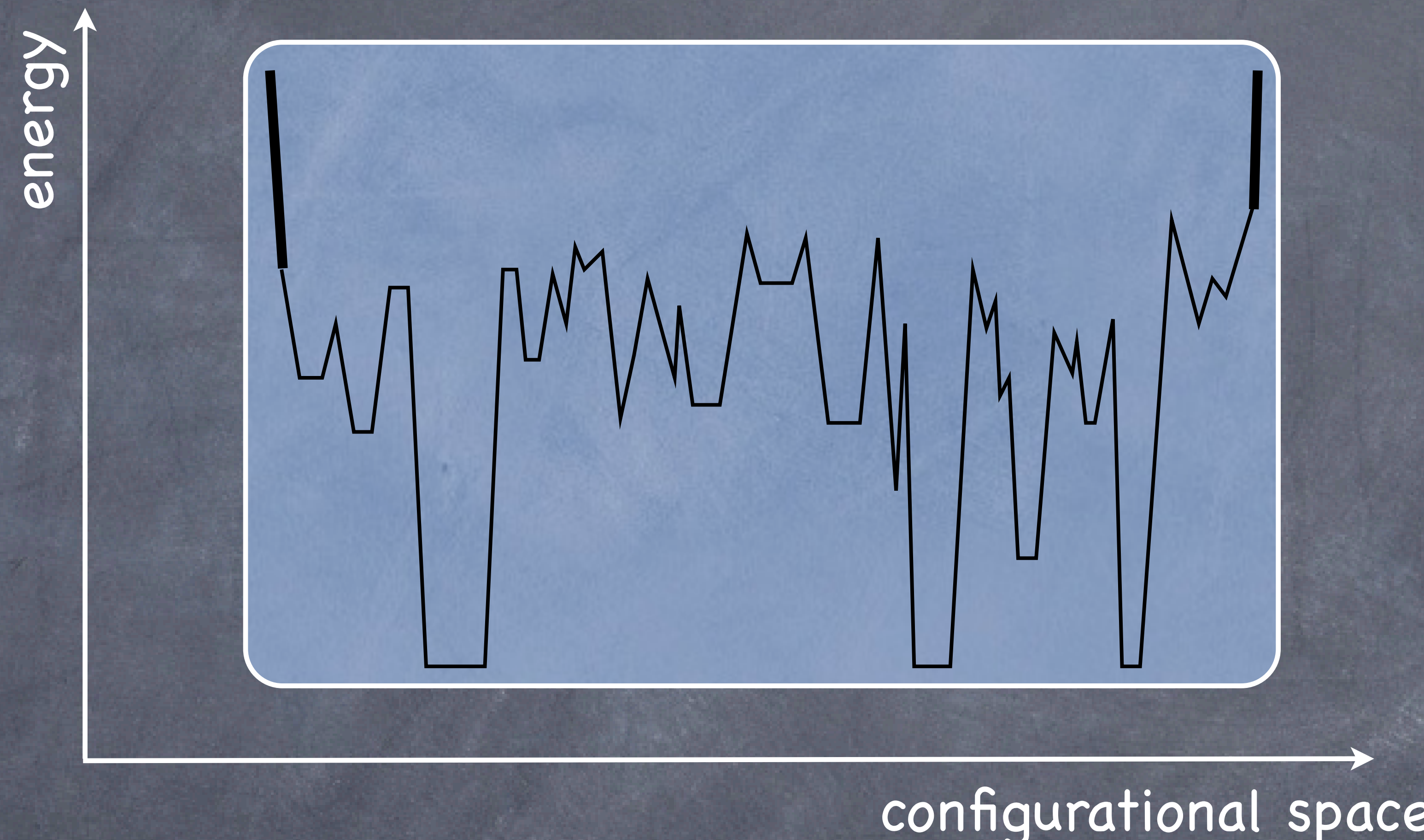
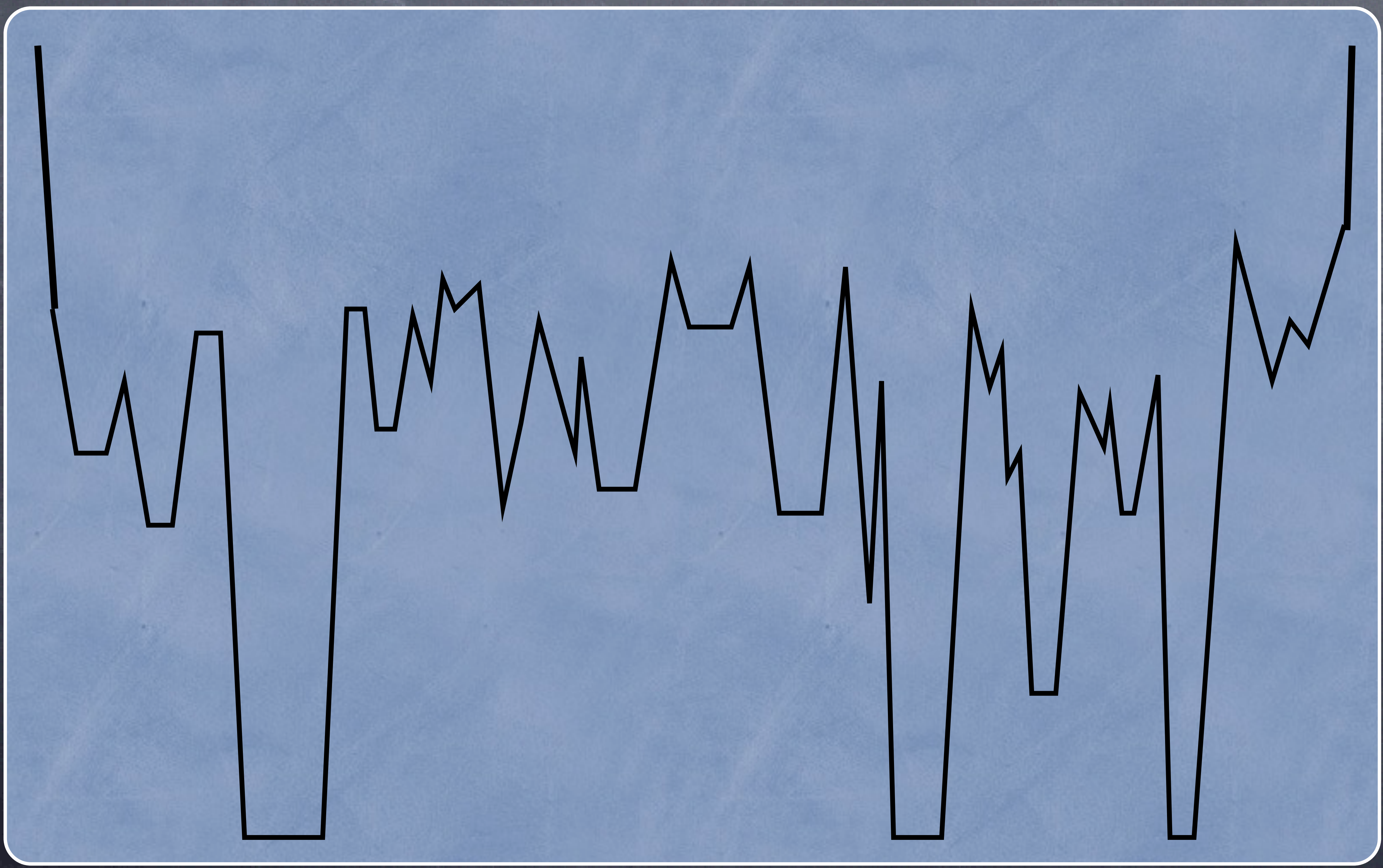


- The information on the landscape is only enumerative...
- ...We do not describe the shape of the valleys...
- ...We cannot use it to get information on the dynamics...
- ...And we do not solve explicitly the dynamics

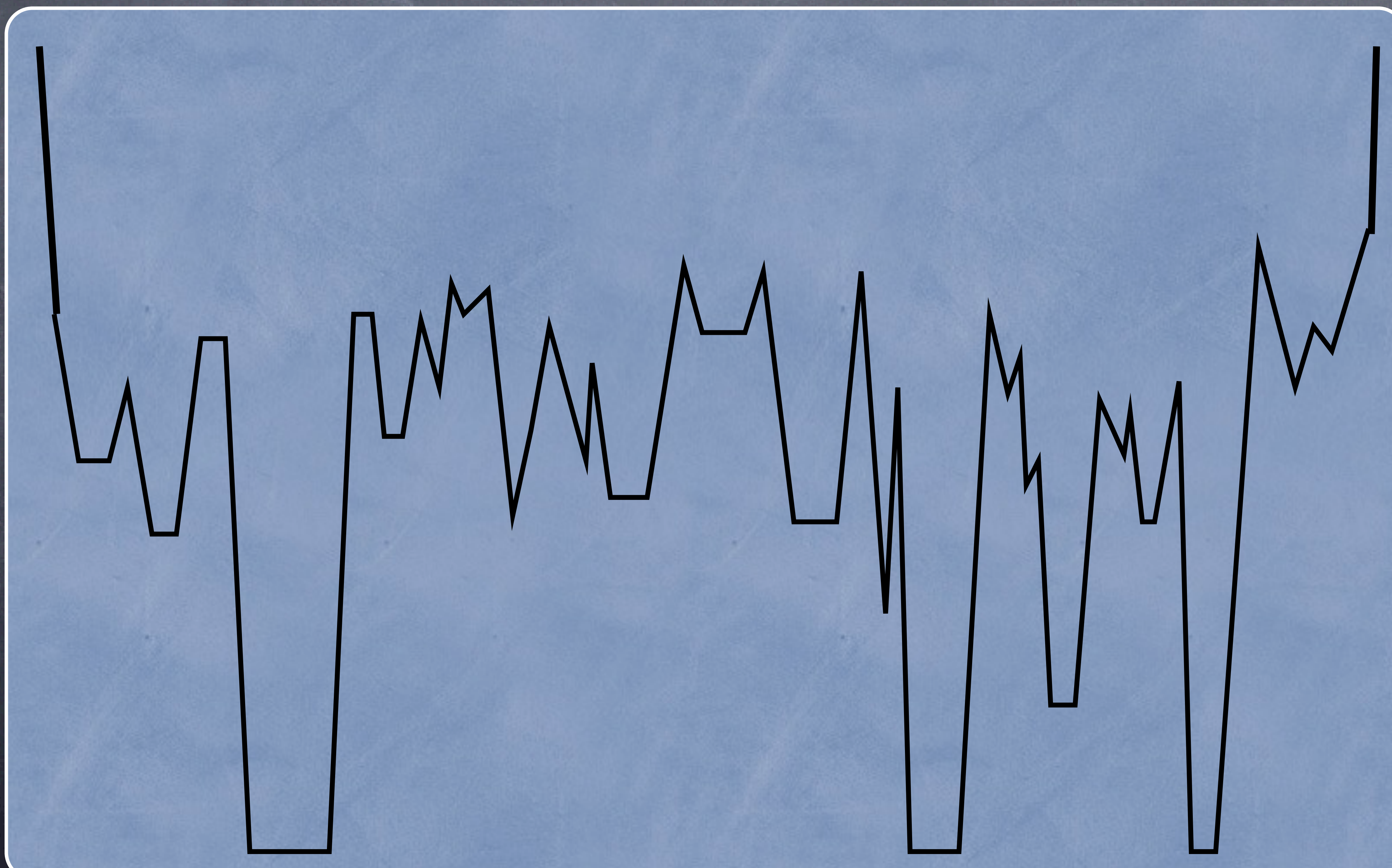
(except for spherical p-spin models, Cugliandolo-Kurchan'93 ...)

Need for a better description of the landscape

How to probe the energy landscape ?
(first in a cartoon)



Choose an energy value.



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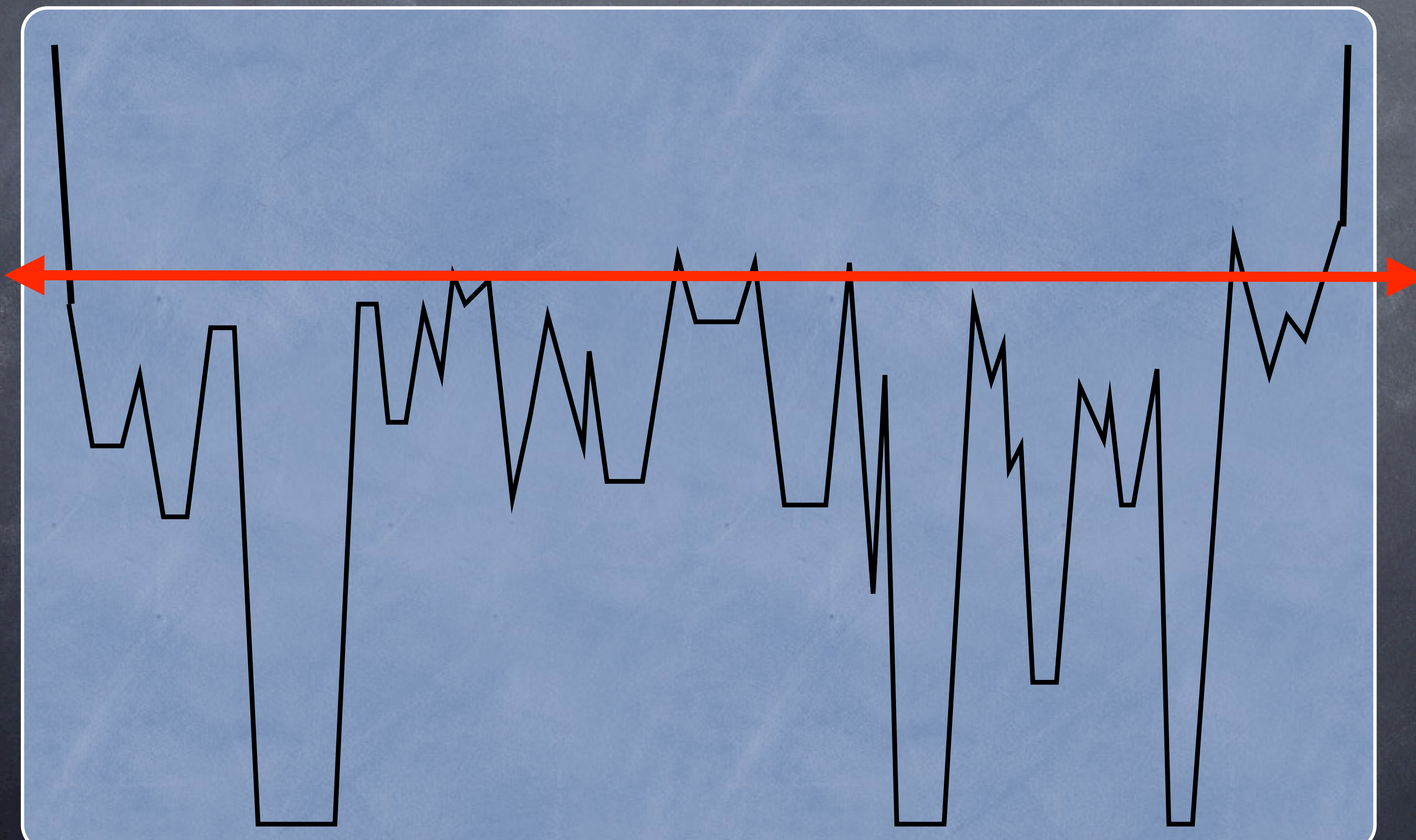
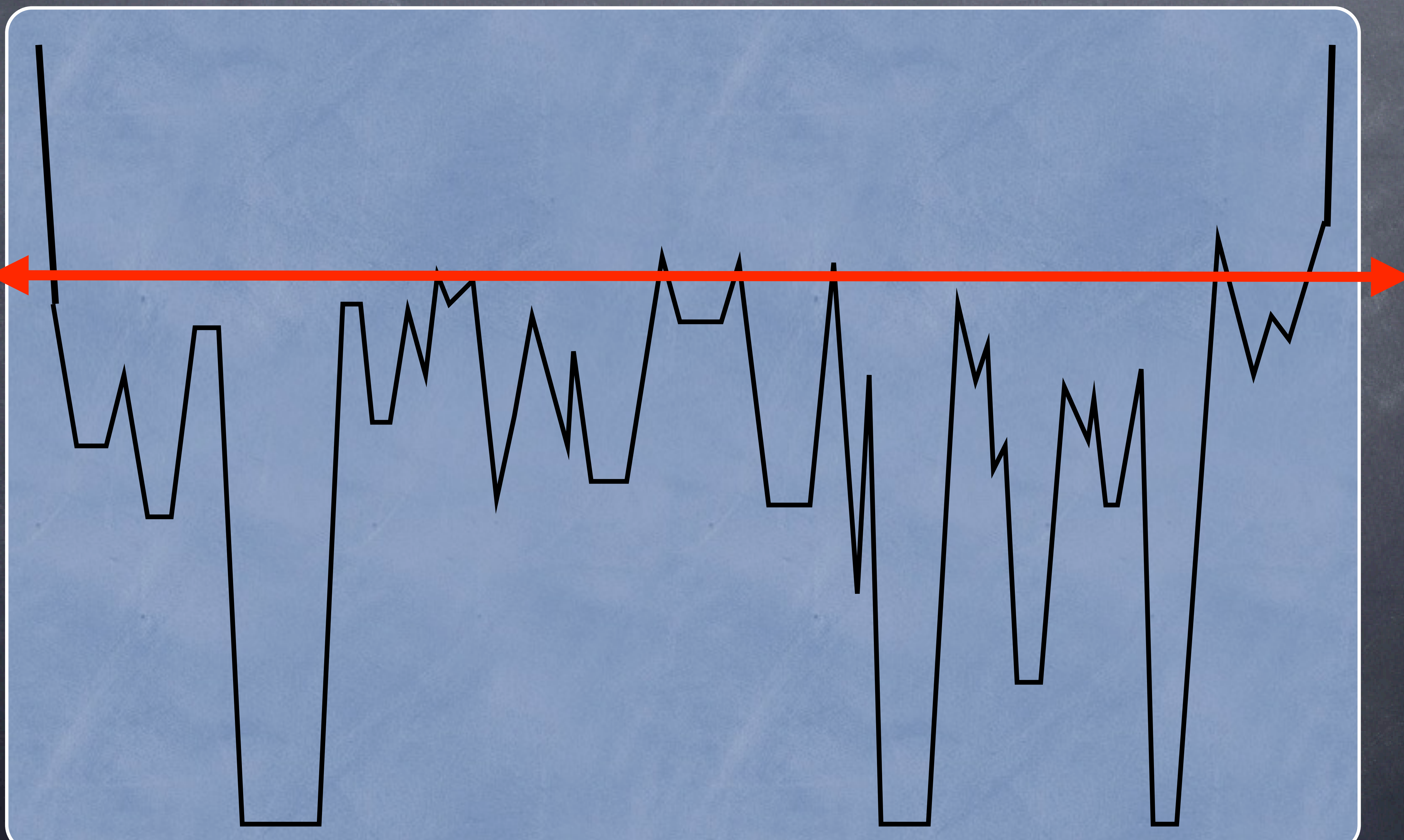


Then take a configuration at random at this energy, the configuration is such that the system is blocked in one of the “states”.



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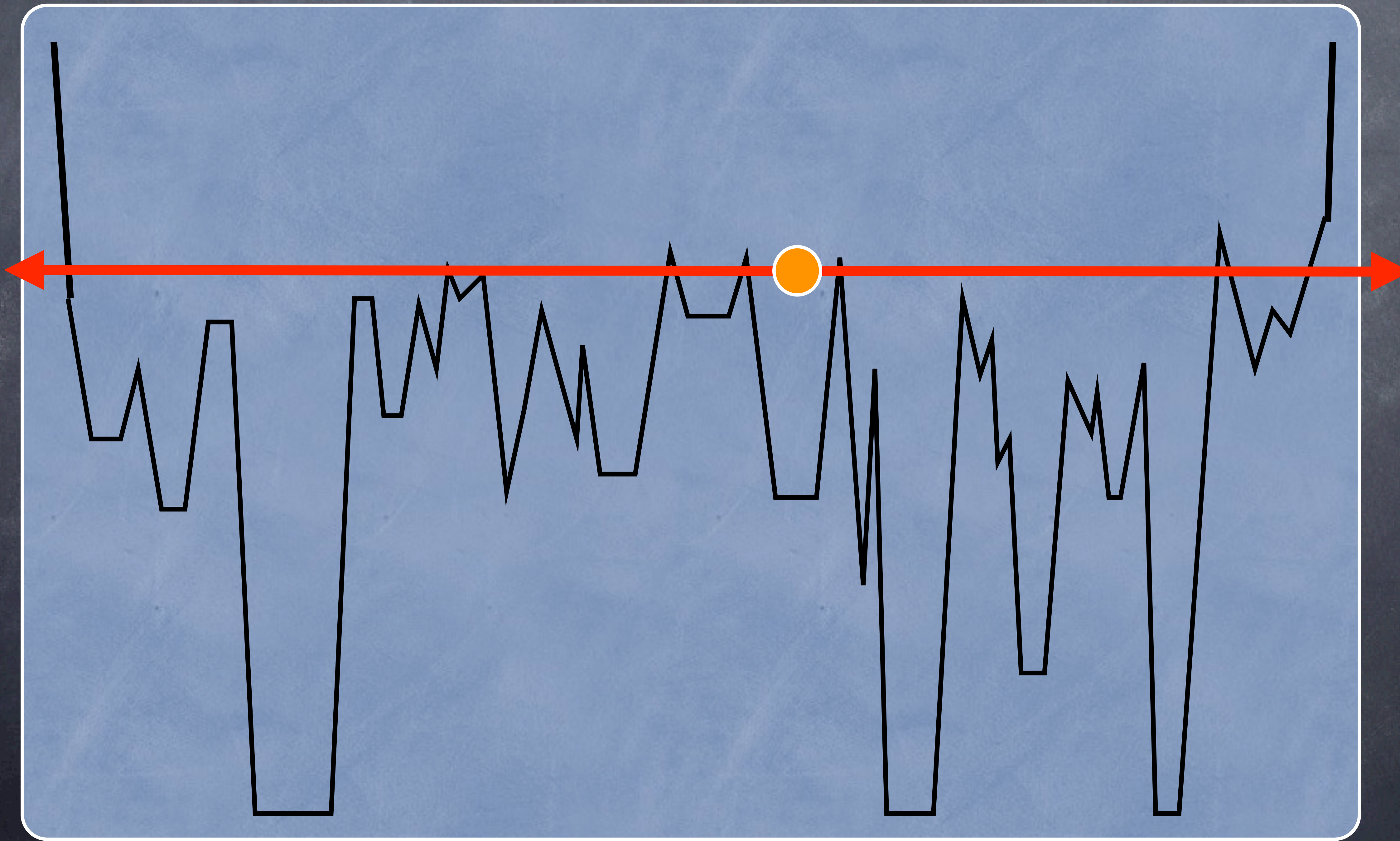
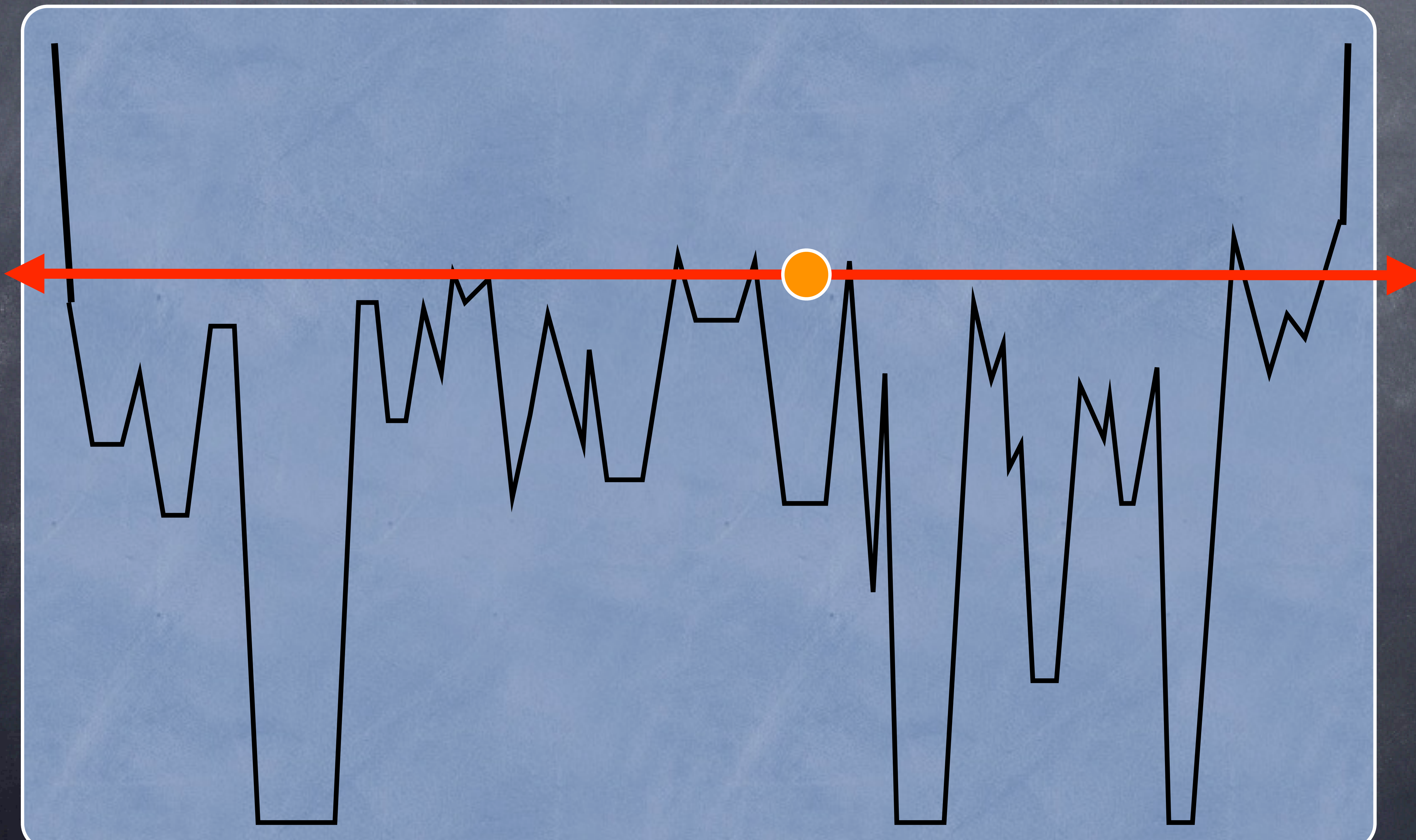


Compute the properties of the state for different energies



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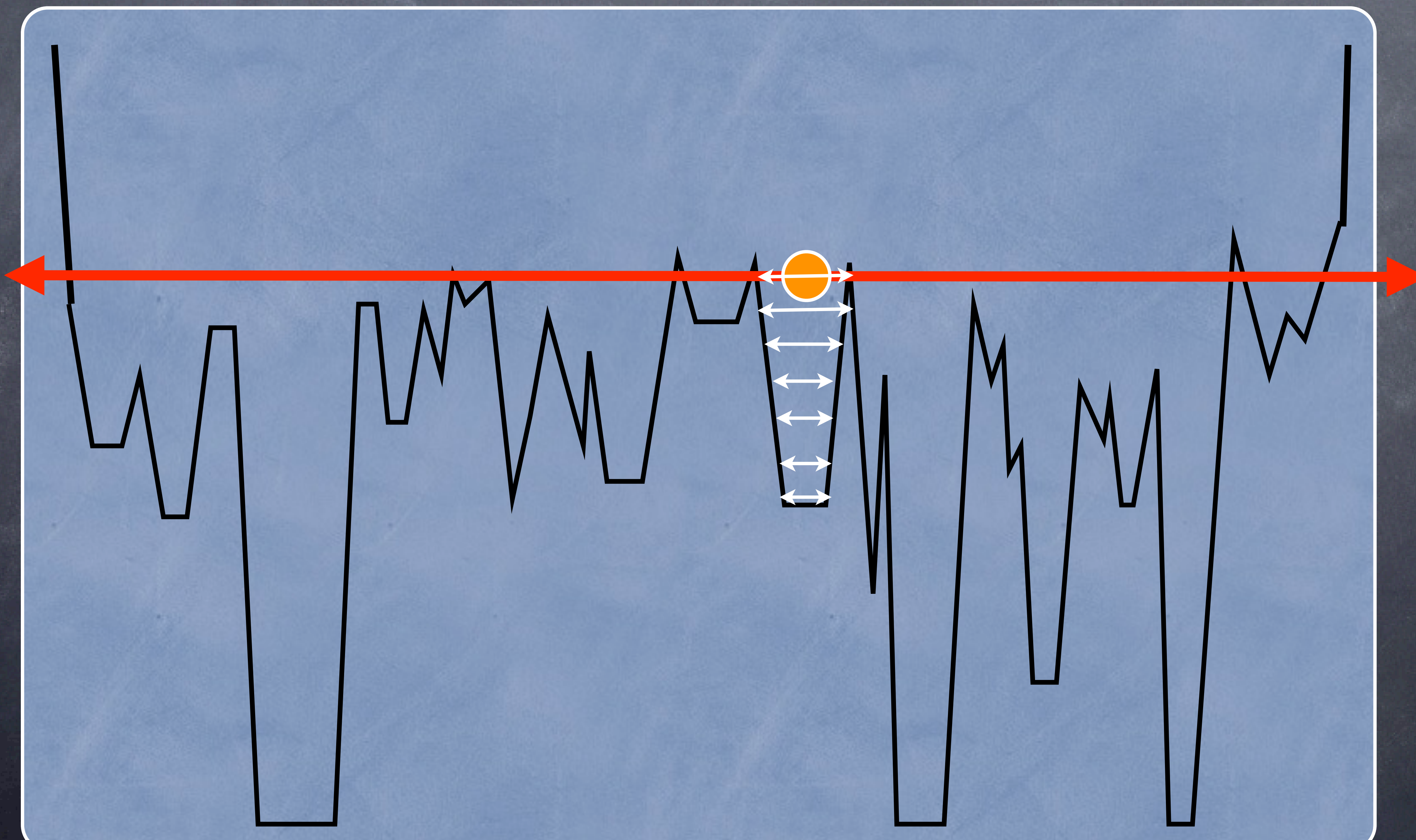
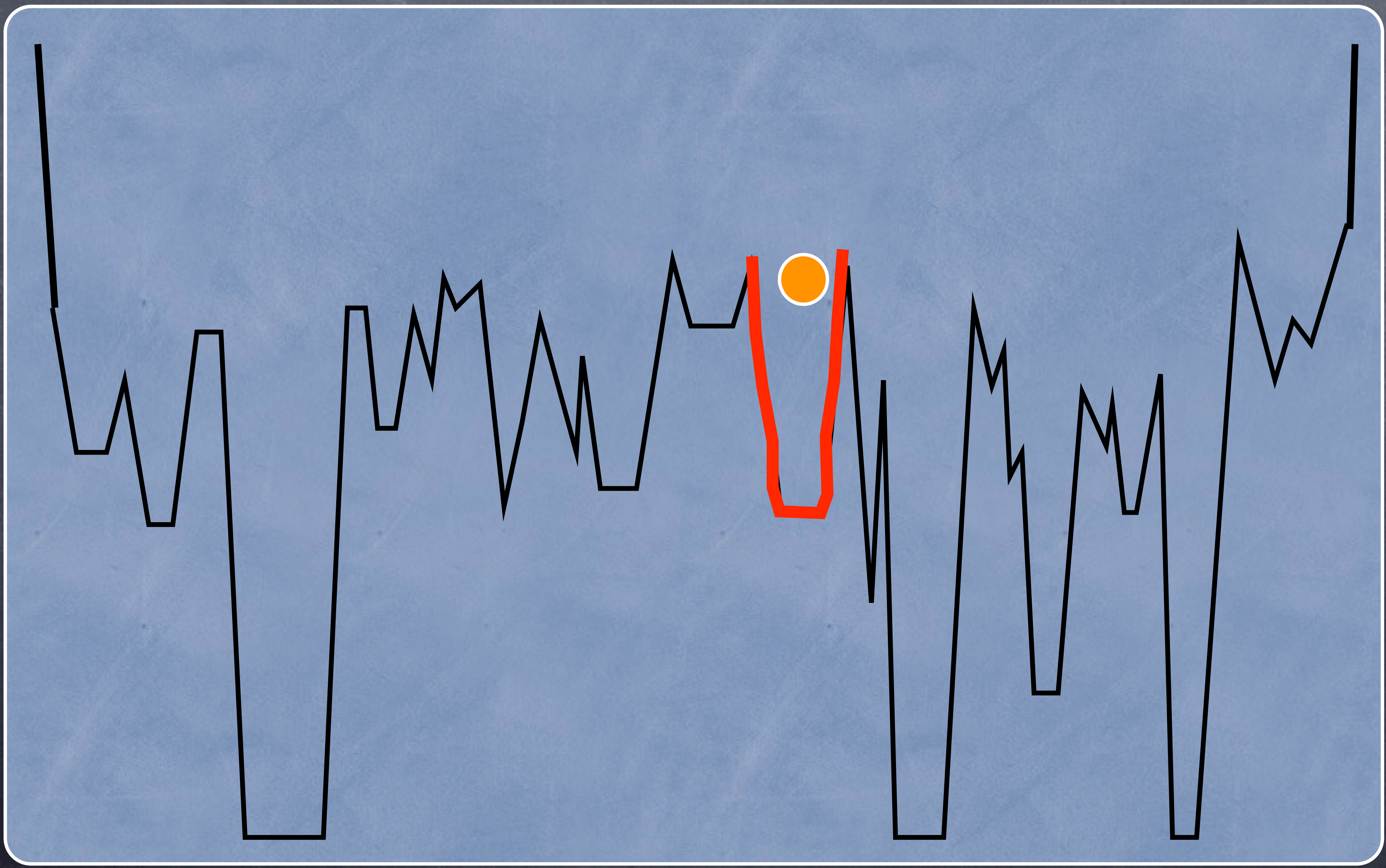
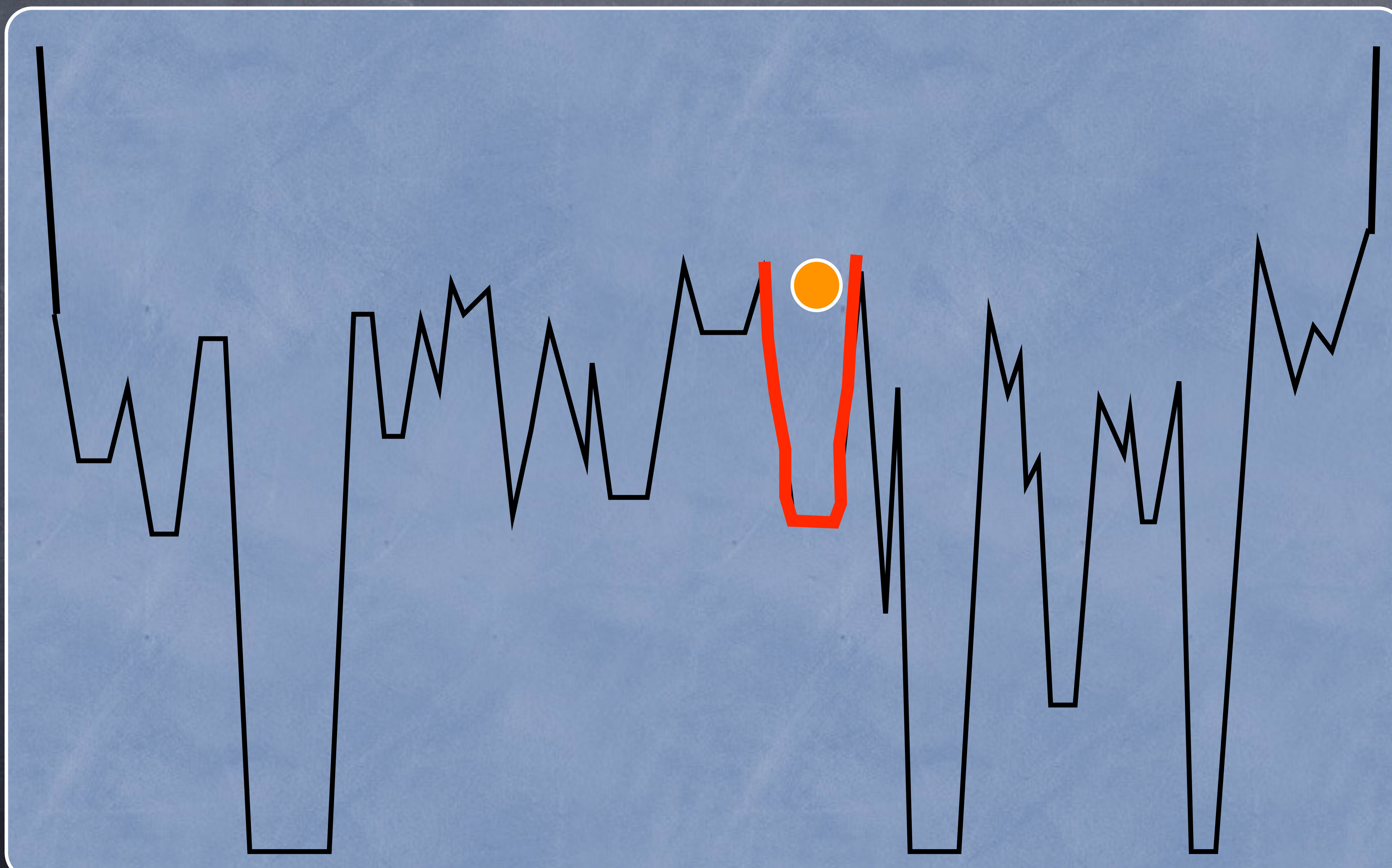


Now, we know what is the shape of an equilibrium state at the temperature we considered



We also know where the slow dynamics will end - at the bottom of the state!



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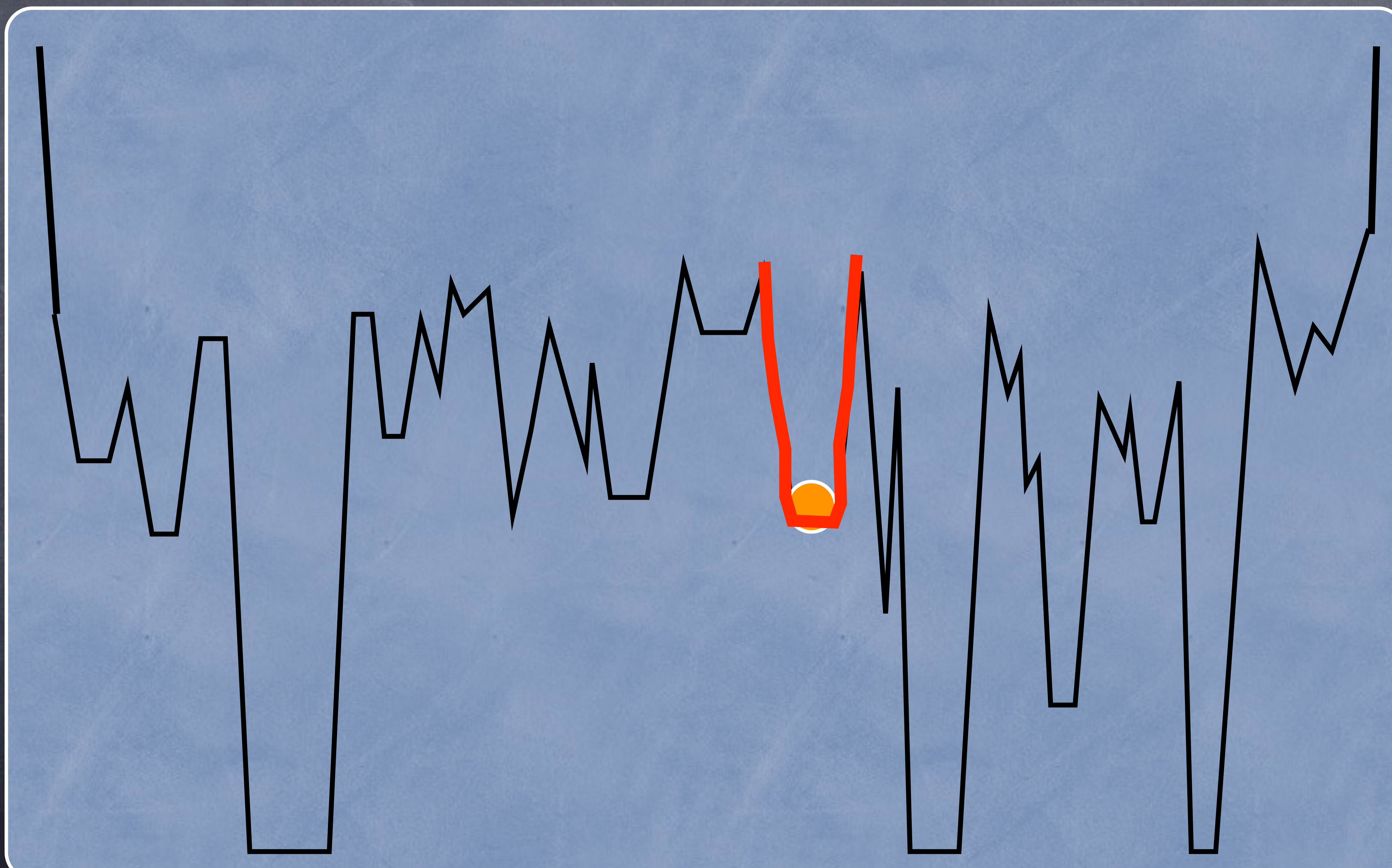


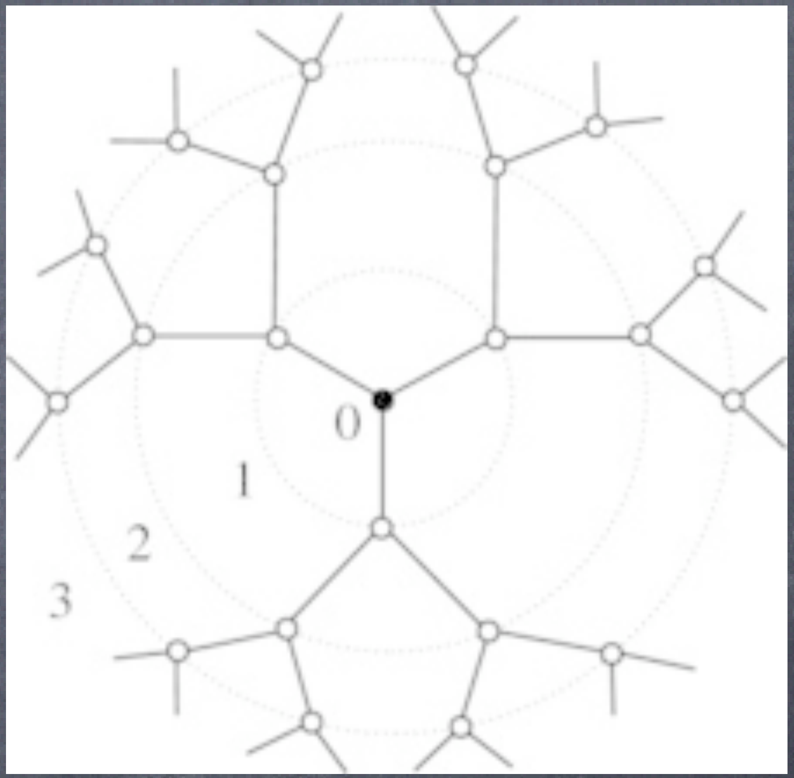
Following states in equations

ex.: the Potts anti-ferromagnet on random graphs

(1) Consider a large tree

(2) Choose a configuration uniformly at random from all those at energy ϵ per link. Corresponding temperature:

$$e^{\beta} = \frac{1-\epsilon}{(q-1)\epsilon} \qquad \beta \leq \beta_K$$



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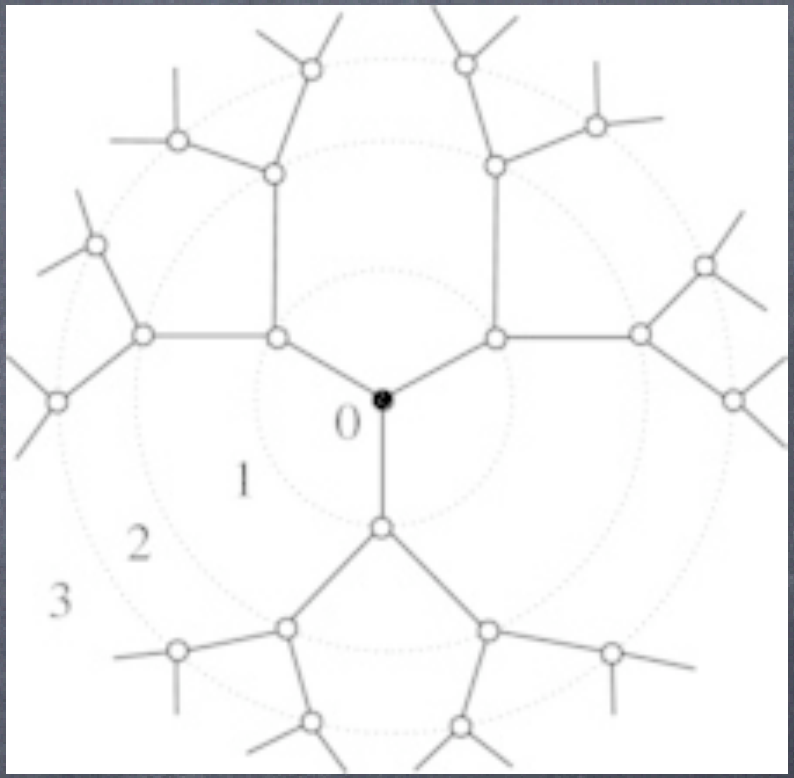
(a) Choose color of the root at random

(b) Iteratively, choose color of a child equal to the color of the parent with probability ϵ , and different with probability $1-\epsilon$



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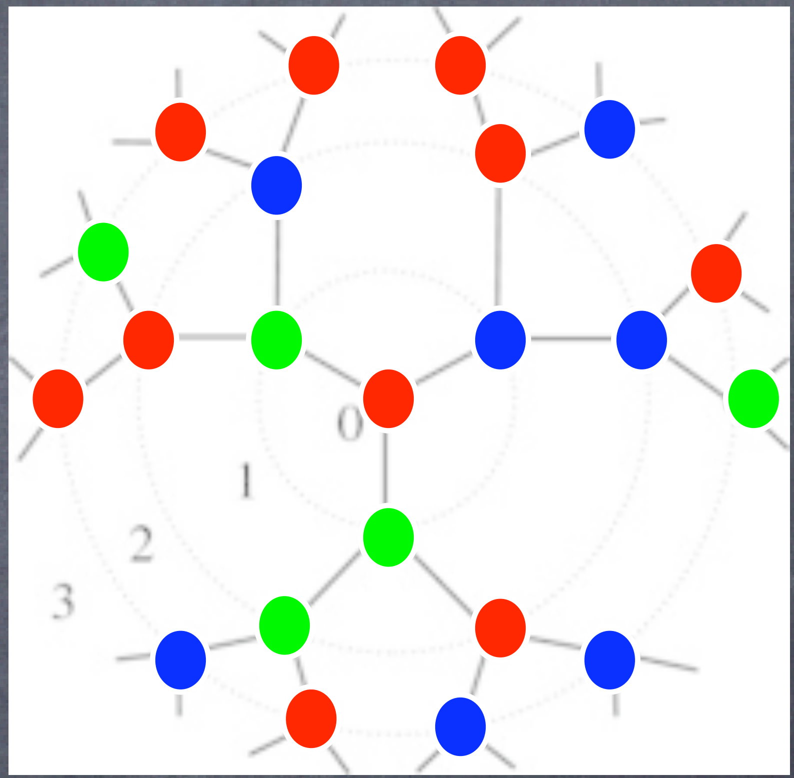

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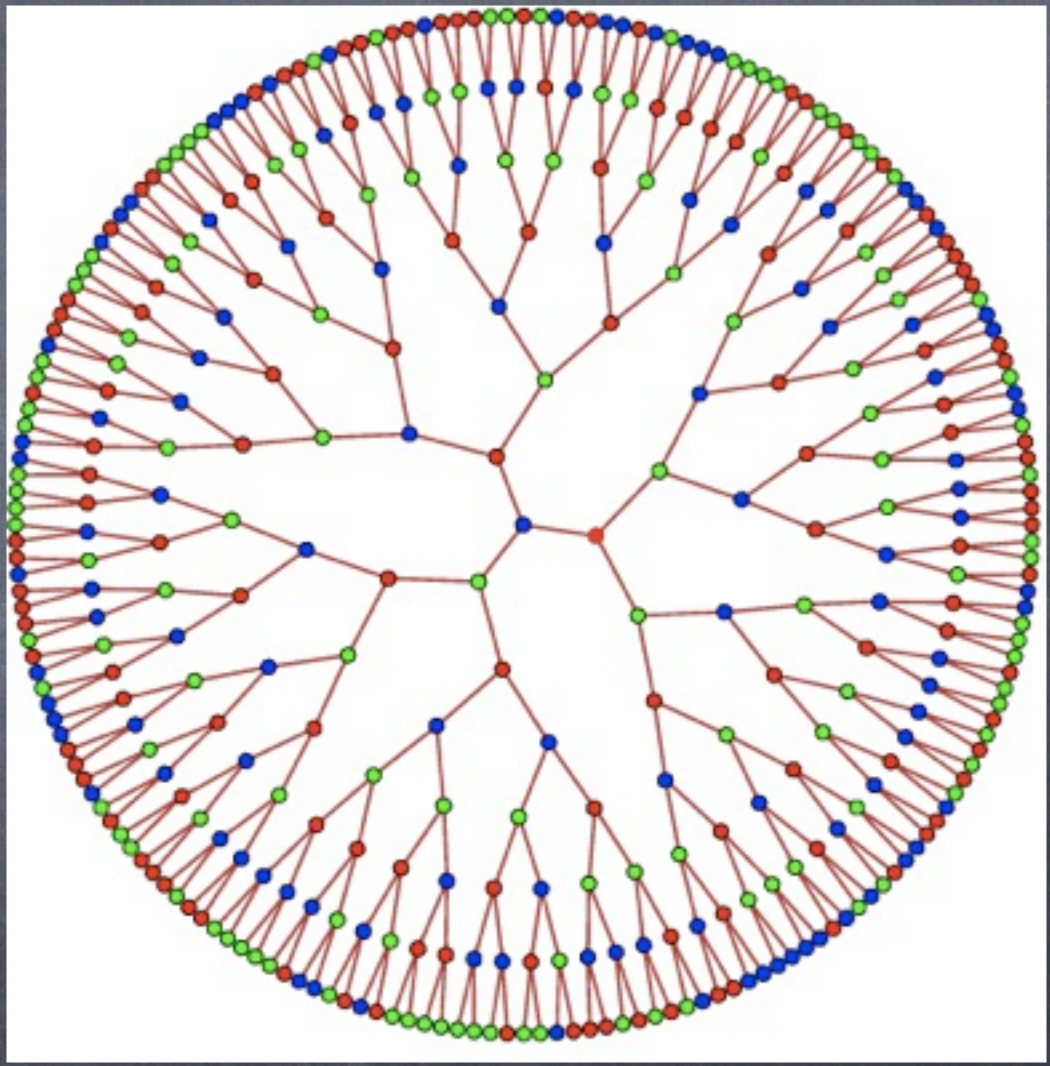

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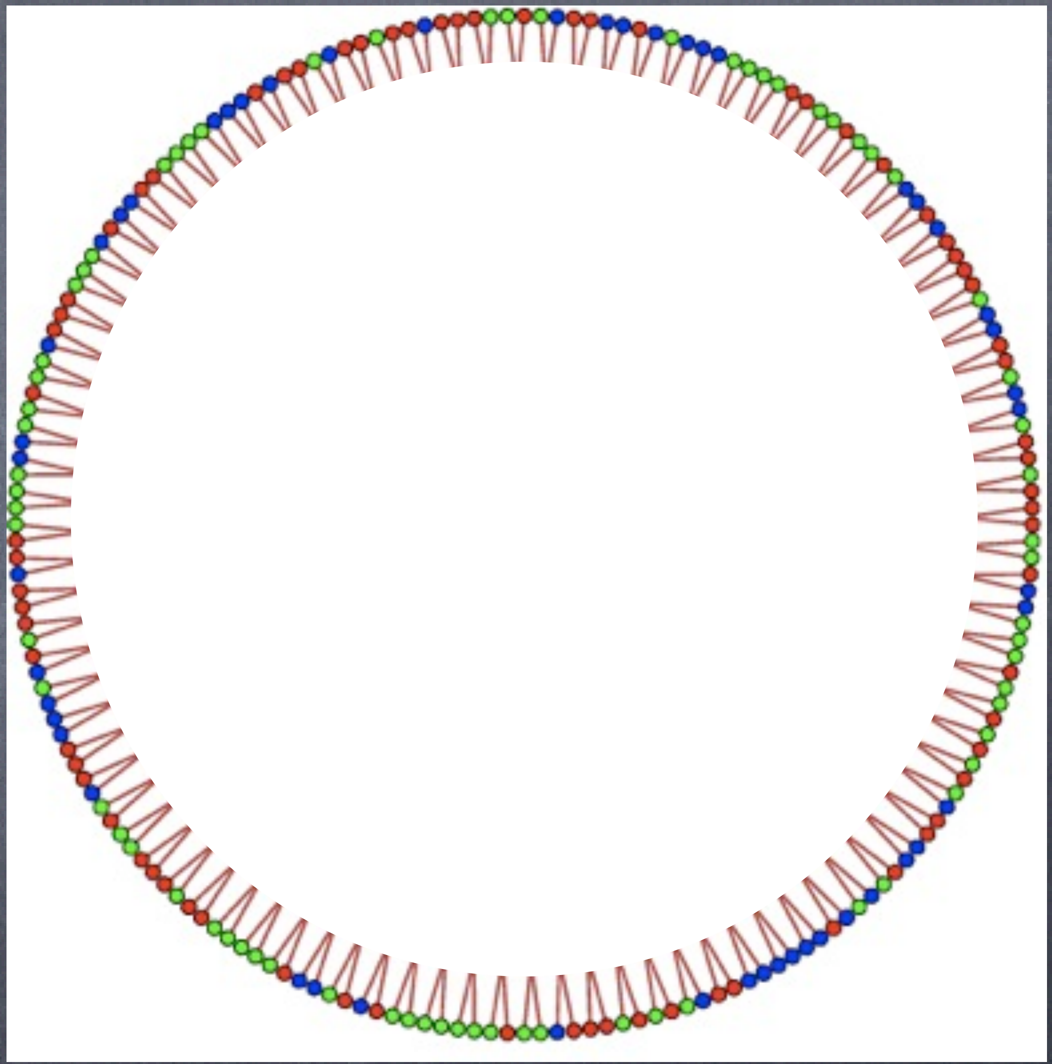

(3) Resulting boundary conditions define the Gibbs state, compute what measure they induce at a **different** temperature.

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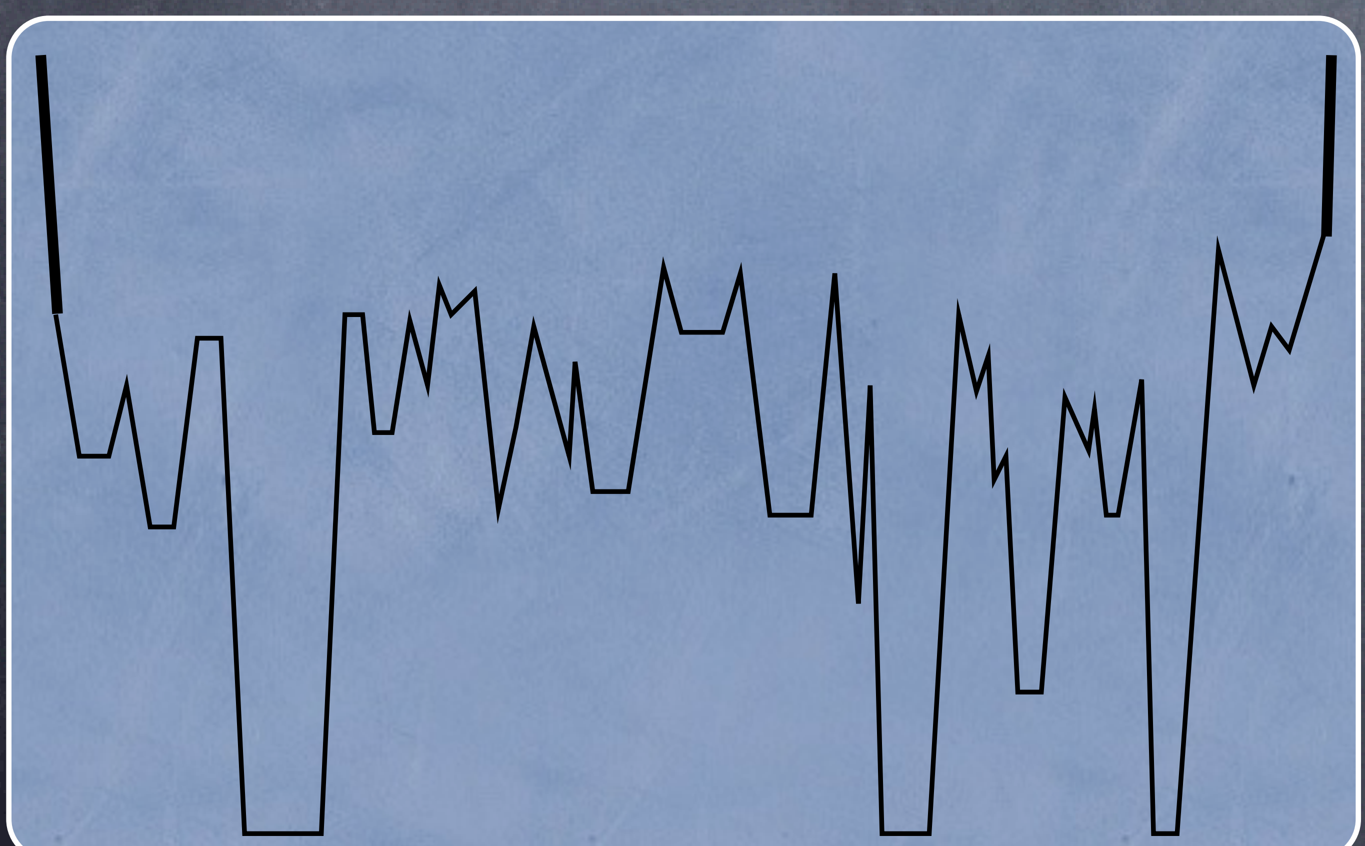
ex.: the p-spin (XOR-SAT) on random graphs



$$H = -\sum_{(ij)} J_{ij} \prod_{i=1}^{p} S_i$$

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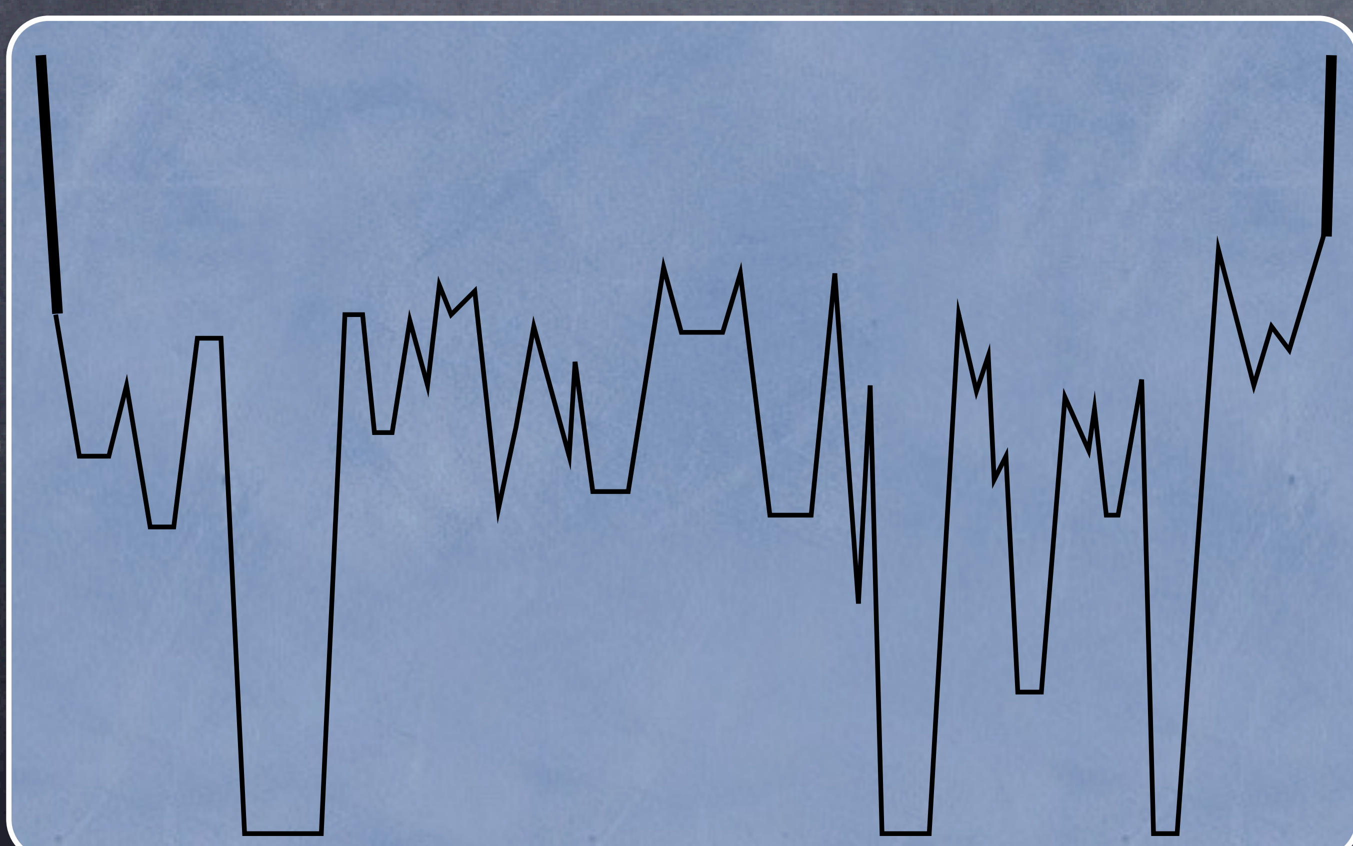
$$\epsilon(T_p) = (1 + e^{1/T_p})^{-1}$$



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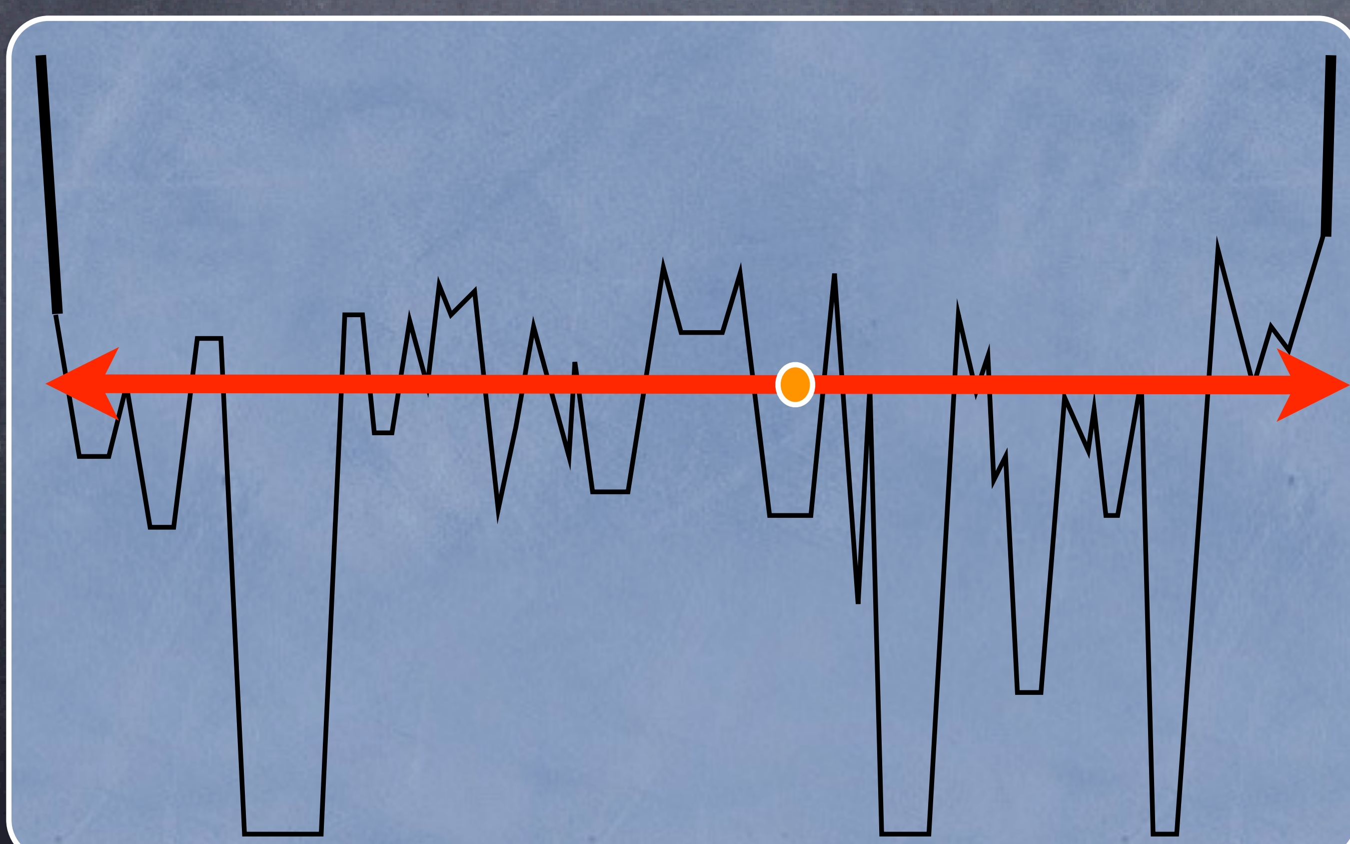

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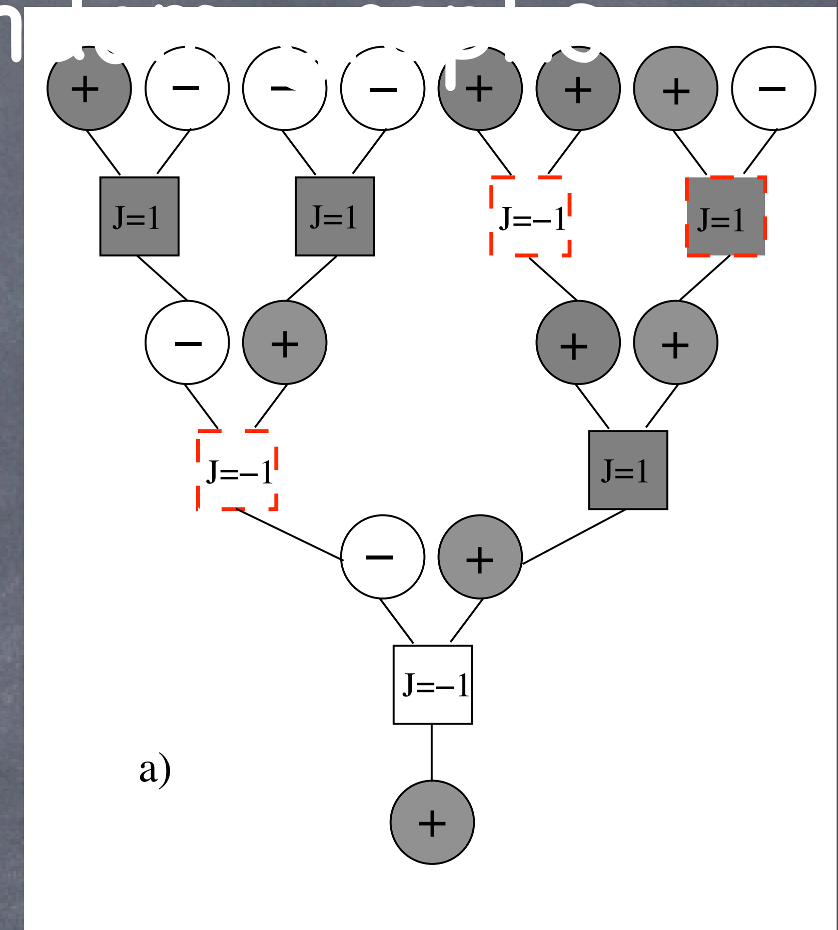

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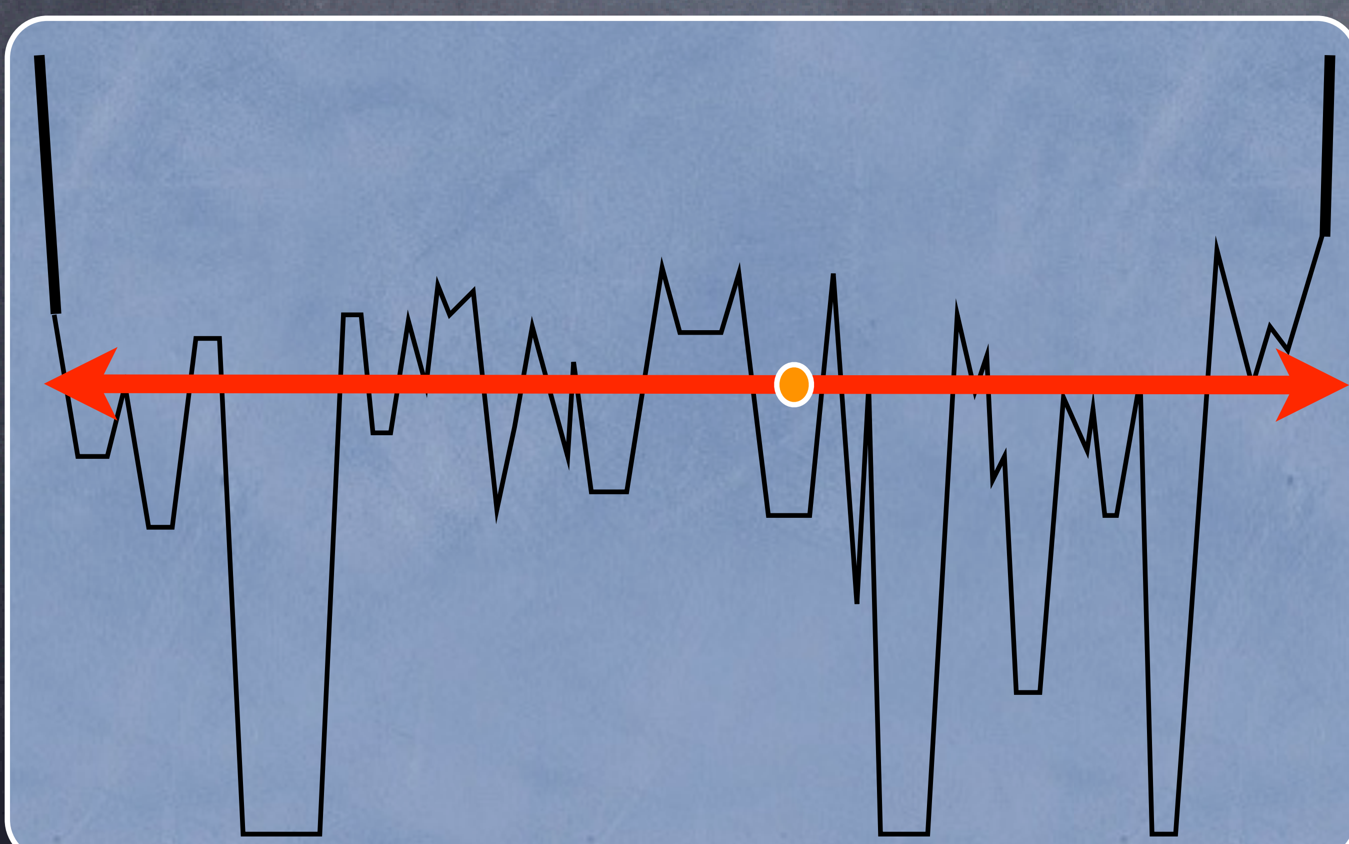

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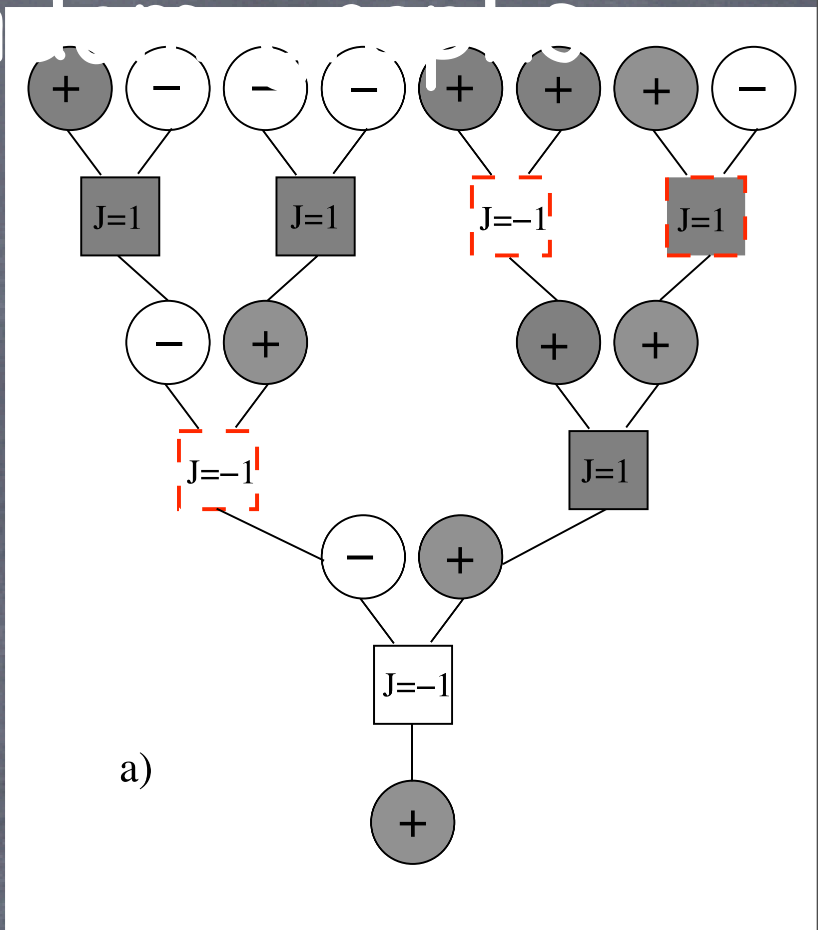

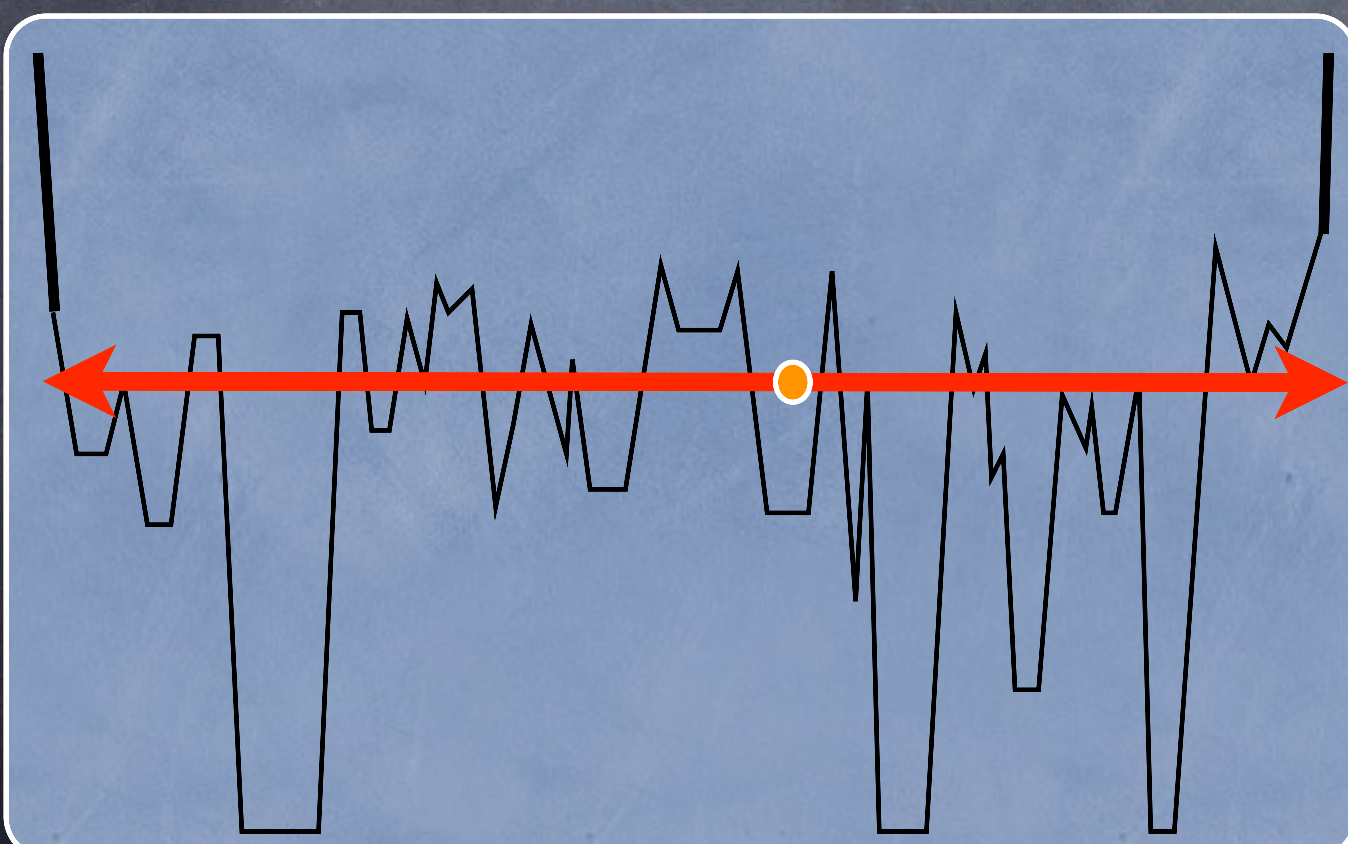

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This construction defines a set of recursive "Bethe-like" equation

$$P^{a\to i}(\psi^{a\to i}) = \frac{1}{\mathcal{Z}^{a\to i}} \int \prod_{j\in\partial a\setminus i} \prod_{b\in\partial j\setminus a} \mathrm{d}P^{b\to j}(\psi^{b\to j}) \left[Z^{a\to i}(\{\psi^{b\to j}\},\beta)\right]^m \delta[\psi^{a\to i} - \mathcal{F}(\{\psi^{b\to j}\},\beta)]$$

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How to make it even simpler ?

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How to make it even simpler ? ⇨ A powerful mapping via a Gauge transformation

A useful and powerful mapping

P-spin model (XORSAT)

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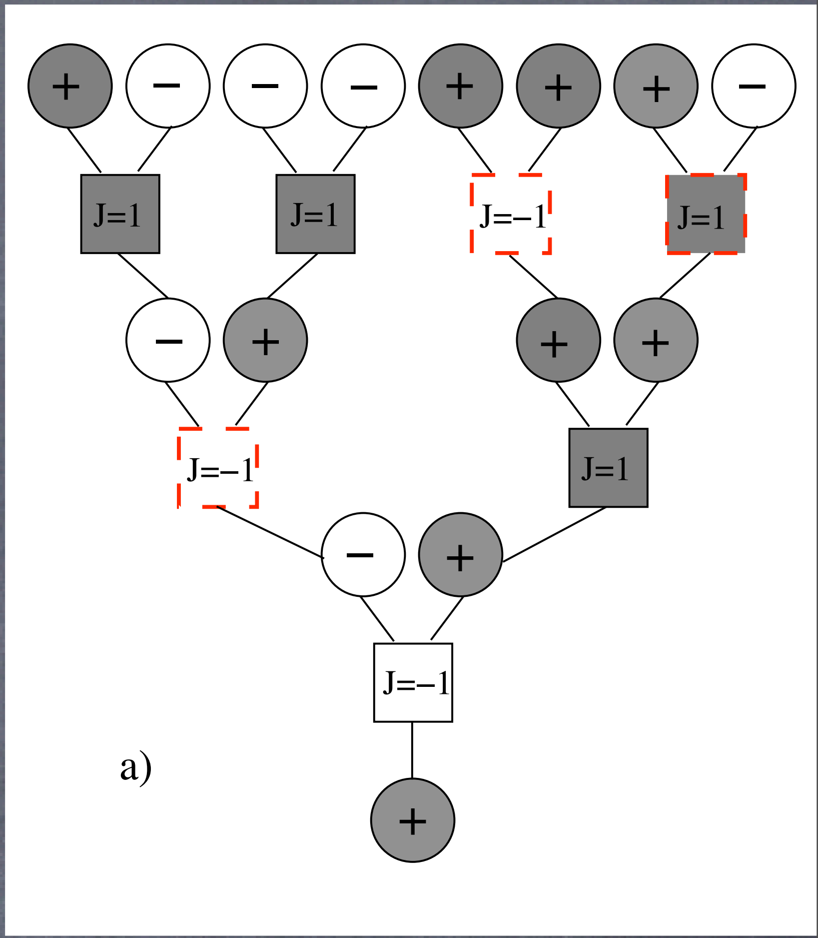
$$\epsilon(T_p) = (1 + e^{1/T_p})^{-1}$$



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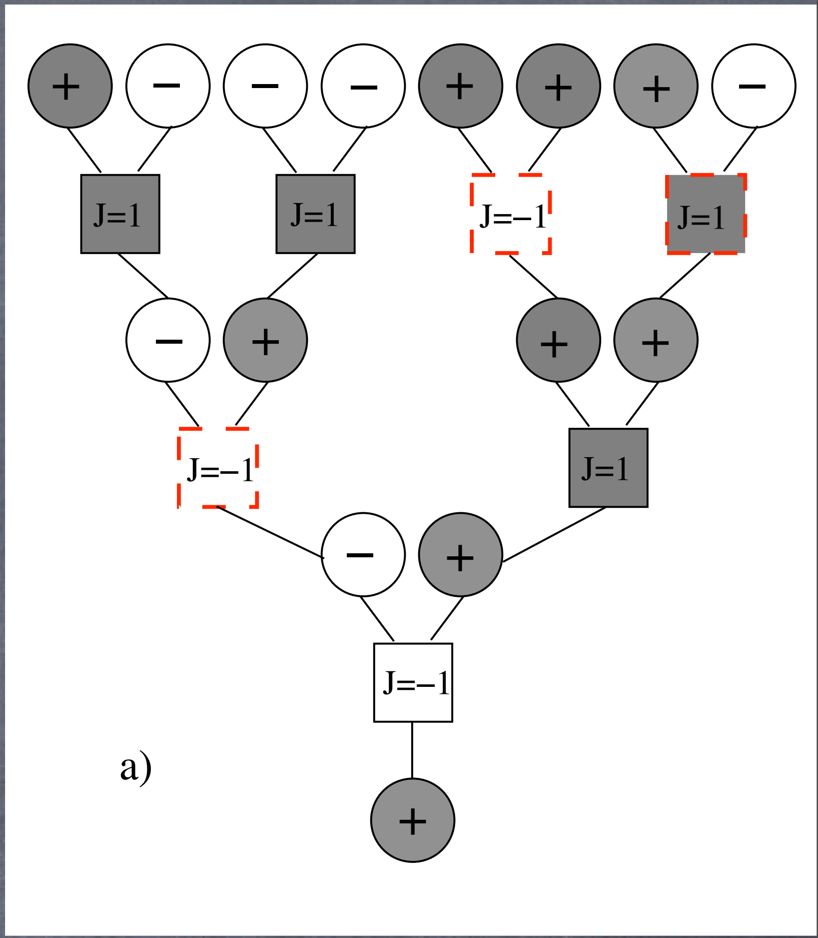

2) Notice the the following Gauge Transform let the Hamiltonian invariant

$$s_i \rightarrow -s_i \text{ and } J_{ij} \rightarrow -J_{ij} \text{ for all } j \in \partial i$$

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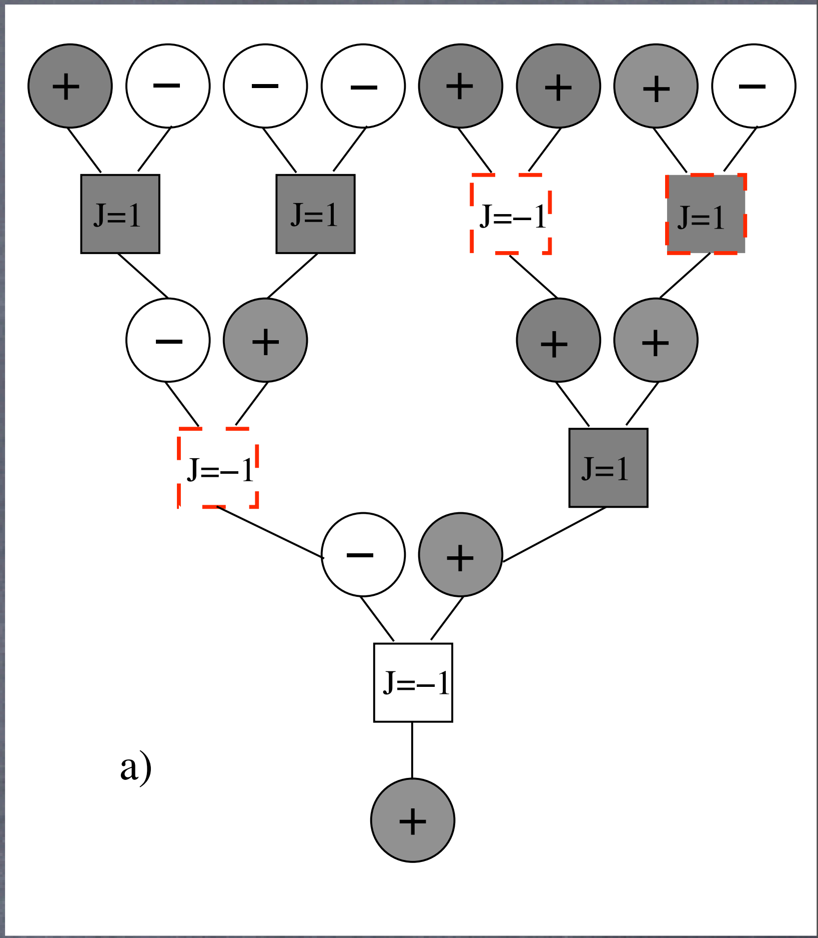

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3) Use the Gauge Transform to put all spins to ↑

$$H = -\sum_{(ij)} J_{ij} \prod_{i=1}^{p} S_i$$

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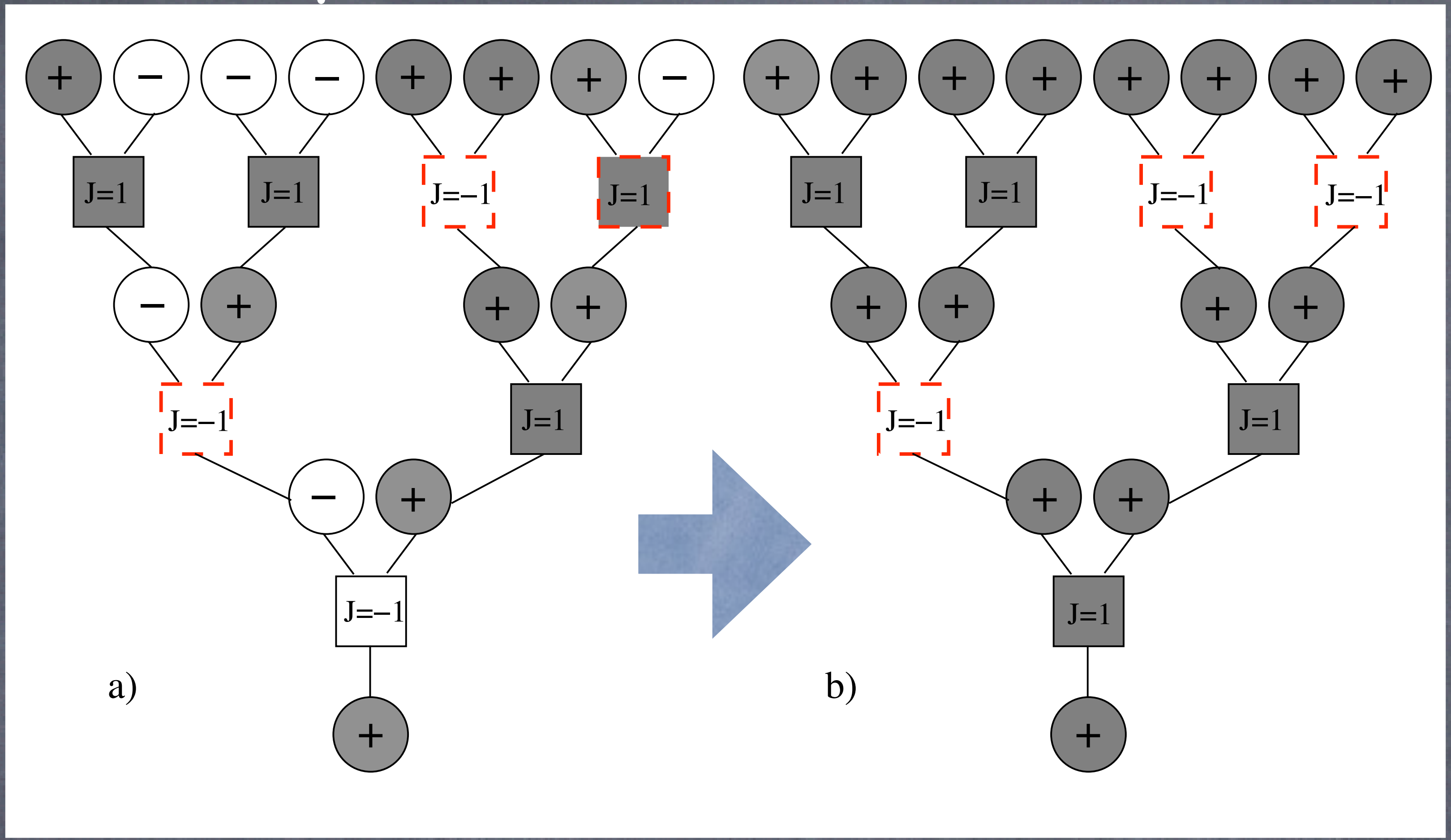

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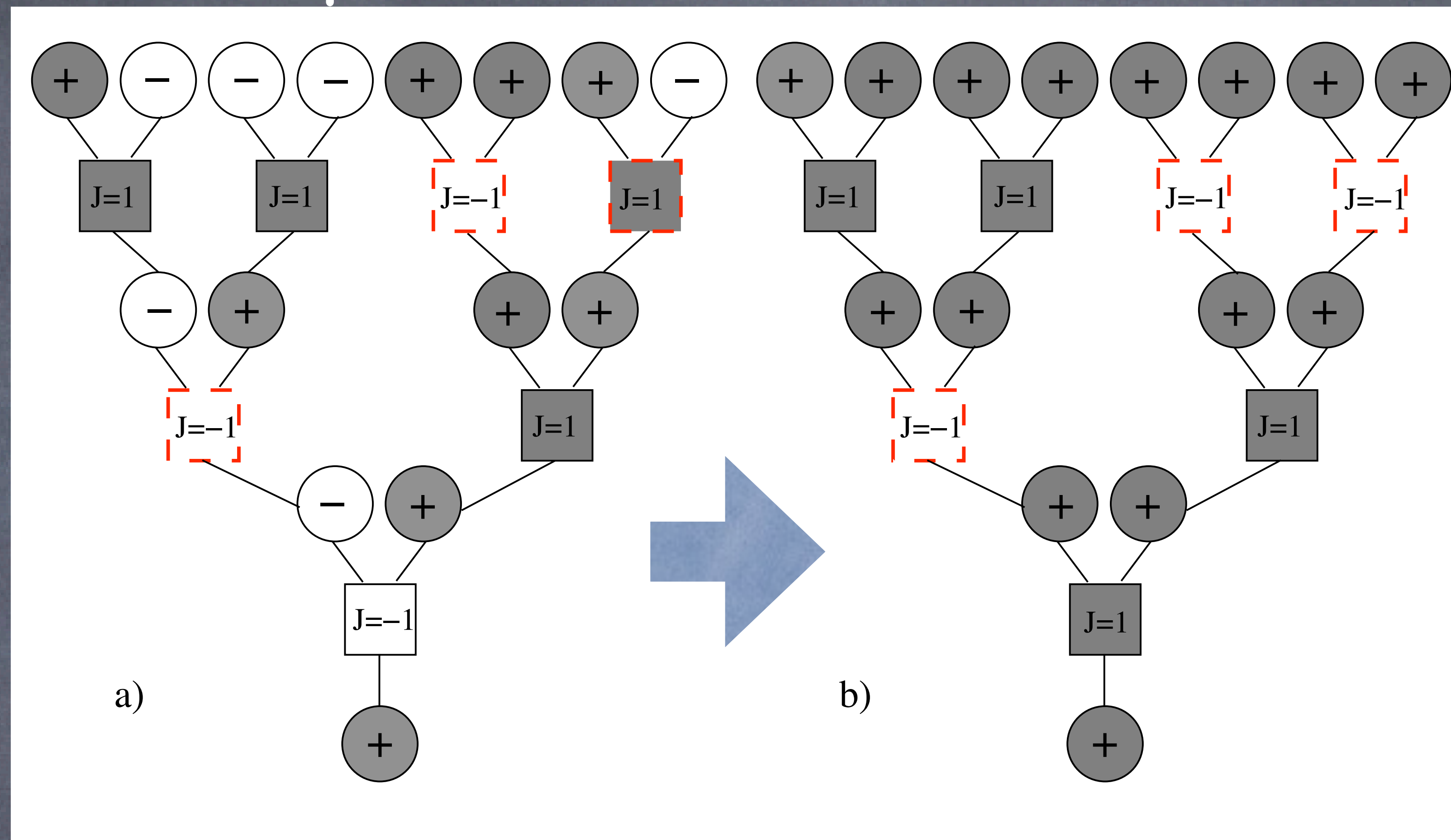

Now one has a trivial “ferromagnetic” border and the distribution of disorder has been transformed to

$$H = -\sum_{(ij)} J_{ij} \prod_{i=1}^{p} S_i$$

$$P_p(J) = \epsilon(T_p)\delta(J-1) + [1-\epsilon(T_p)]\delta(J+1)$$

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In order to study how an equilibrium spin glass"state" at temperature Tp behave at temperature T

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↓

You just need to study a ferromagnetic model with a fraction $\epsilon(T_p) = (1 + e^{1/T_p})^{-1}$ of negative interactions

↓

The phase diagram and the long time dynamics are trivially given by a simple equilibrium computation

Outline

I. Glassy landscapes

II. A new method to describe the landscape

III. Result I: Following states and the long time dynamics

IV. Result II: Analyzing simulated annealing: Canyons versus Valleys.

V. Result III: Presence of temperature chaos in the glass phase.

Ex.: Fully connected p-spin

(Derrida'81; Gross, Mezard'84; Kirkpatrick, Thirumalai'87)

$$\mathcal{H} = -\sum_a J_a \prod_{i \in \partial a} s_i \,,$$

$$\langle J_a \rangle = 0$$

$$\langle J_a^2 \rangle = J^2 p! / (2N^{p-1})$$

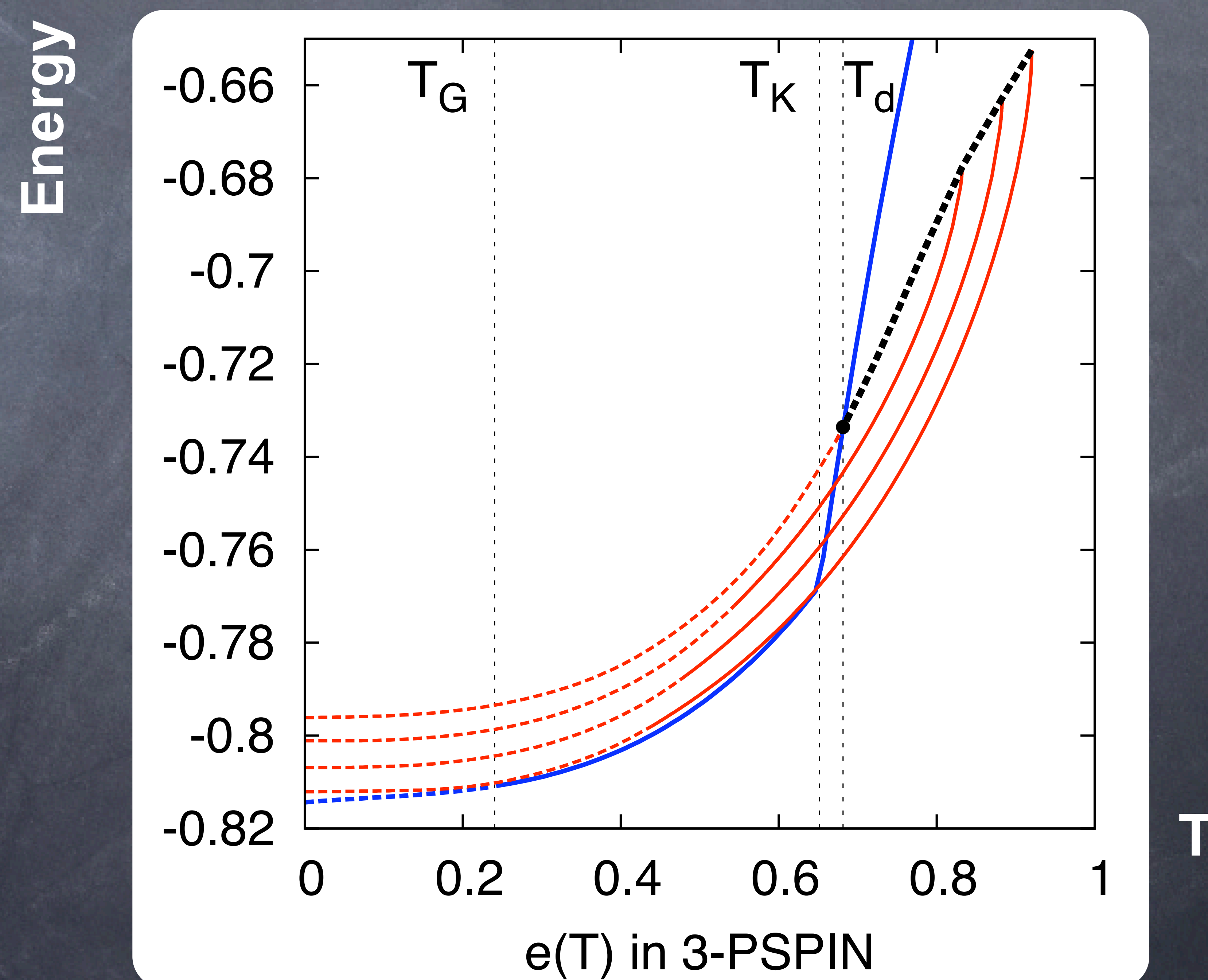
Properties of state equilibrium at β, at temperature $\tilde{\beta}$

$$m = \int_{-\infty}^{\infty} \mathcal{D}y \tanh\left(\tilde{\beta} J y \sqrt{pq^{p-1}/2} + \tilde{\beta}\beta J^2 p m^{p-1}/2\right)$$

$$q = \int_{-\infty}^{\infty} \mathcal{D}y \tanh^2\left(\tilde{\beta} J y \sqrt{pq^{p-1}/2} + \tilde{\beta}\beta J^2 p m^{p-1}/2\right)$$

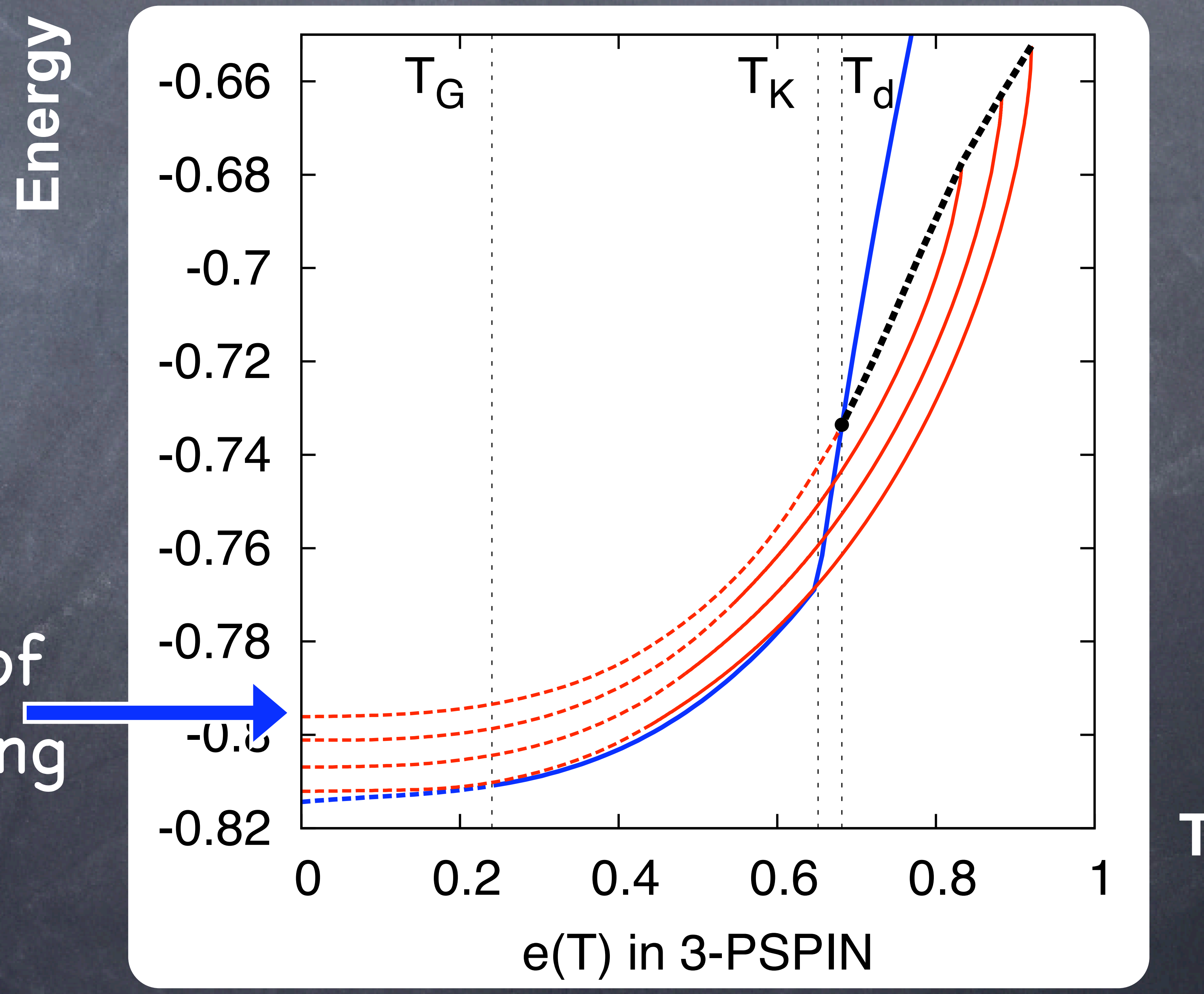
$\tilde{\beta} = \beta \quad \Rightarrow \quad m = q$ due to the Nishimori condition

Results for the fully connected p-spin

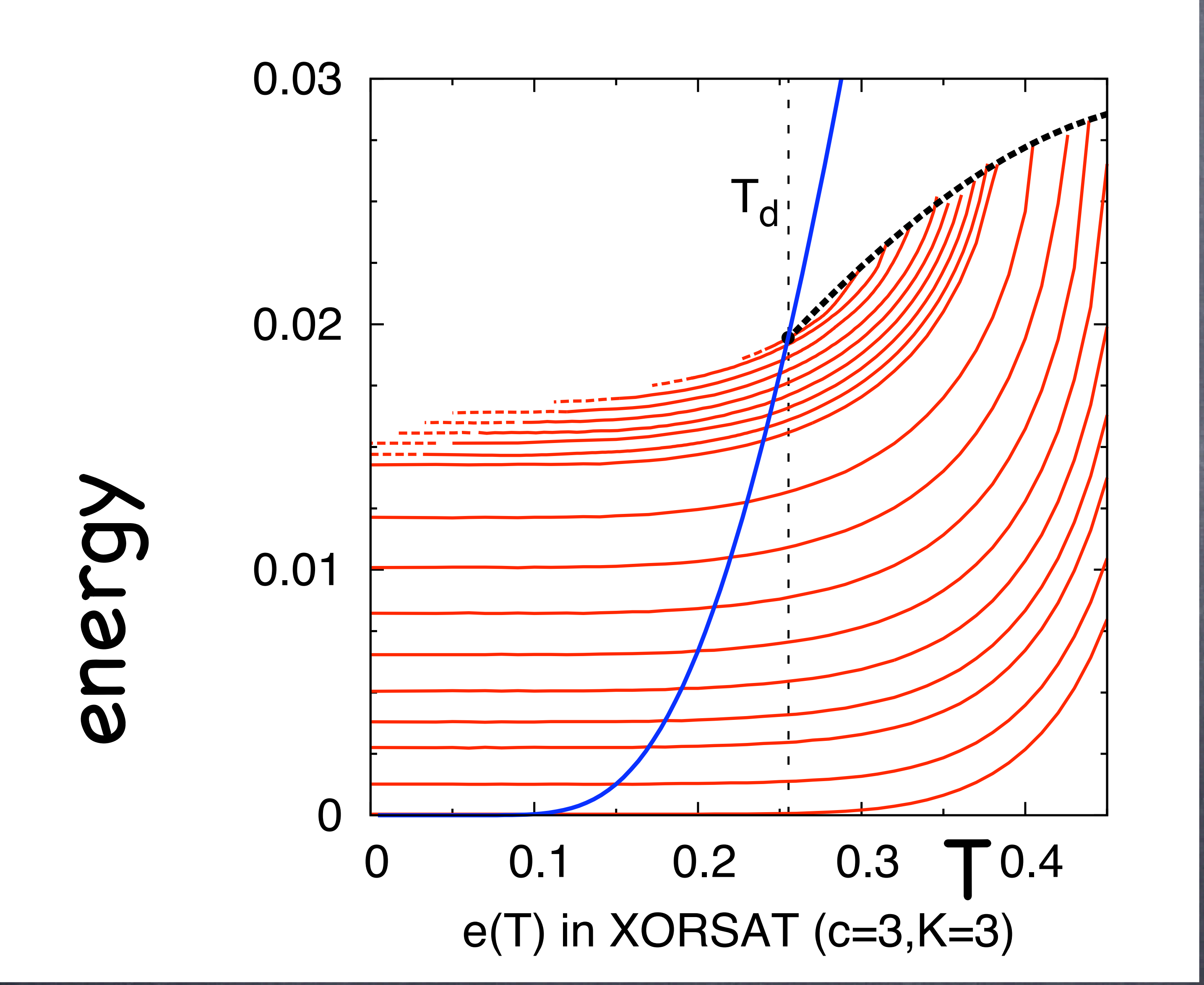


Results for the fully connected p-spin

Limiting energy of very slow annealing

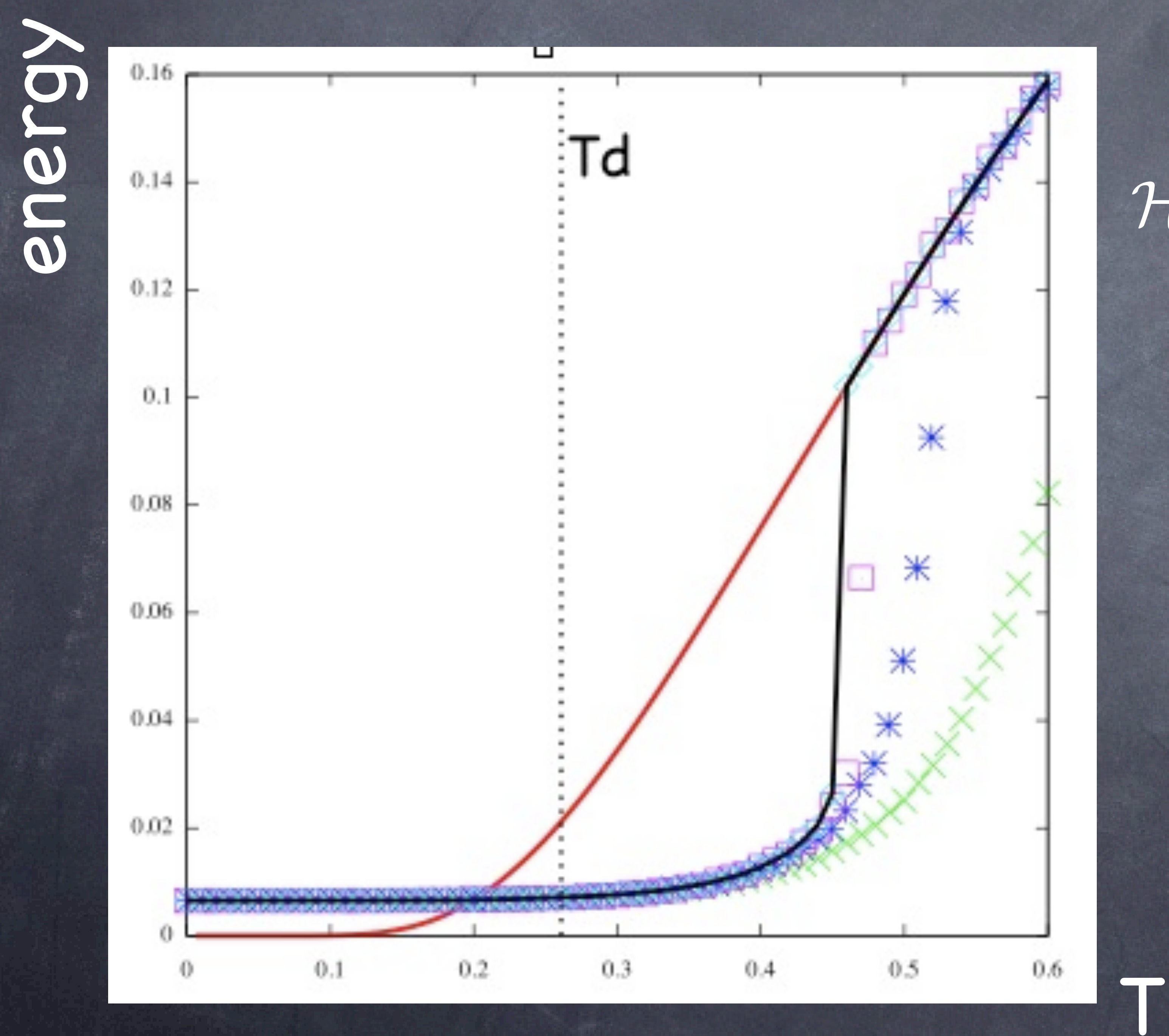


Results for the diluted connected p-spin



Comparison with Monte Carlo dynamics

(equilibrated at T=0.2 using the Planting Method)



$$\mathcal{H}(\{S\}) = \sum_{ijk} \frac{1 + J_{ijk} S_i S_j S_k}{2}$$

coordination z=3

N=200 000 spins

MC annealings starting from equilibrium at T=0.2

Long time dynamics

- The long time dynamics starting from equilibrium is given by a "static" computation.
- This can be checked directly by Monte-Carlo simulation
- Our method allow to recover easyly the exact results on the dynamics of spherical models (Cugliandolo-Kurchan 93, Franz-Parisi 97...)

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Usual answer: Hard to find ground state in a glassy landscape.

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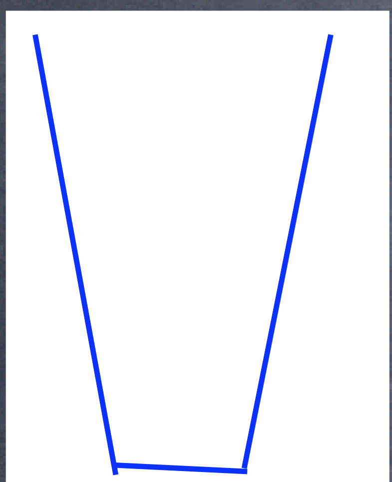

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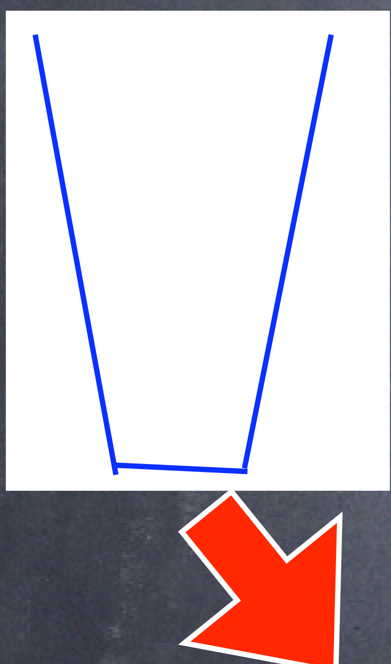

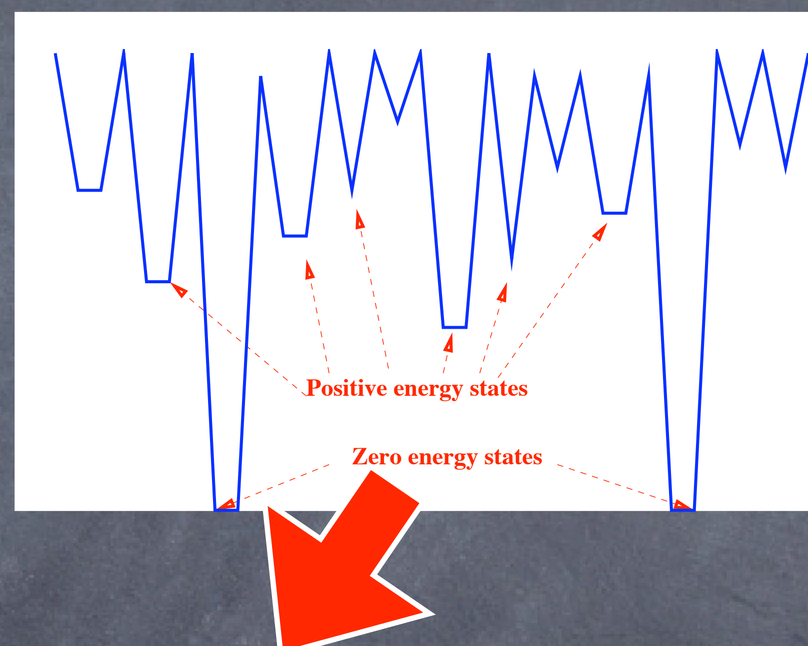

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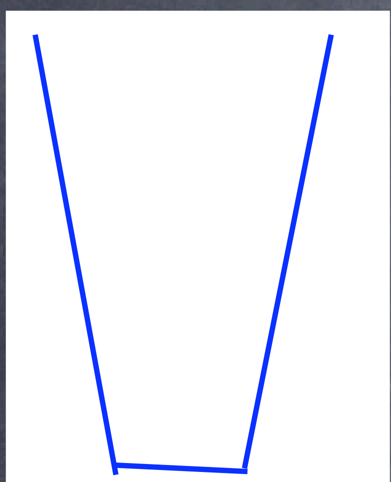

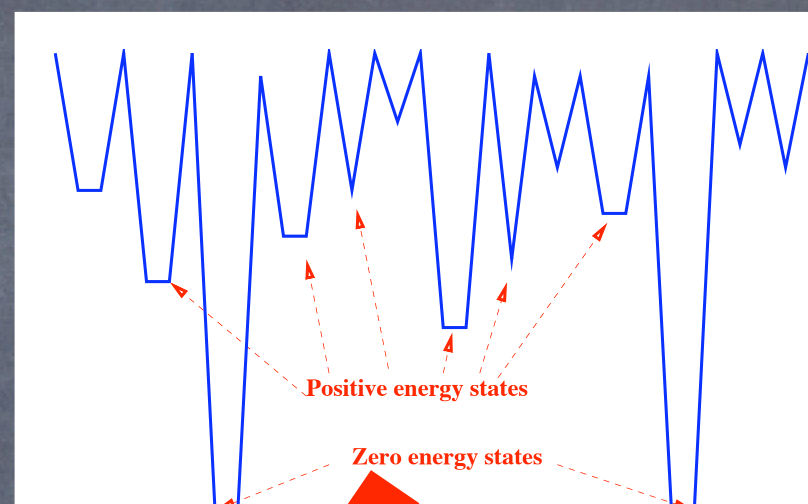

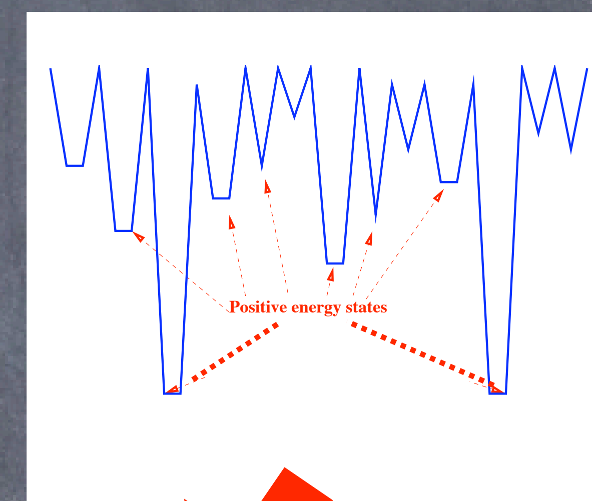

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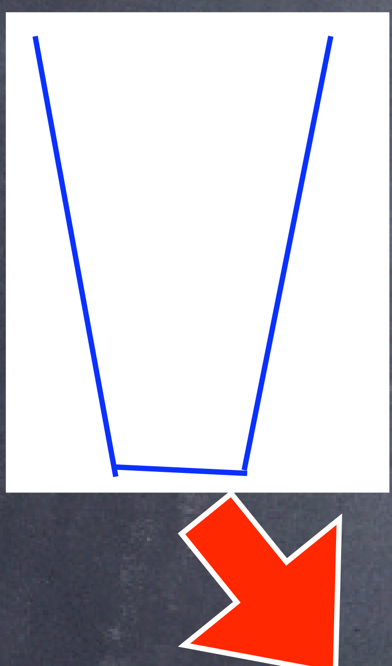

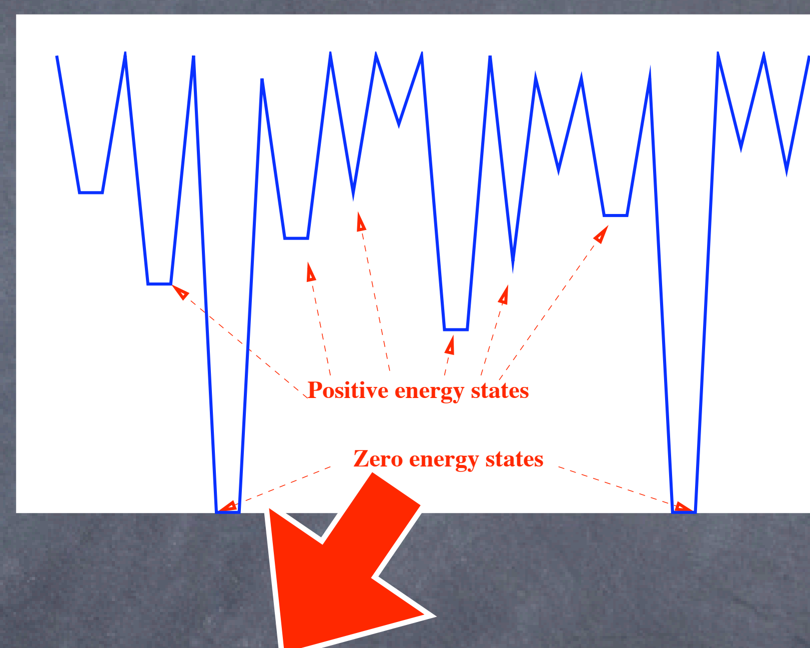

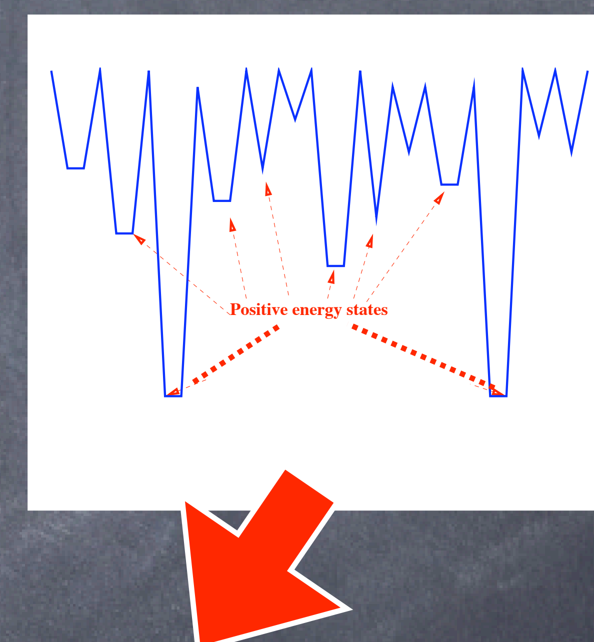

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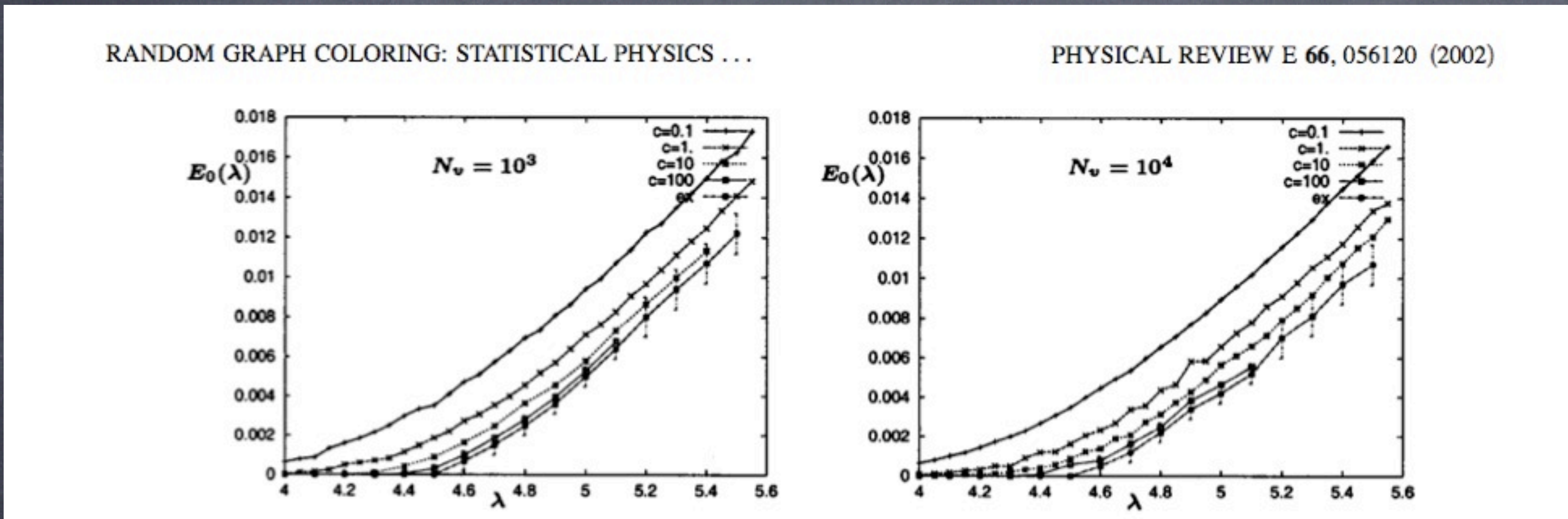

3-col: Monte Carlo annealing finds EASYLY ground states in the glassy region (Saad, Van Mourik 02')

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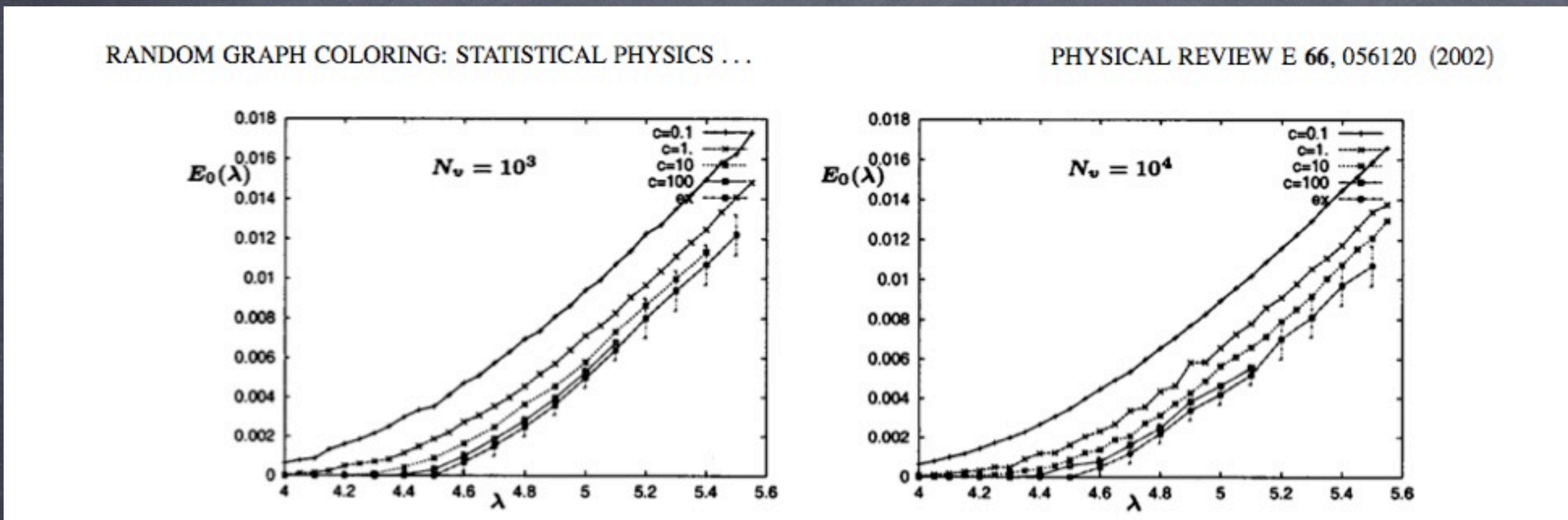

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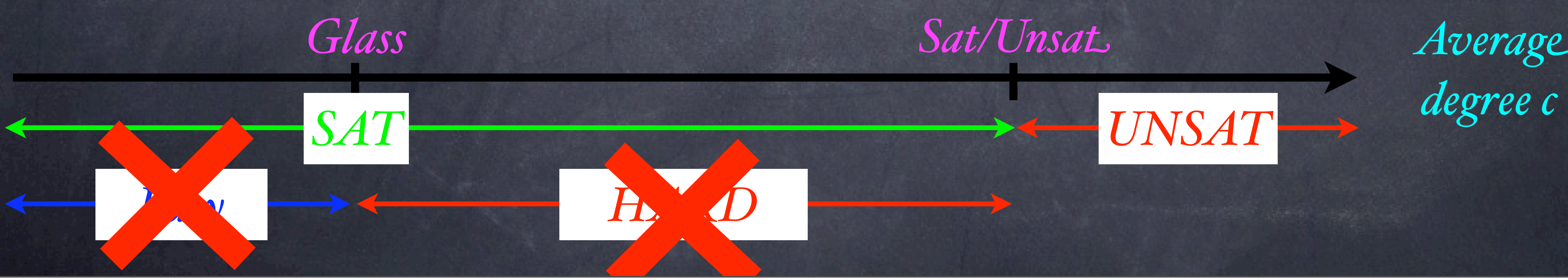

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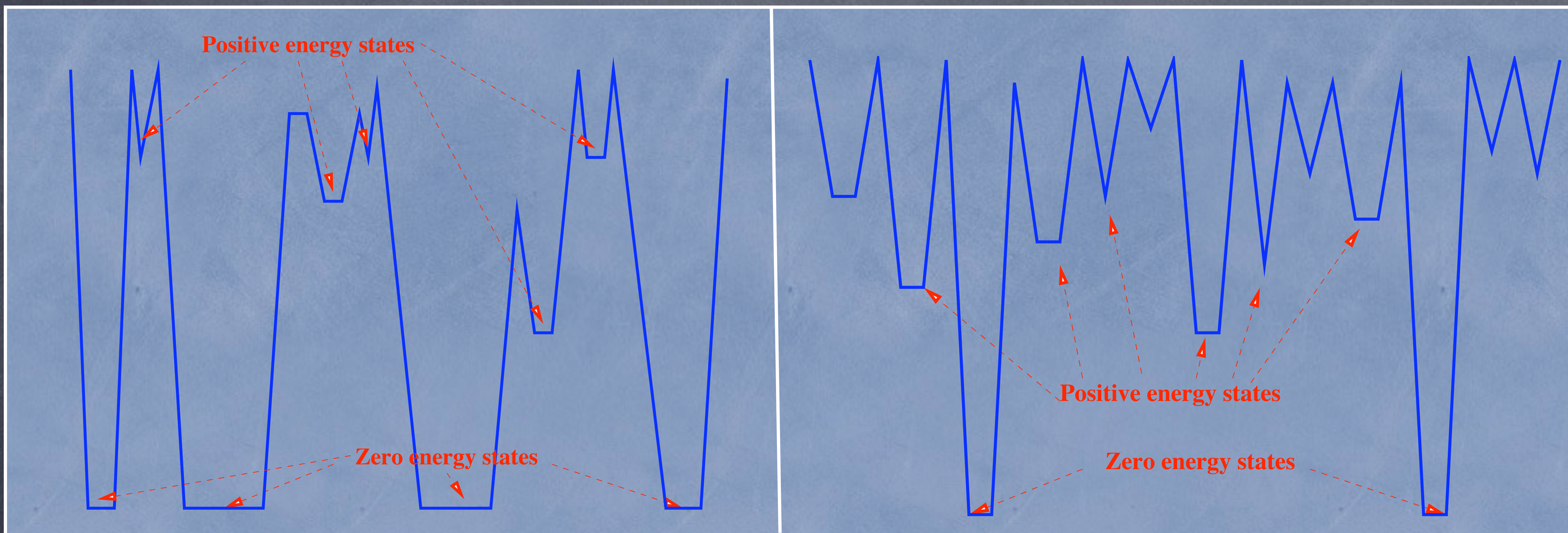
Landscapes: canyons, and valleys...

A question of basins of attraction

Canyon dominated vs. Valley dominated

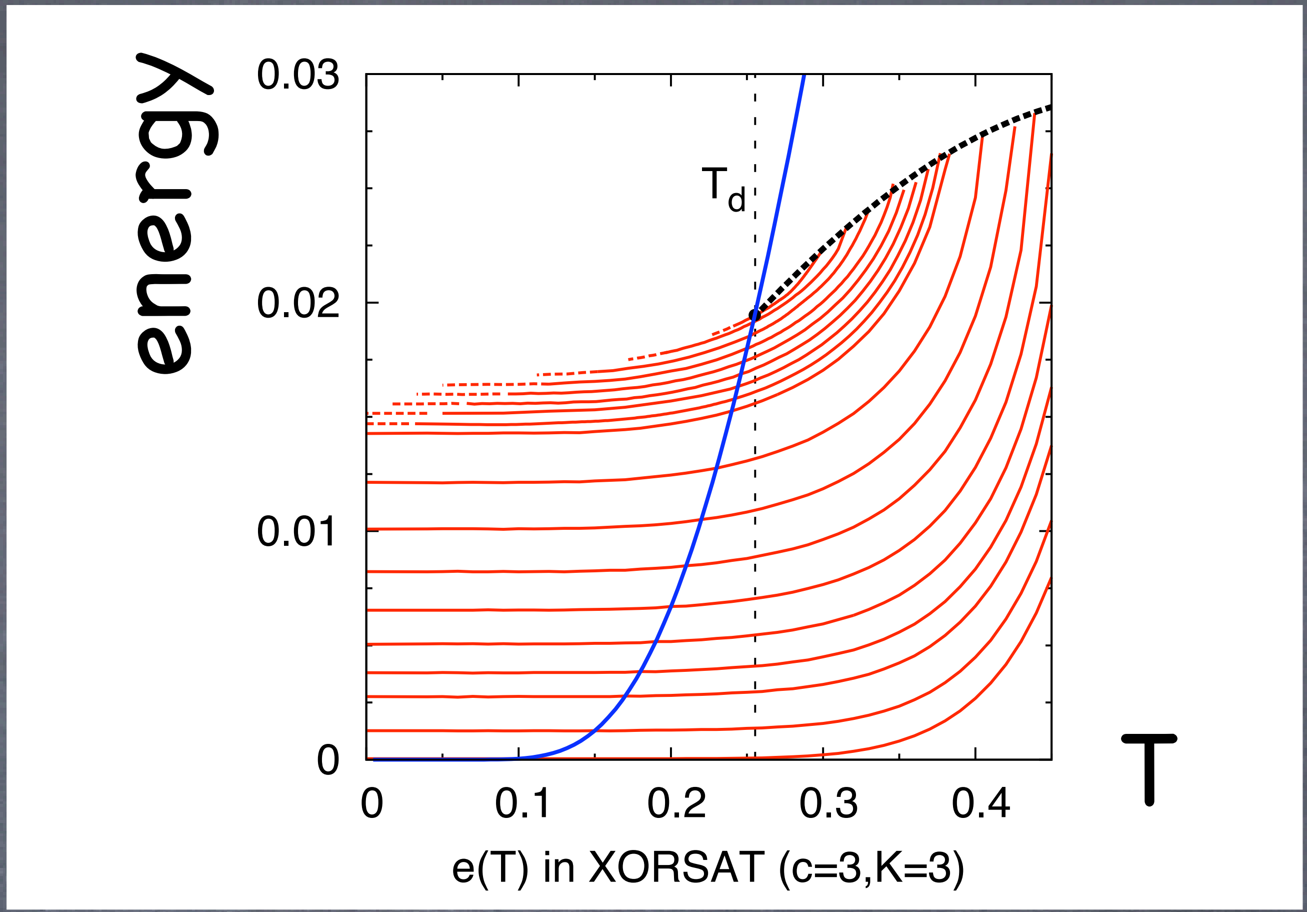


EASY vs HARD

Where is the bottom of a state typical at E_d?

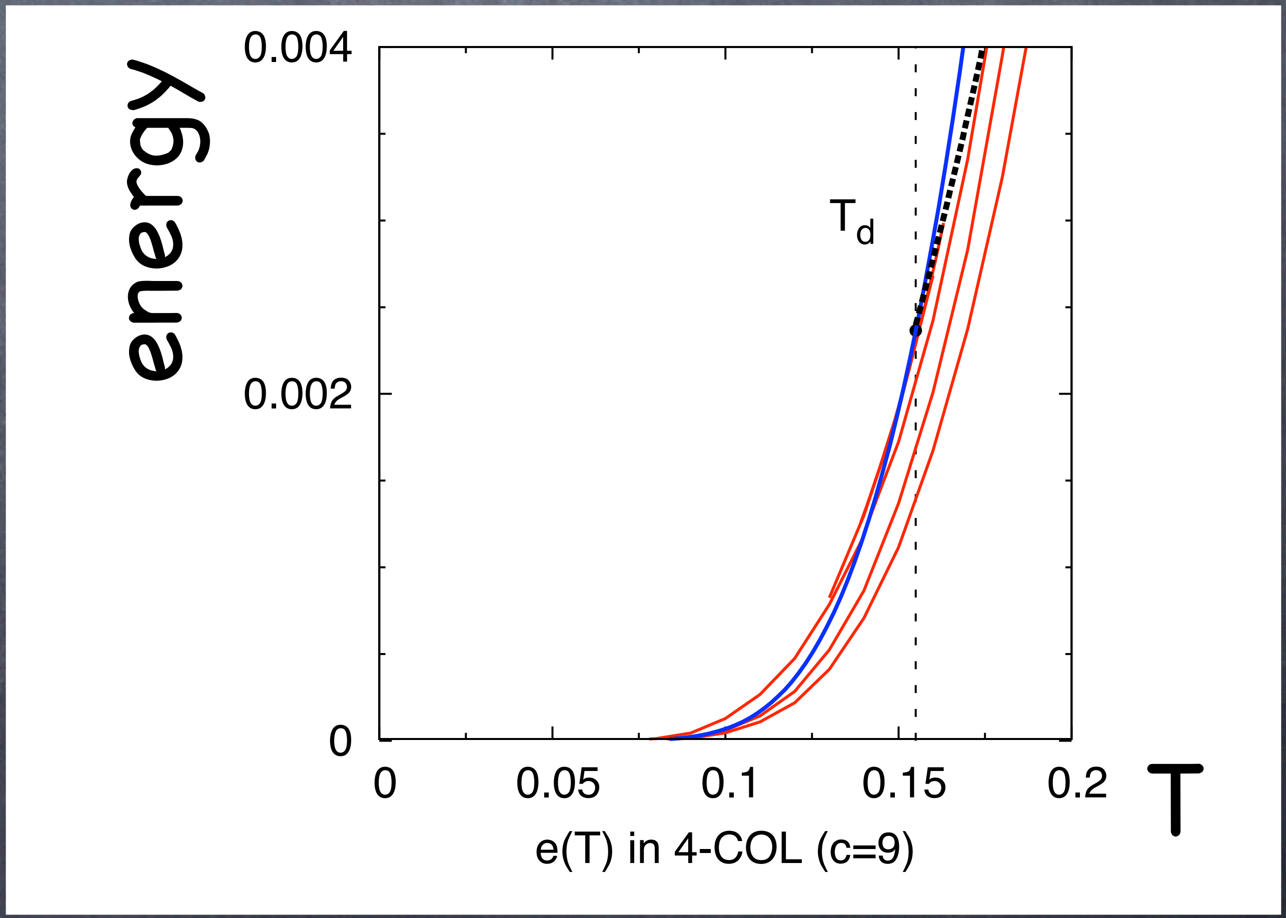
Valleys

3-XOR-SAT with L=3



Canyons

4-coloring of 9-regular random graphs



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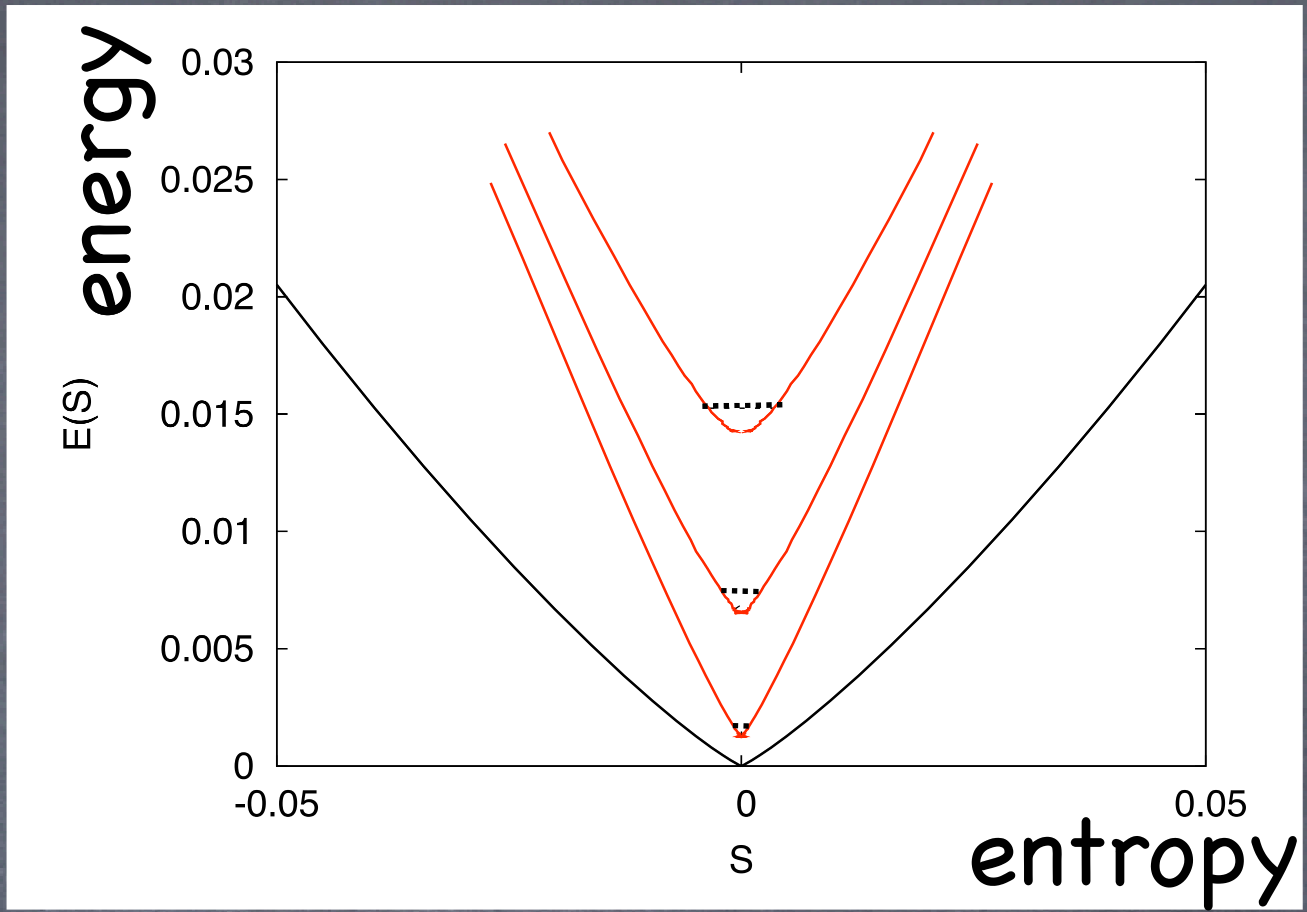

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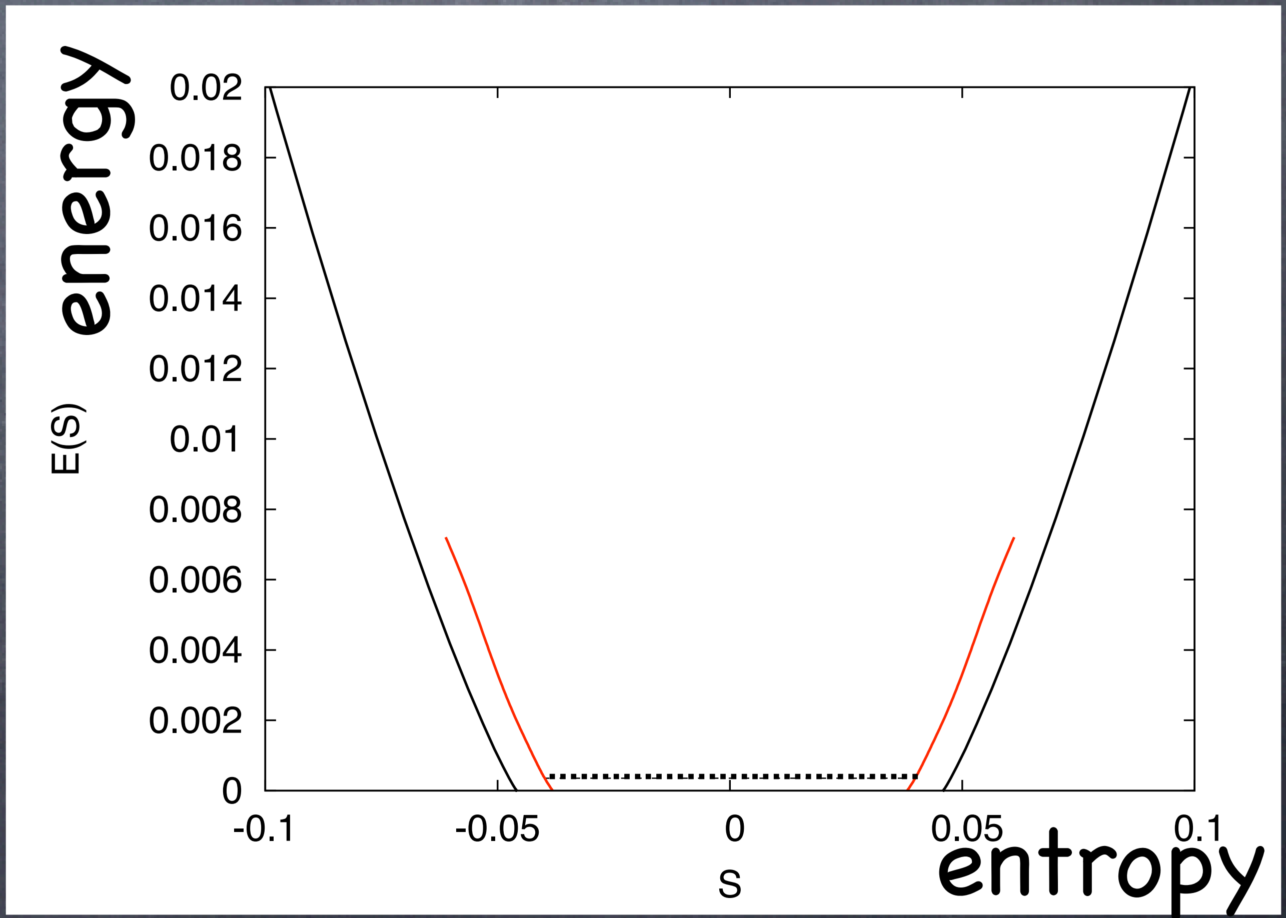

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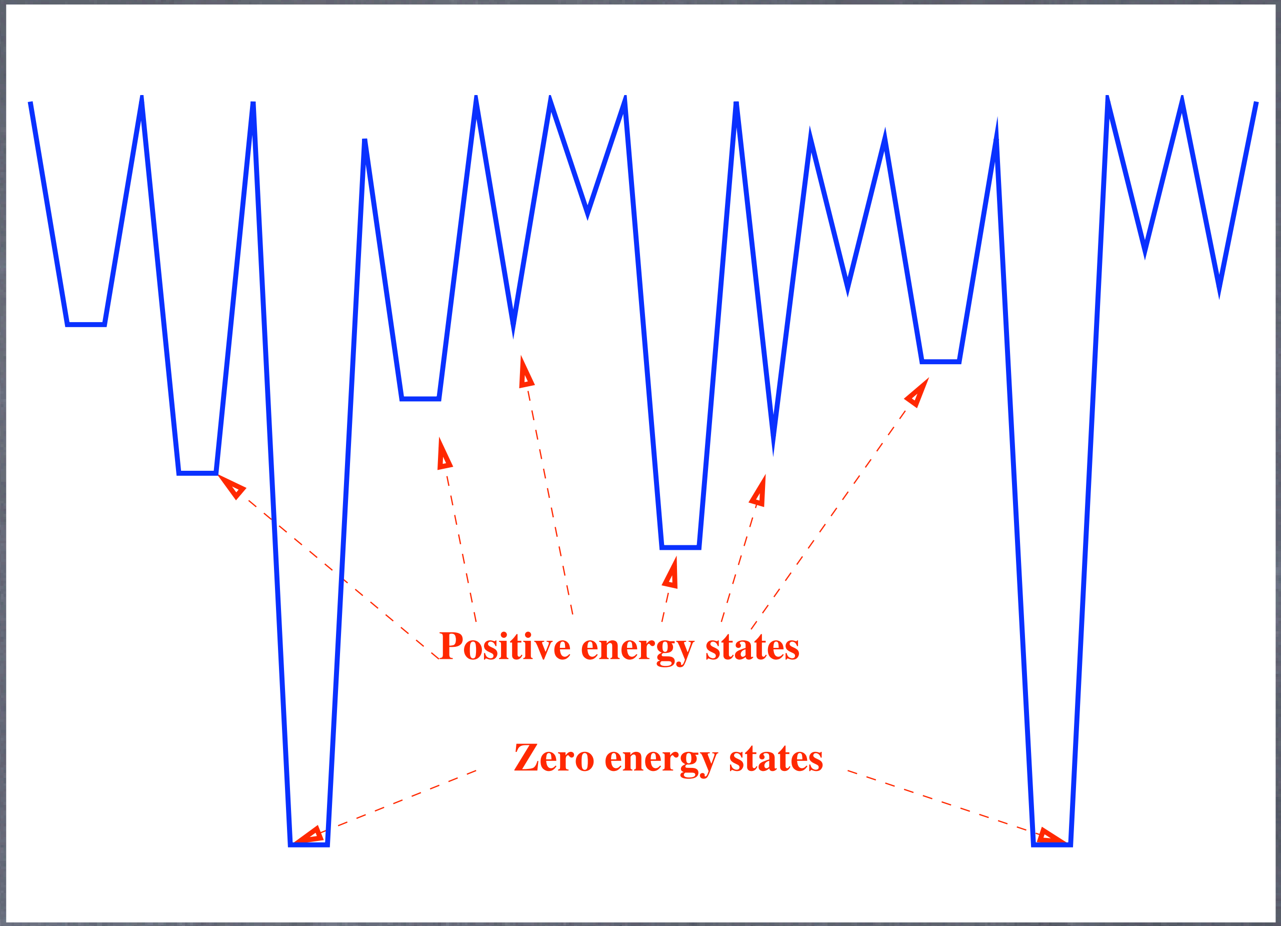

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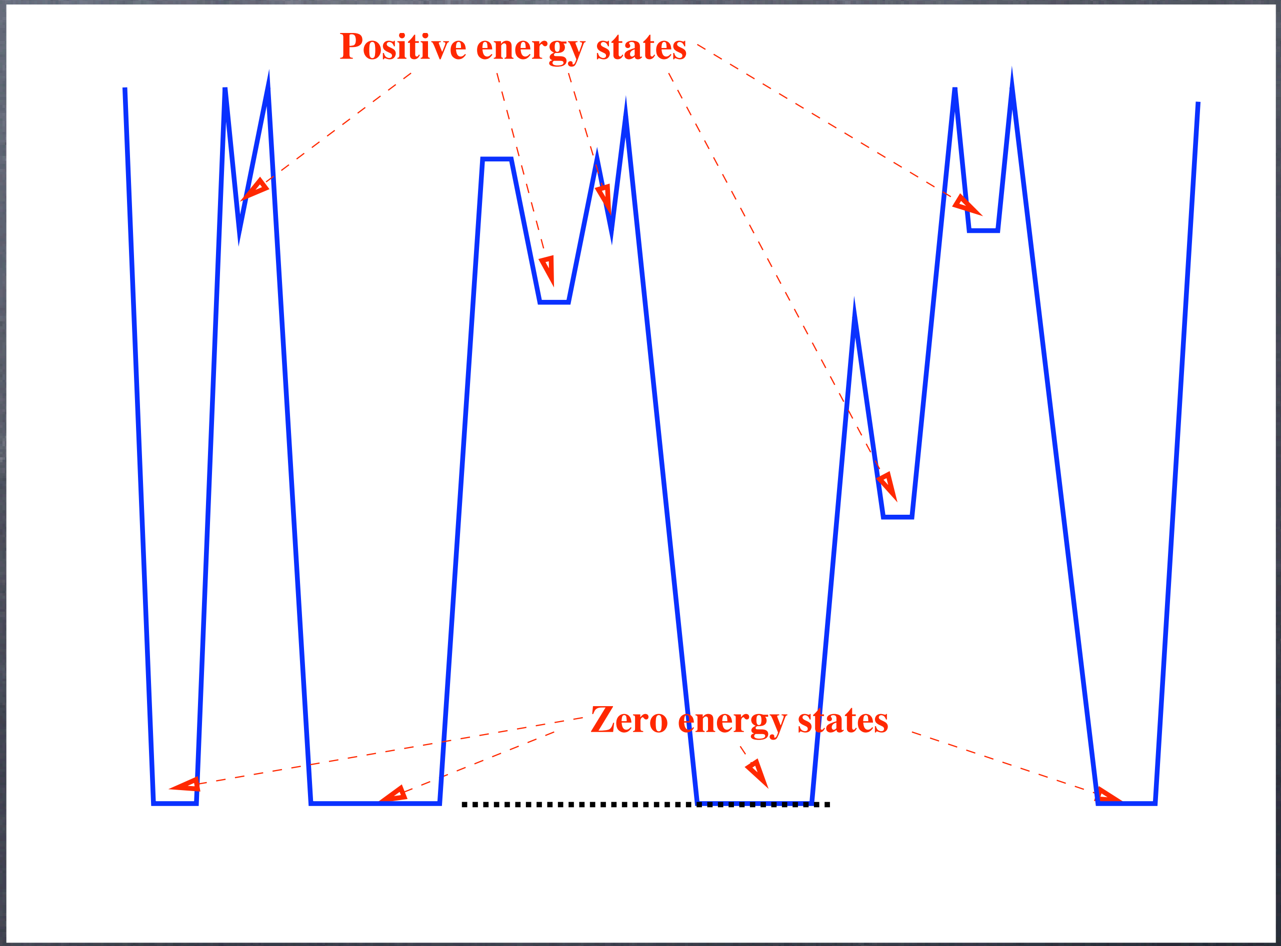
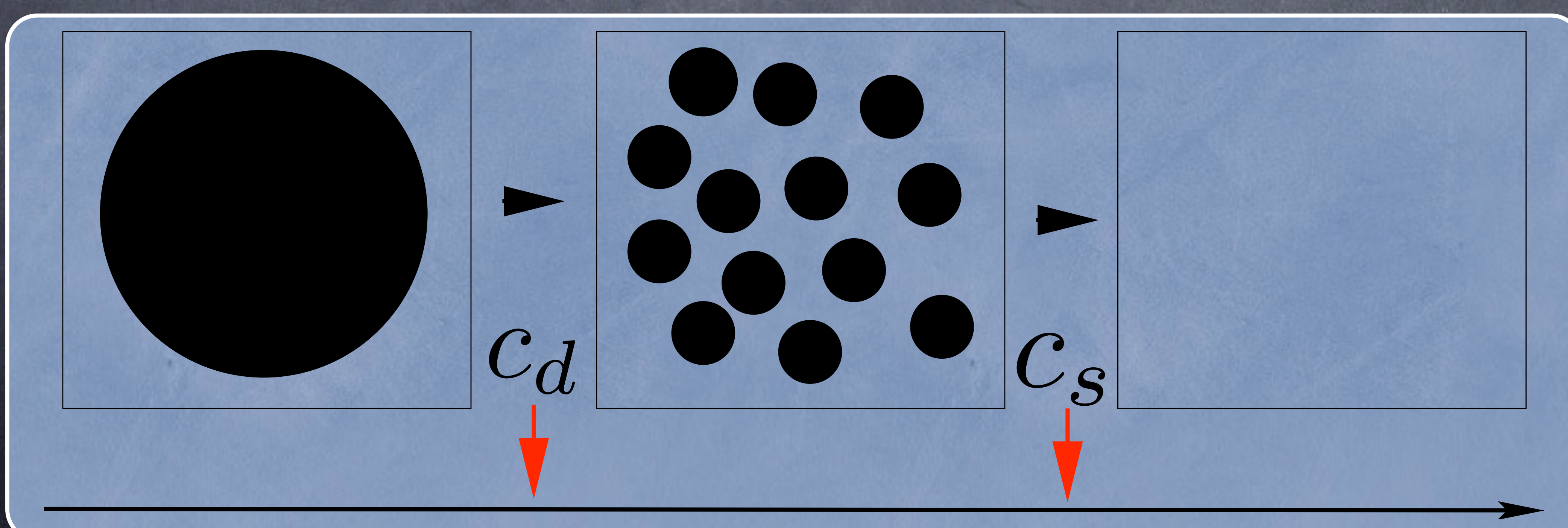


Landscape of random optimization problems



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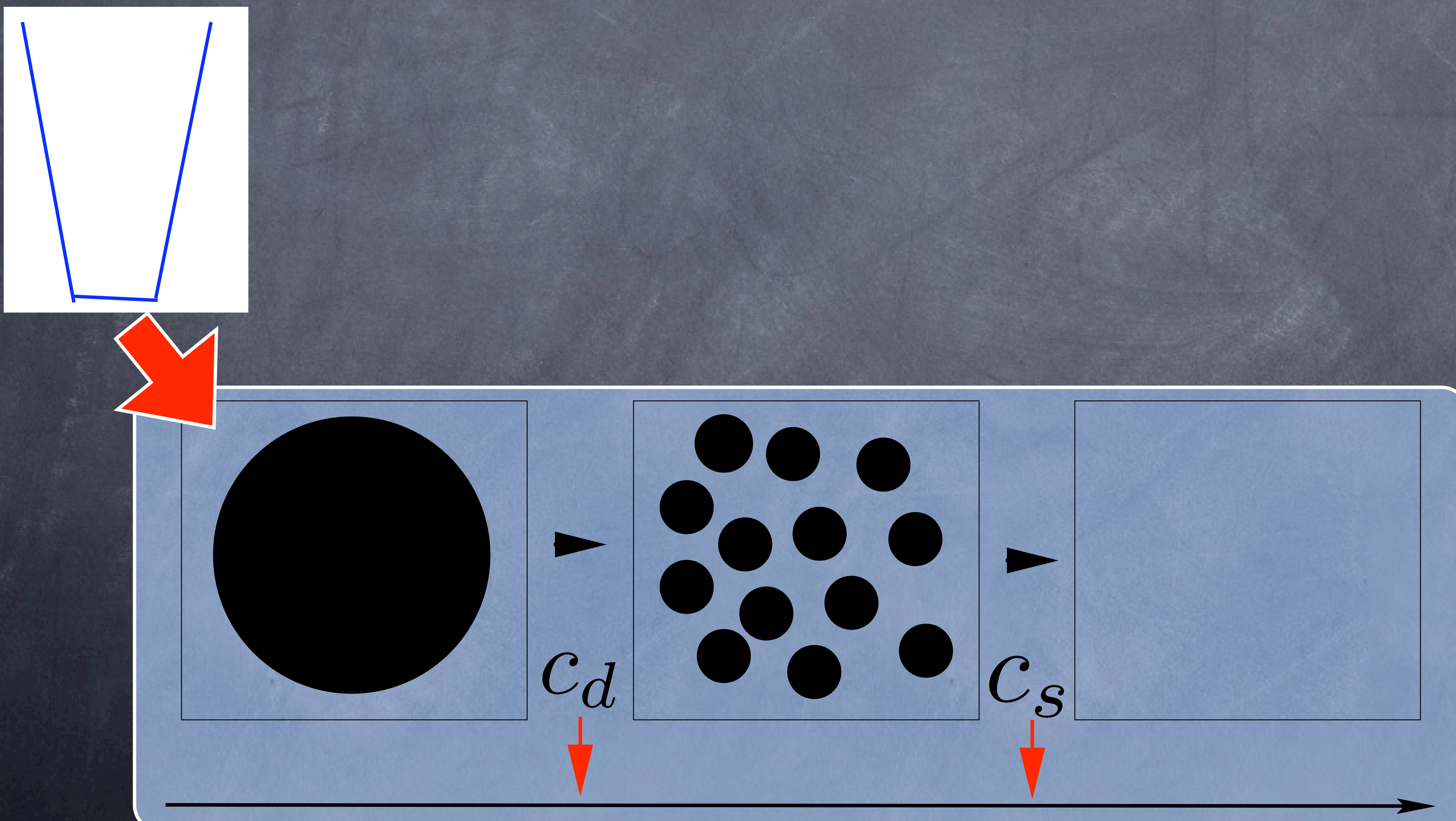

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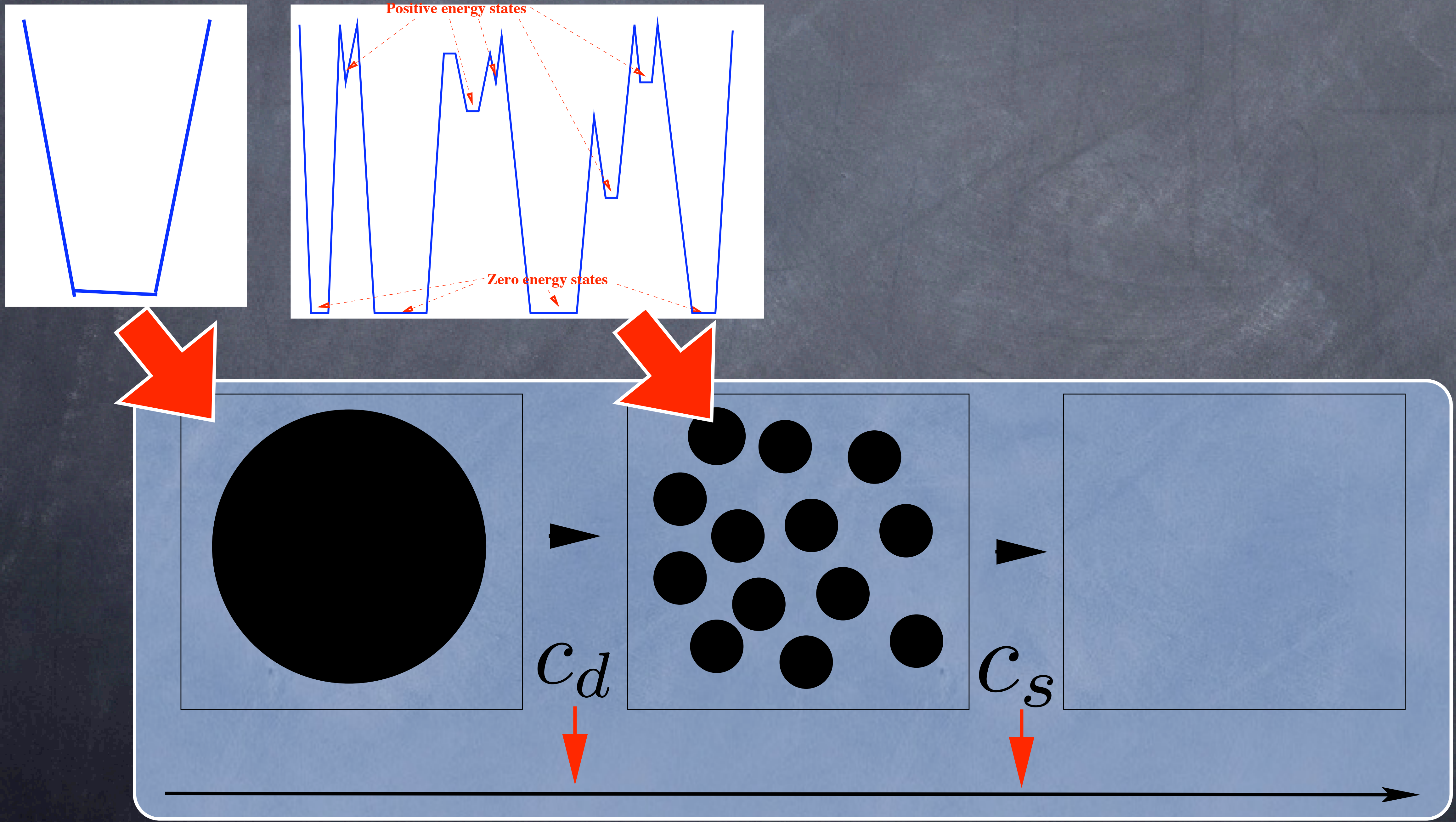

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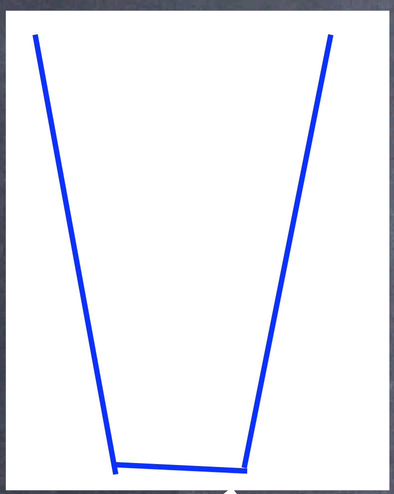

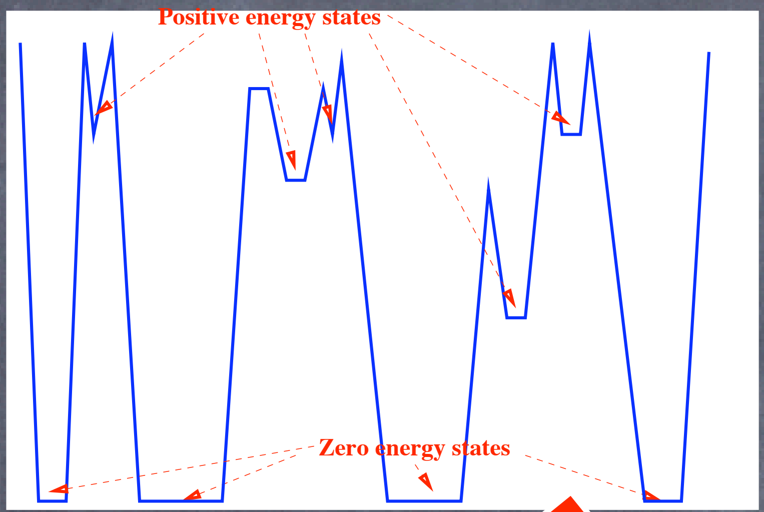

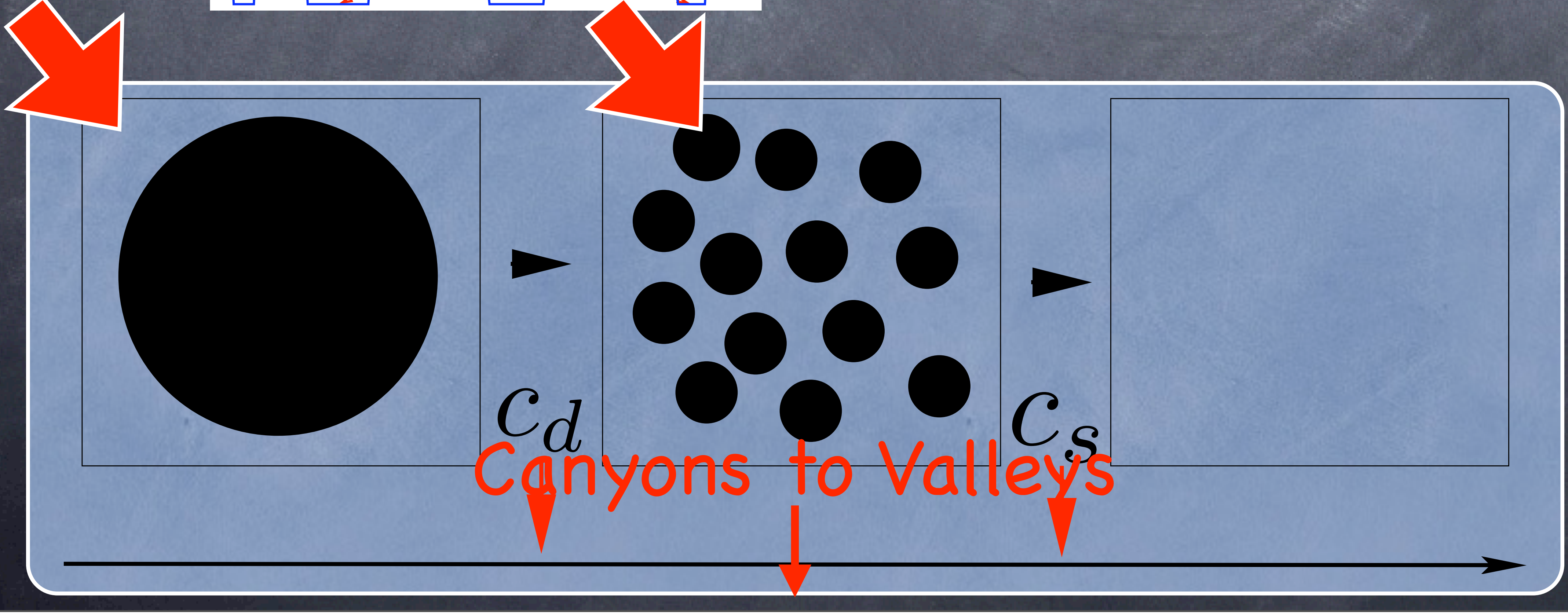

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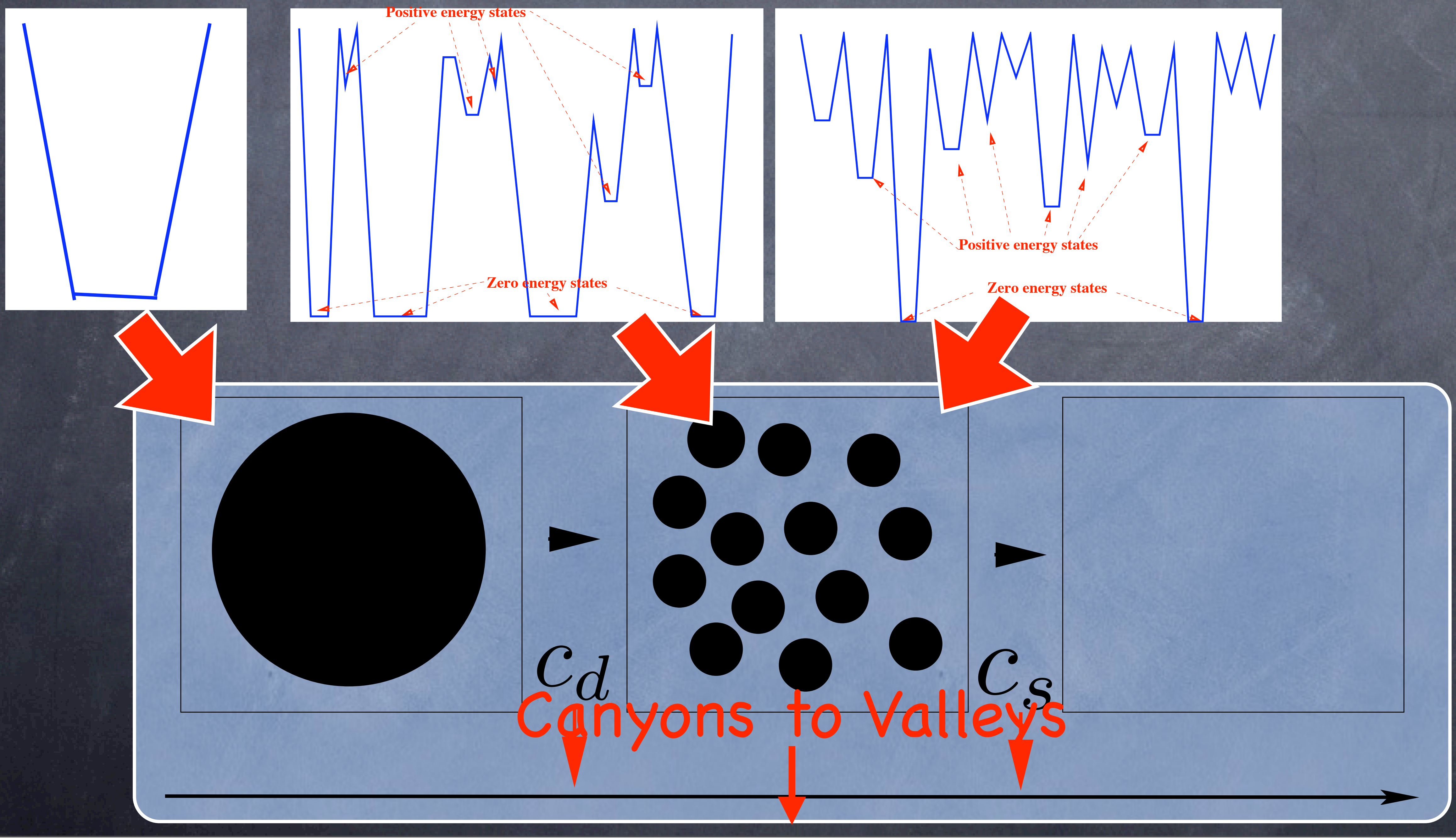

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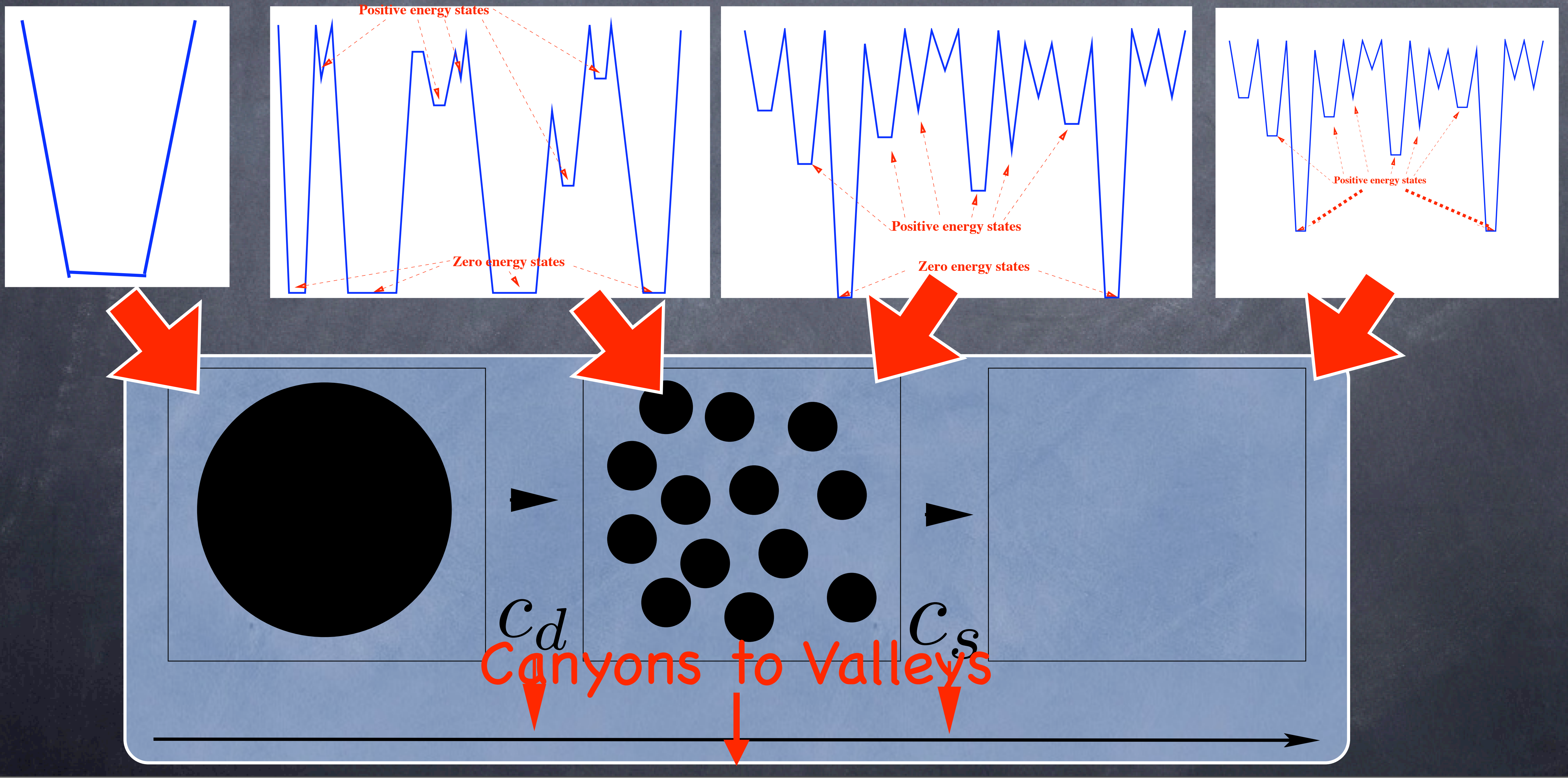

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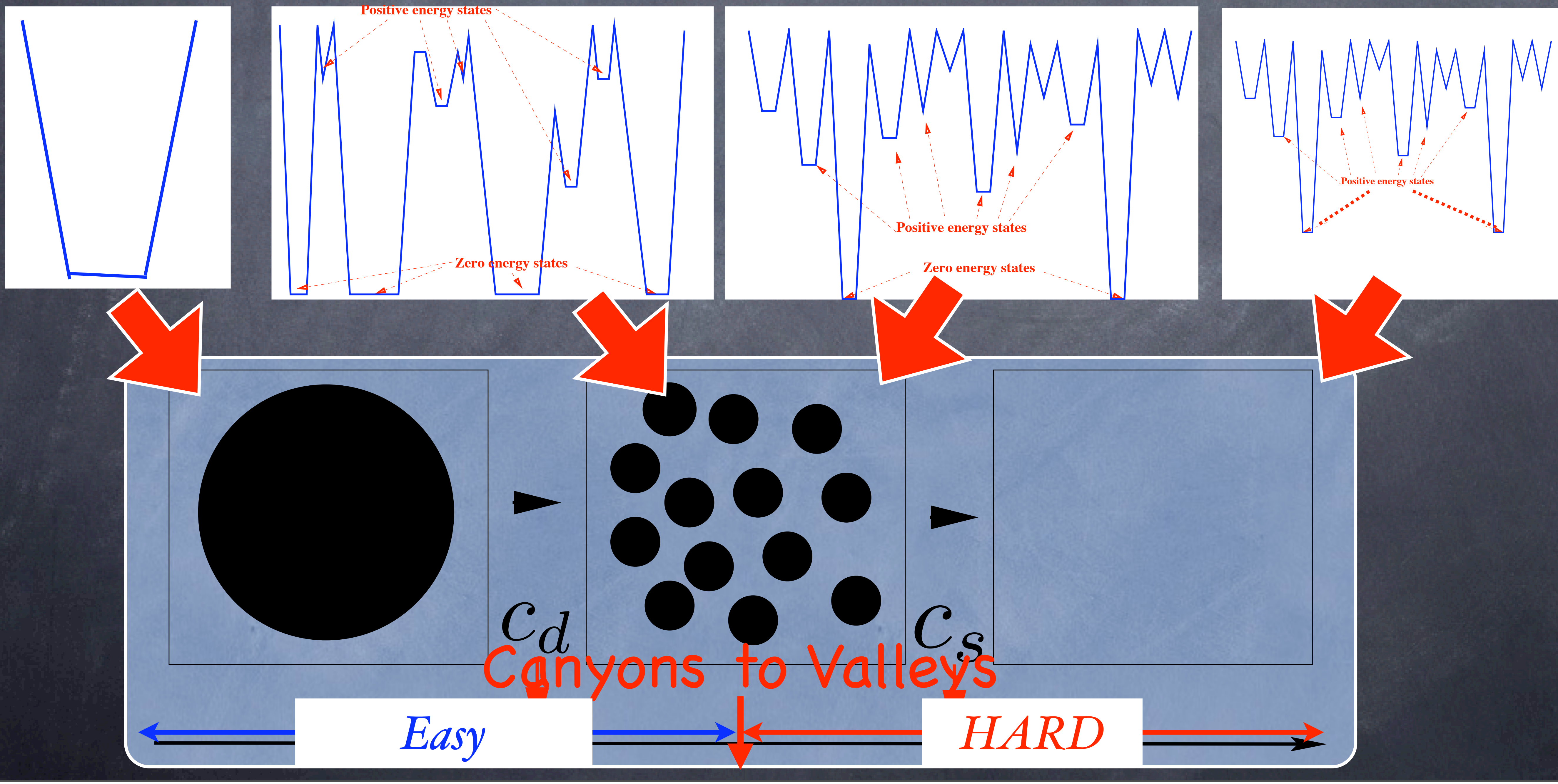

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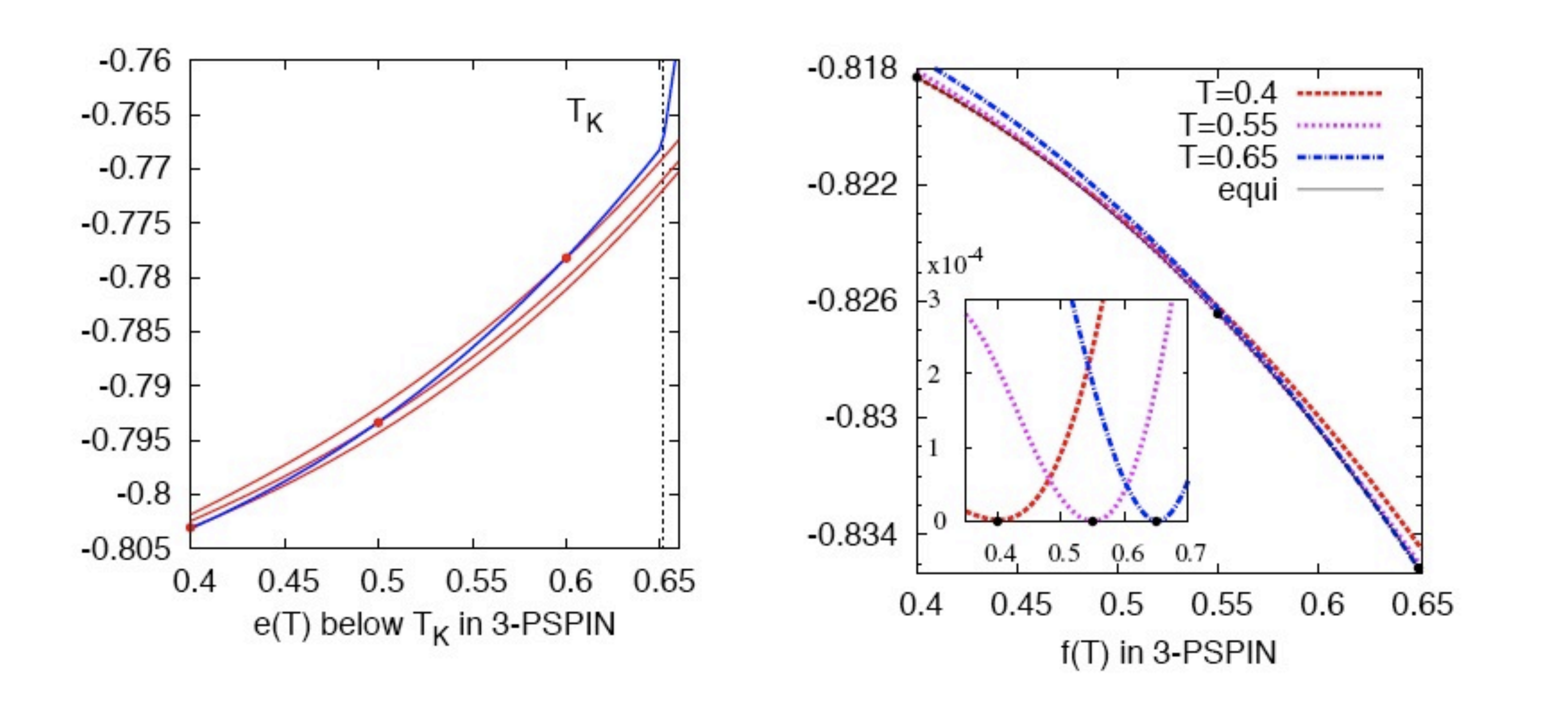
Temperature chaos in spin glasses

- Temperature chaos ≡ the equilibrium state changes completely when the temperature is slightly changed
- Present in renormalization group studies of spin glasses (Bray-Moore 87'; Nifle, Hilhorst 92')
- Usual explanation for many experimentally observed effects in glassy systems (ex: memory and rejuvenation)

Chaos and level crossing, in the glass phase



What can we do more?

- Jamming points - in mean field models for hard spheres following states in density (instead of temperature)
- Generalization to follow states in magnetic field, transverse quantum field, coordination number, ...
- Equilibrating in systems where it is impossible to equilibrate - via quiet planting, if $\mathbb{E}(\log Z) = \log \mathbb{E}(Z)$

Conclusions

- Method for following states: a cavity-like detailed description of the landscape:
- Gives access to long time dynamics...
- .... predicts average algorithmic hardness ...
- ... and the presence of temperature chaos ...
- ... allows to see the landscape ....
- ... and more to come !

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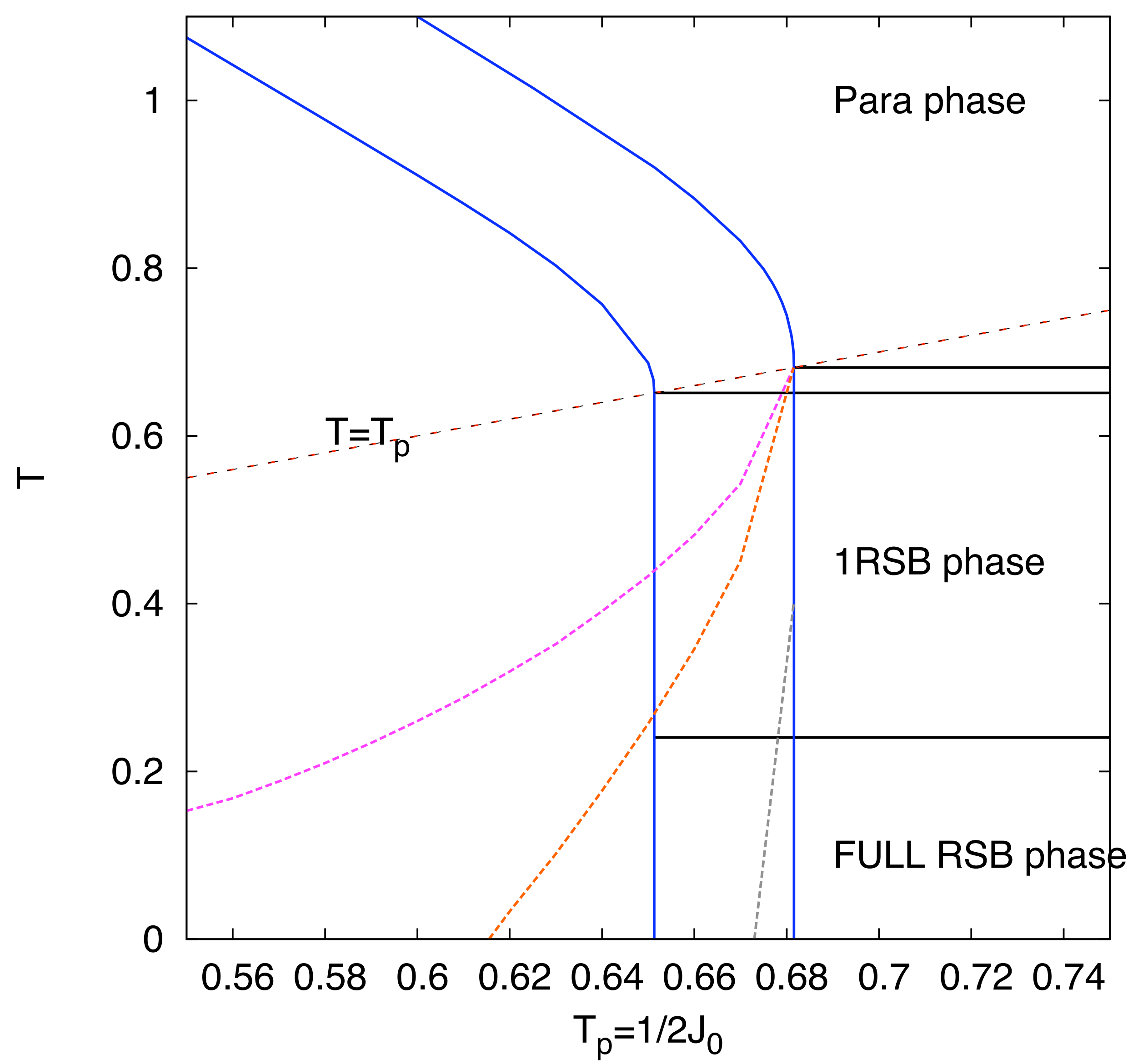
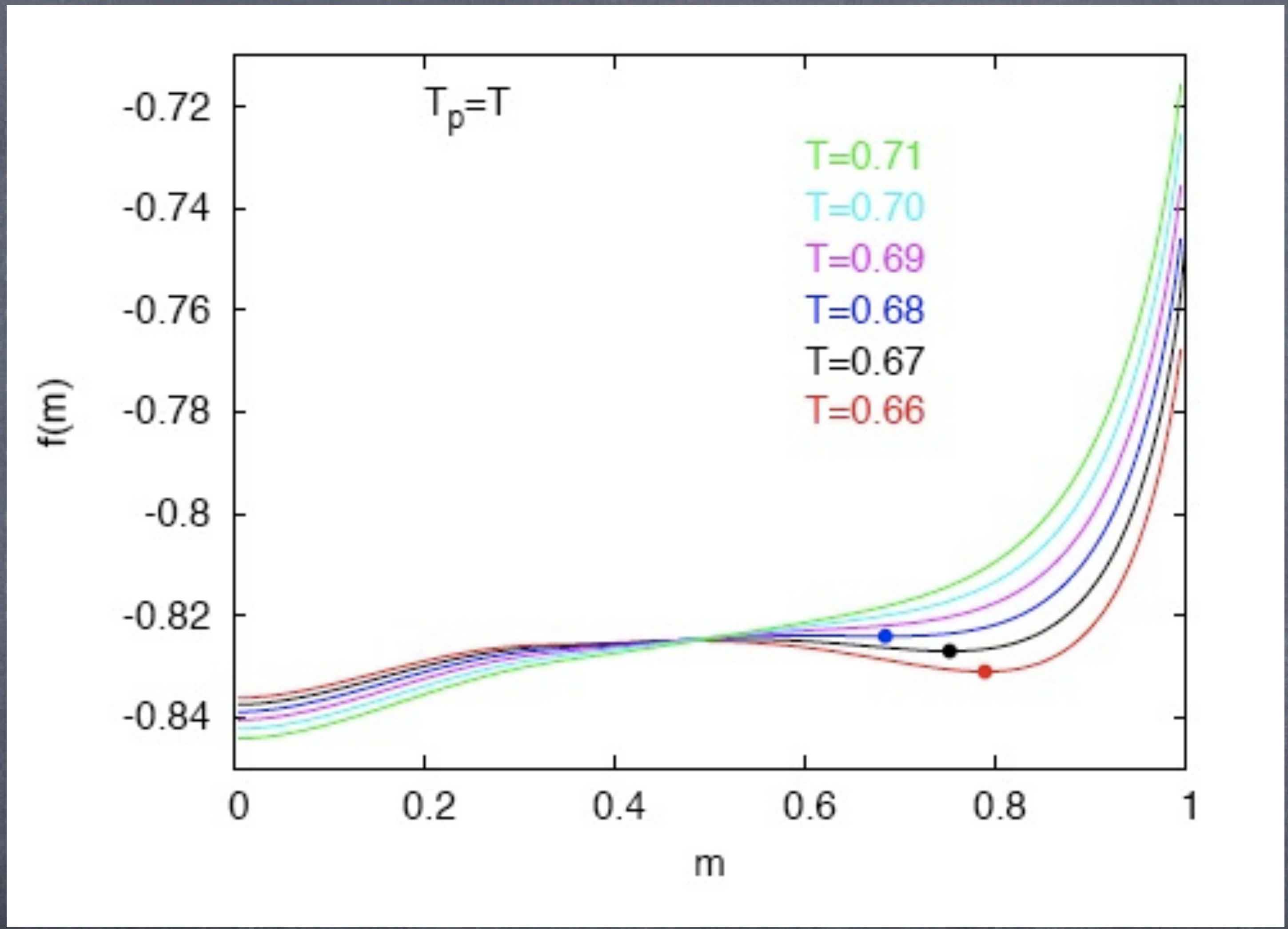
Thank you for your attention!

Phase diagram with ferromagnetic bias...



Relation to the Franz-Parisi potential

(Franz, Parisi'97)



Our method is looking directly at the minimum.
Easily tractable in particular in the diluted systems.

Following states in equations

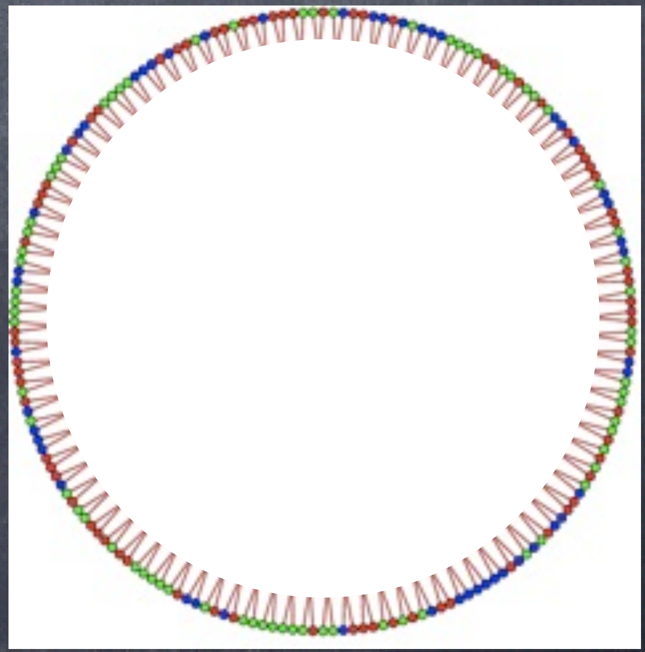
ex.: the Potts anti-ferromagnet on random graphs

(3) Resulting boundary conditions define the Gibbs state, compute what measure they induce at a different temperature.

$$P_s(\psi) = \sum_{\{s_i\}} \frac{e^{-\beta \sum_{i=1}^{c-1} \delta_{s,s_i}}}{(q-1+e^{-\beta})^{c-1}} \int \prod_i \mathrm{d}P_{s_i}(\psi^i)\delta[\psi - \mathcal{F}(\{\psi^i\},\tilde{\beta})]$$

$$\mathcal{F}_s(\{\psi^i\},\beta) \equiv \frac{\prod_i [1-(1-e^{-\beta})\psi_s^i]}{\sum_r \prod_i [1-(1-e^{-\beta})\psi_r^i]}$$

$$\beta \leq \beta_K$$



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General formulas

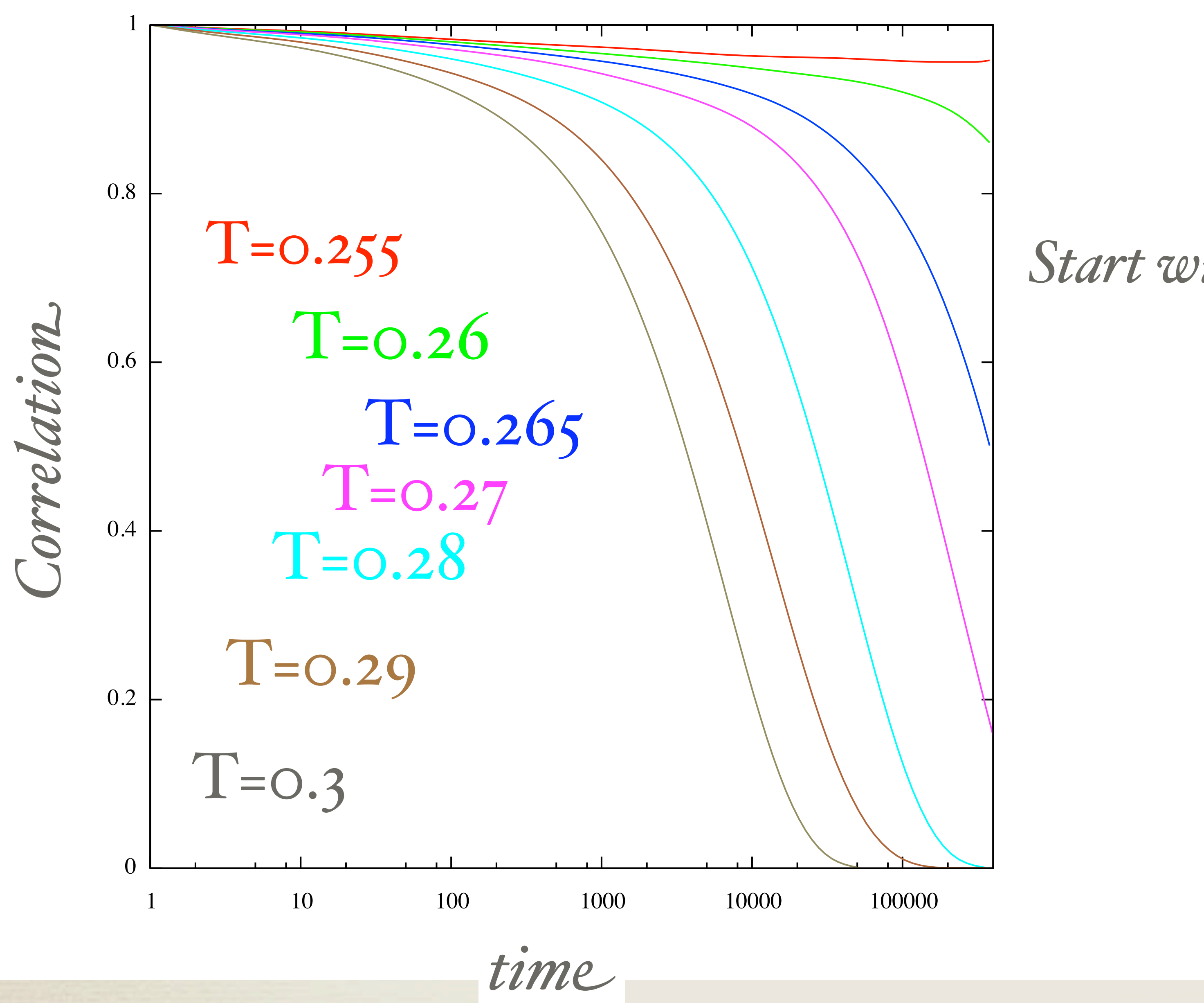
$$P^{a\to i}(\psi^{a\to i}) = \frac{1}{\mathcal{Z}^{a\to i}} \int \prod_{j\in\partial a\setminus i} \prod_{b\in\partial j\setminus a} \mathrm{d}P^{b\to j}(\psi^{b\to j}) \left[Z^{a\to i}(\{\psi^{b\to j}\},\beta)\right]^m \delta[\psi^{a\to i} - \mathcal{F}(\{\psi^{b\to j}\},\beta)]$$

$$\tilde{P}^{a\to i}(\tilde{\psi}^{a\to i}) = \frac{1}{\tilde{\mathcal{Z}}^{a\to i}} \int \prod_{j\in\partial a\setminus i} \prod_{b\in\partial j\setminus a} \mathrm{d}\tilde{P}^{b\to j}(\tilde{\psi}^{b\to j}) \left[Z^{a\to i}(\{\psi^{b\to j}\},\beta)\right]^m \delta[\tilde{\psi}^{a\to i} - \mathcal{F}(\{\tilde{\psi}^{b\to j}\},\tilde{\beta})]$$

Works in all systems where 1RSB can be identified (random graphs or fully connected)

Solving these equations: via population dynamics, only as difficult as ordinary 1RSB solution (in many models above T_K mapping to RS equations).

Testing the cavity predictions for the clustering transition



A better Approach:

Start with an equilibrated initial condition

Many temperatures:

Divergence of the relaxation time

Prediction: beyond the so-called "dynamic" threshold, the Monte-Carlo Dynamic is trapped!

Ex: 3-XORSAT, T_d=0.255