Spin Glasses:

A frustrating problem for statistical physics

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Collaborators

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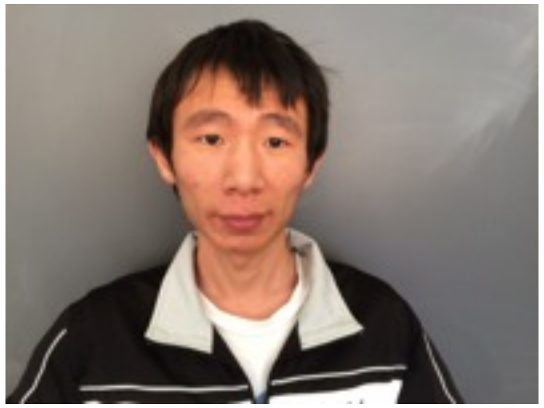


Outline

- Statistical Physics
- Spin Glasses
- Population Annealing
- Results
- Questions/Conclusions

Statistical Physics

- The study of the emergent properties of many component systems using probabilistic methods.
- Objects of study are statistical ensembles of system states or histories:
  - Thermal Equilibrium--Gibbs distribution:

$$P[\sigma] = \frac{1}{\mathcal{Z}} \exp(-H[\sigma]/k_B T)$$

  - Non-equilibrium--stochastic dynamics

Gibbs Distribution

Thermal equilibrium: asymptotic stationary state in the absence of net fluxes of energy or mass. Described by a few parameters, e.g. temperature.

$$P[\sigma] = \frac{1}{\mathcal{Z}} \exp(-H[\sigma]/k_B T)$$

$$P\left[\sigma\right] = \text{ probability of state } \sigma$$

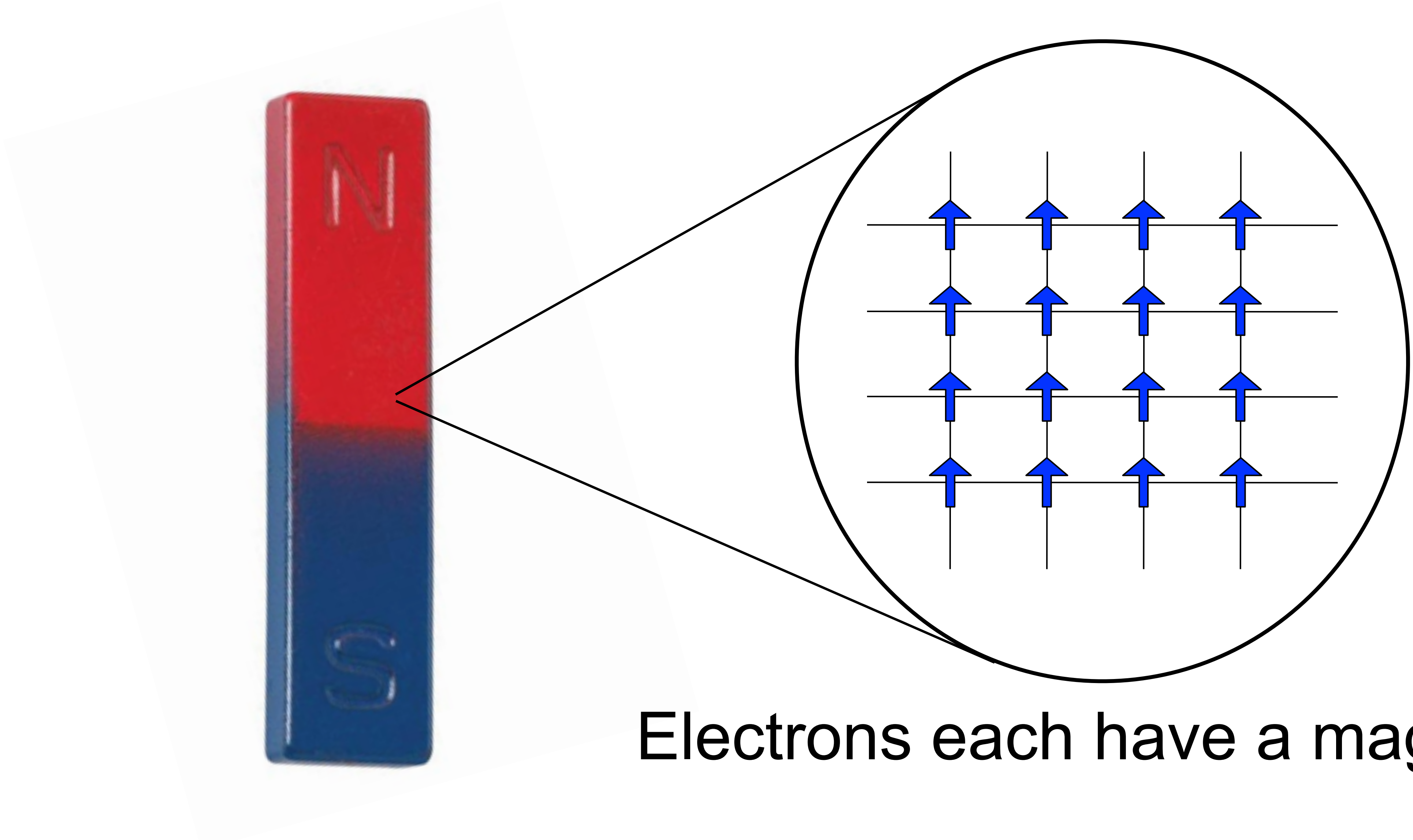
$$H\left[\sigma\right] = \text{ energy of state } \sigma \qquad T = \text{temperature}$$

$$\mathcal{Z} = \text{normalization (partition function)}$$

$$k_B = \text{Boltzmann's constant}$$

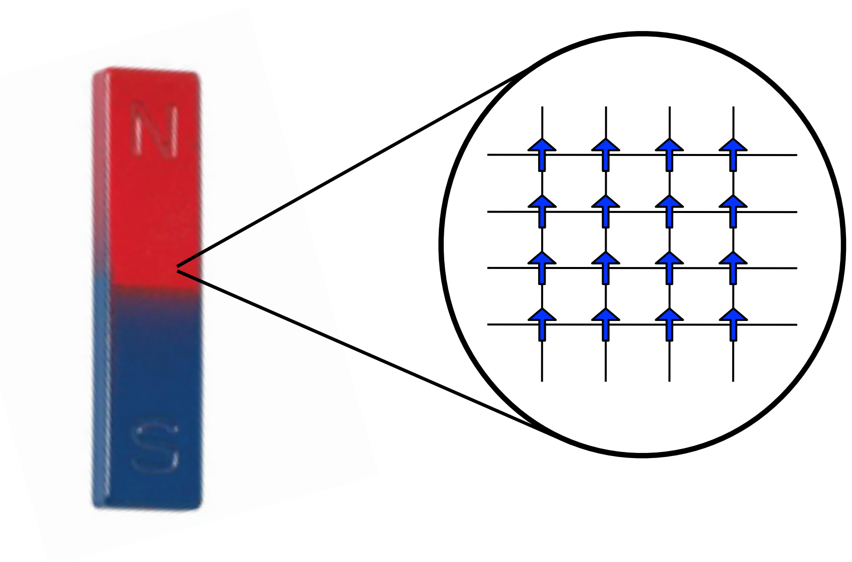
The Partition Function
and
Free energy

Magnetism



Electrons each have a magnet moment.

Ferromagnetism



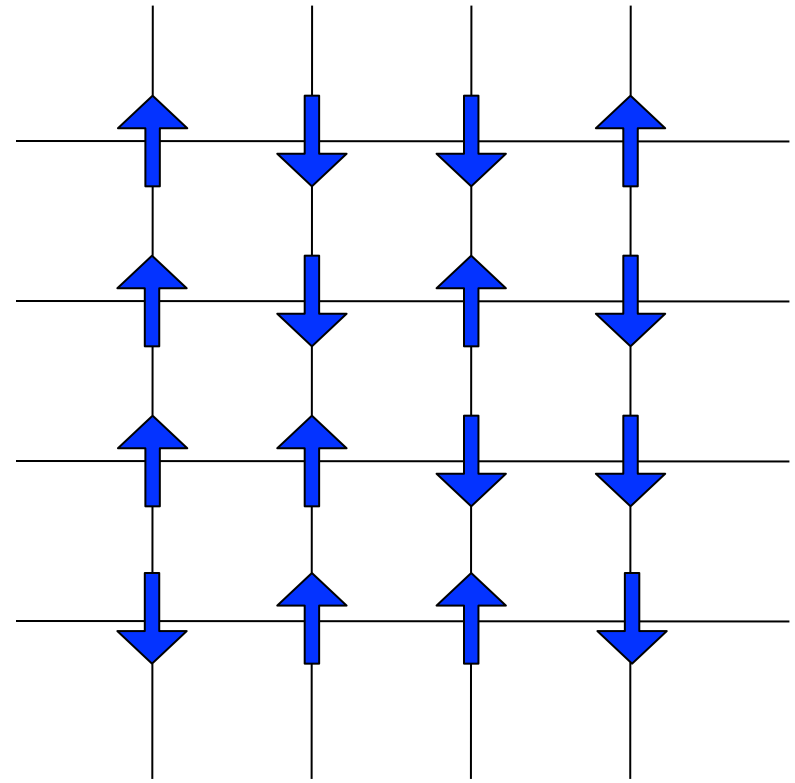
- Ferromagnetism (permanent magnetism) arises from the alignment of electron magnet moments, aka "spins."
- Alignment is maintained over microscopic distances while the coupling distance between electrons is microscopic.

Ising Model

$$H\left[\sigma\right] = -J \sum_{(i,j)} s_i s_j$$

$$\sigma = \{s_i | i = 1, \ldots, N\}$$

$s_i = \pm 1$ $\qquad$ $\uparrow = +1$ $\downarrow = -1$



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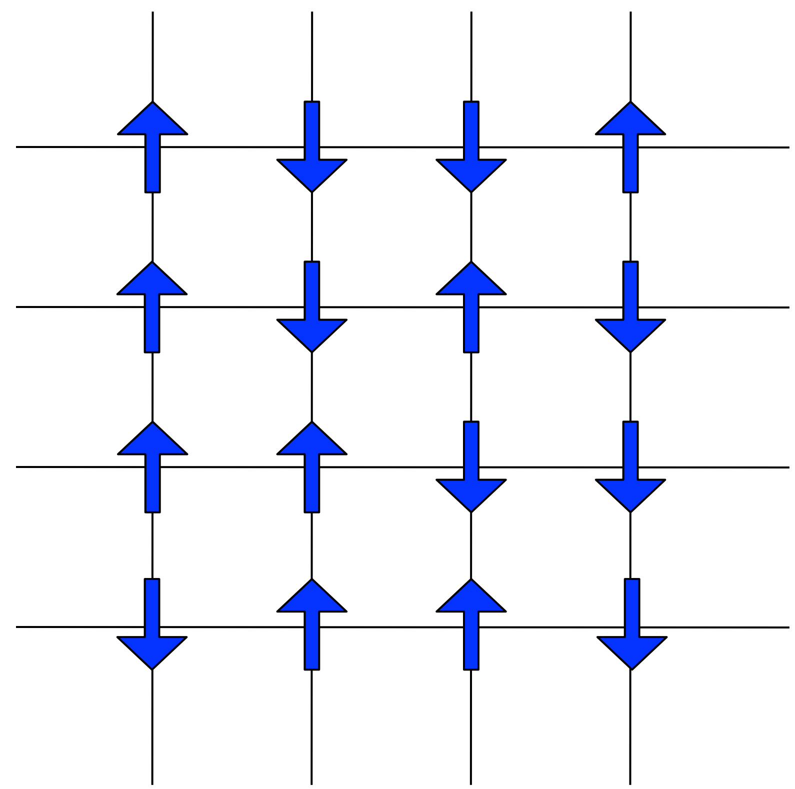

$$\sigma = \{s_i | i = 1, \ldots, N\}$$

$s_i = \pm 1$ $\quad \uparrow = +1 \quad \downarrow = -1$

Aligned spins lower the energy and vice versa:

$\uparrow\!-\!\uparrow$ or $\downarrow\!-\!\downarrow$ $\quad -J$

$\uparrow\!-\!\downarrow$ or $\uparrow\!-\!\downarrow$ $\quad +J$

Ising Model

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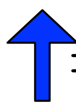
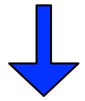
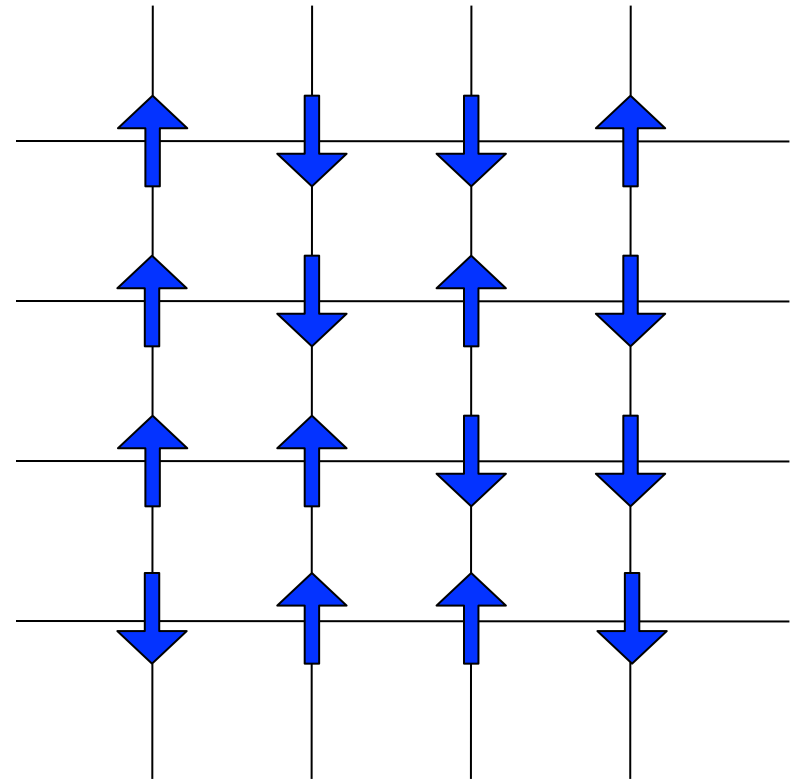
$s_i = \pm 1$  $= +1$  $= -1$



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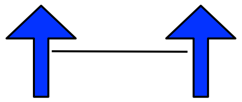
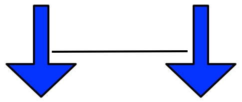
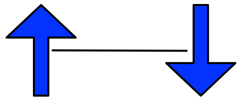
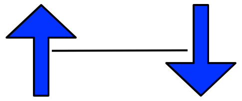
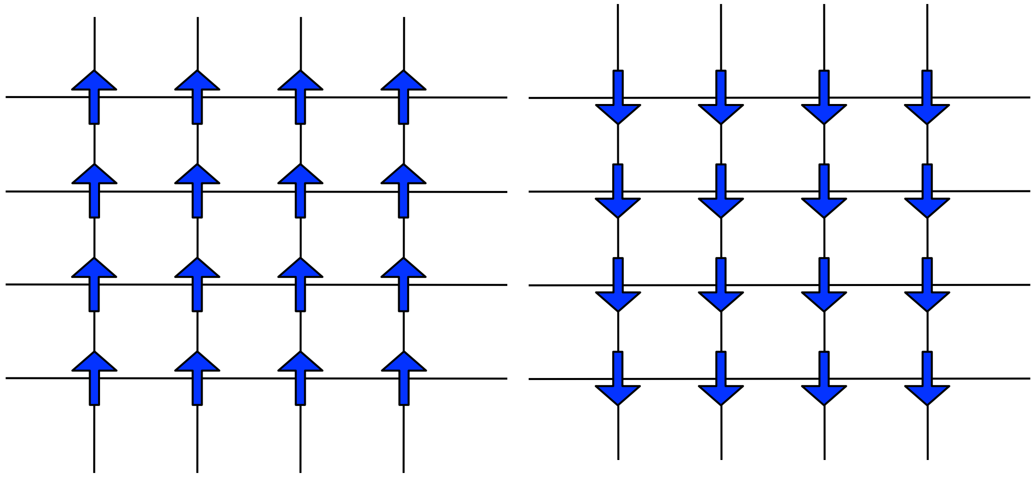
 or  $-J$

 or  $+J$

Two ground states:

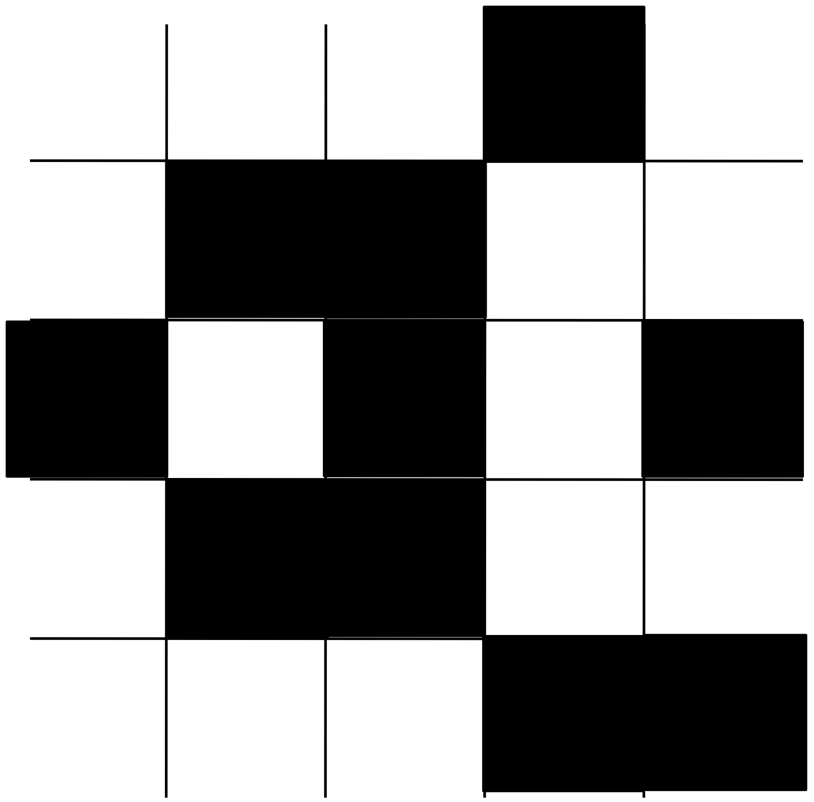


Ising Model Behavior

$$H\left[\sigma\right] = -J \sum_{(i,j)} s_i s_j$$

$$P\left[\sigma\right] = \frac{1}{\mathcal{Z}} \exp(-H\left[\sigma\right]/k_B T)$$

Gibbs Distribution



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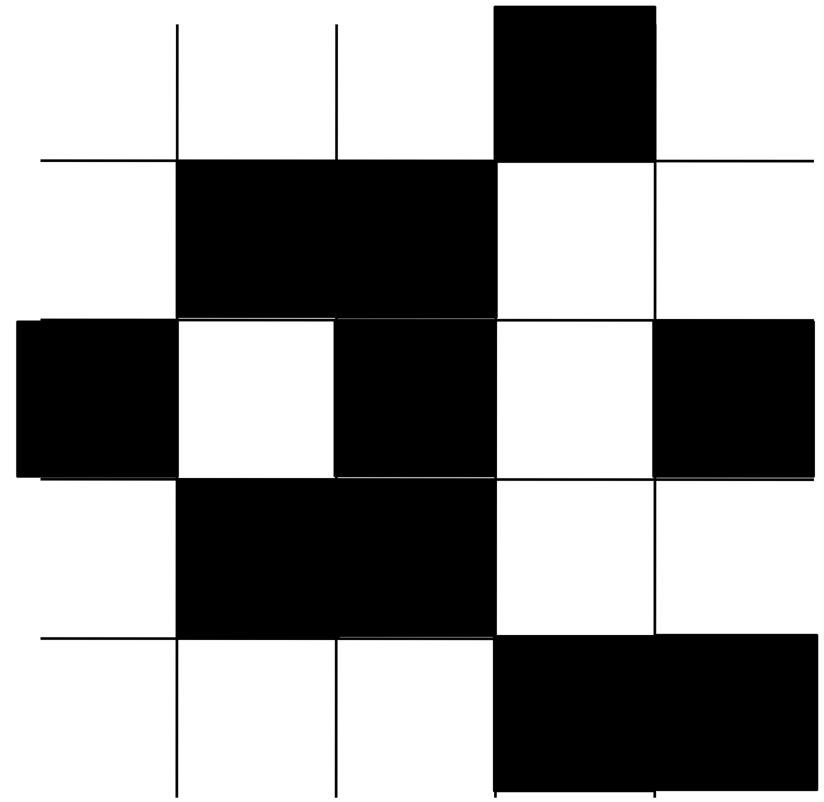
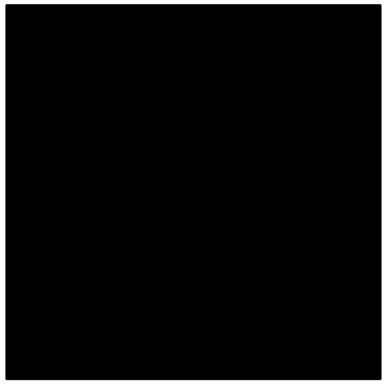
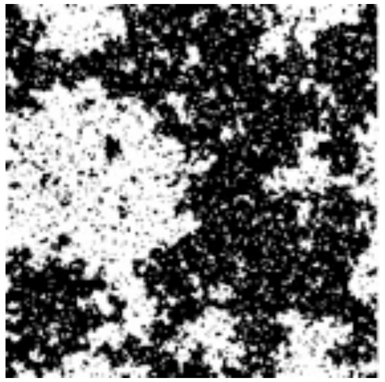
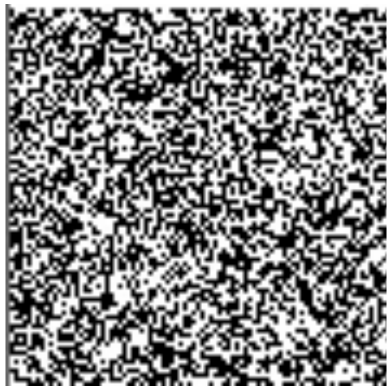




$T = 0$



$T = T_c$



$T = \infty$

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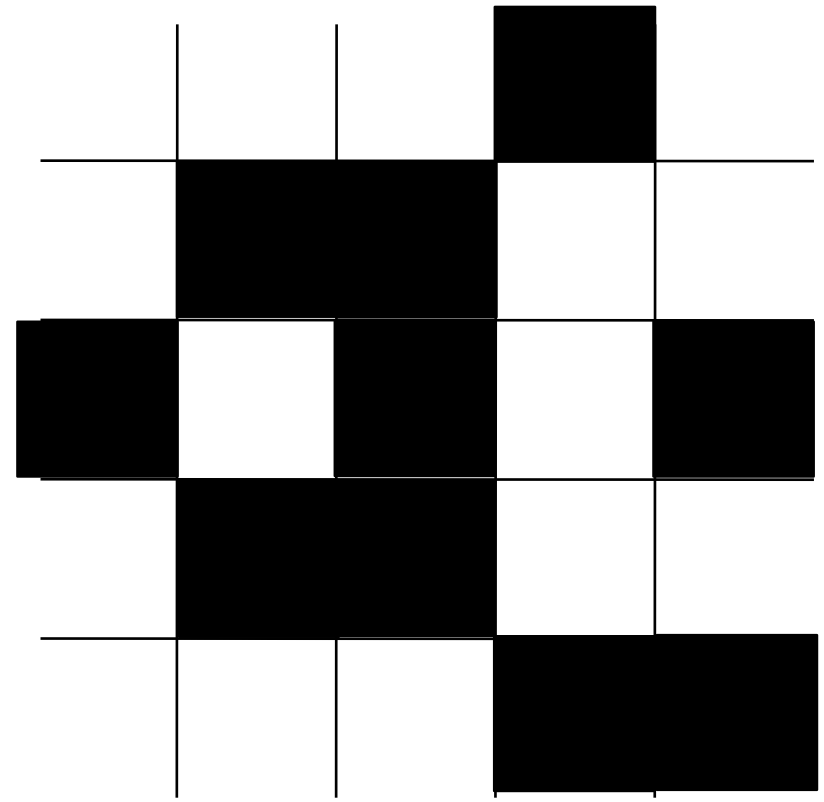
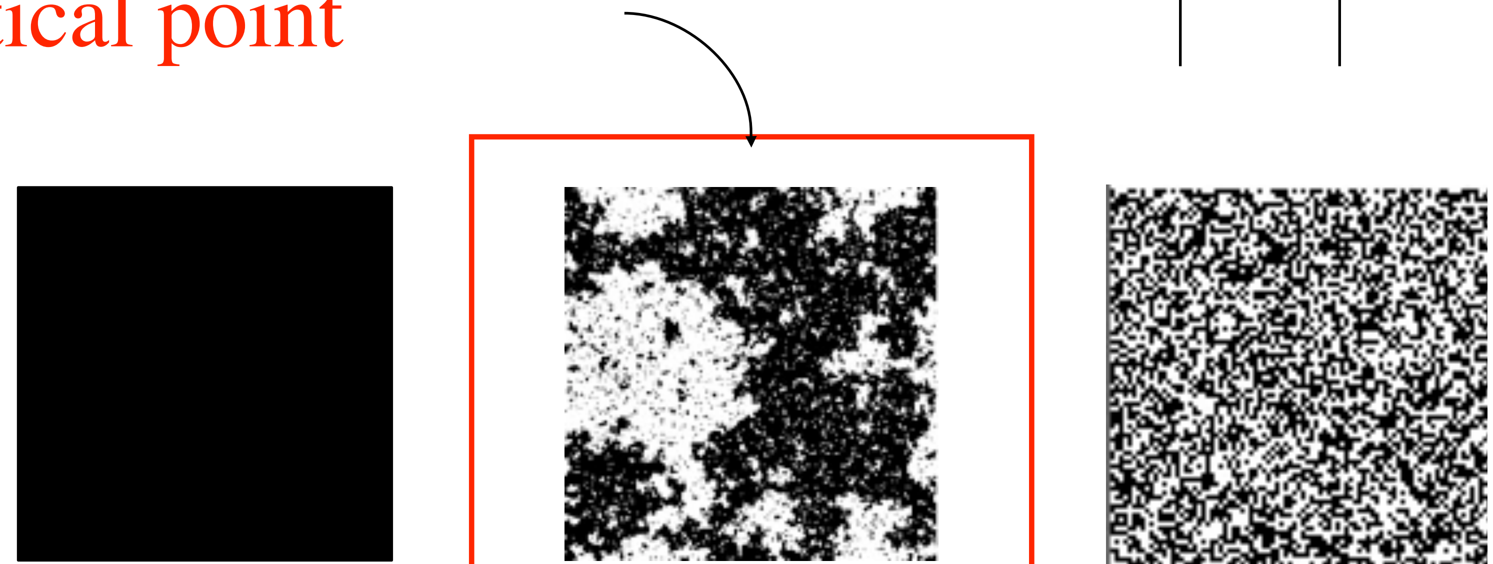
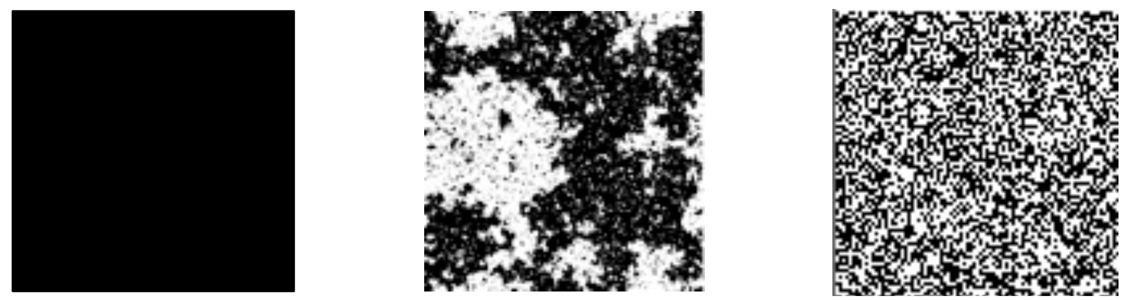


Critical point



$T = 0$ $T = T_c$ $T = \infty$

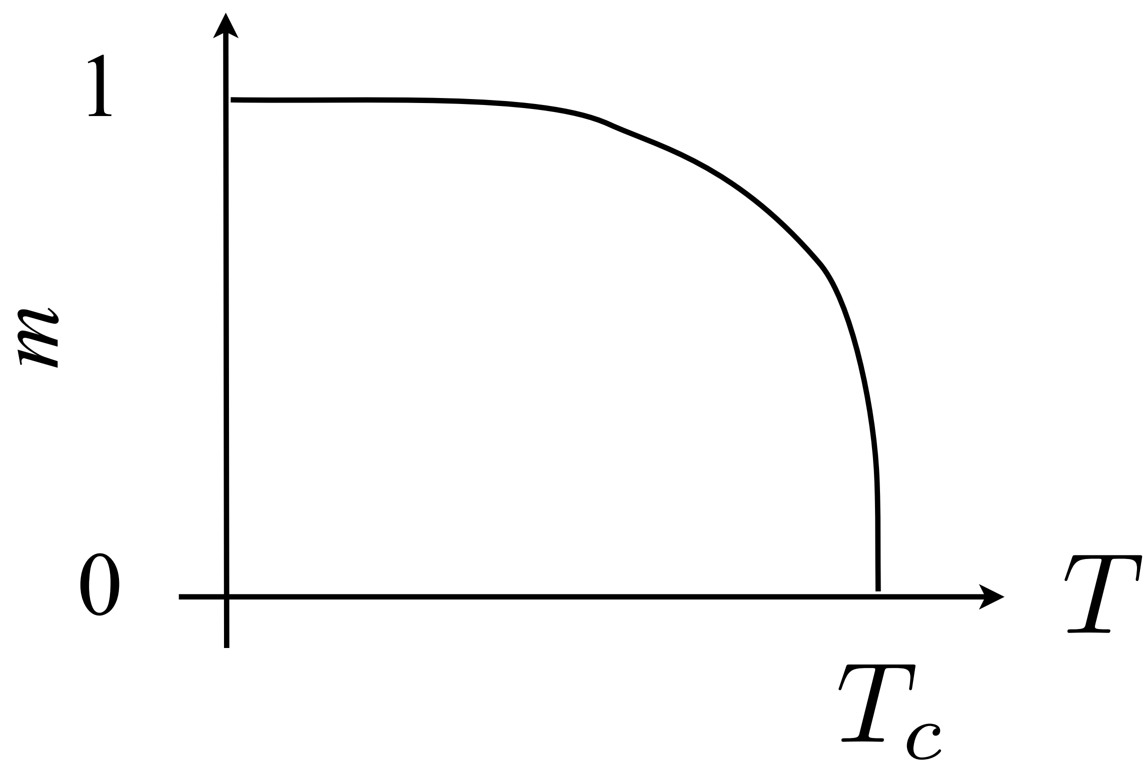
Order Parameter



$T \ll T_c$ $T = T_c$ $T \gg T_c$

Order parameter
(magnetization)

$$m = (1/N)\langle \left| \sum_i s_i \right| \rangle$$

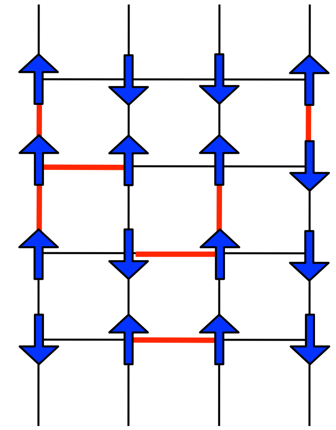


Pure States

- At low temperature the Gibbs distribution for the Ising model can be decomposed into a linear combination of two “pure states,” one mainly spin up and the other mainly spin down. The two pure states are related by the up-down symmetry of the energy function.

Spin Glasses

- Random magnetic alloys: CuMn, ...
- Ising spin glass (Edward-Anderson model, 1975)



$J > 0$, ferromagnetic

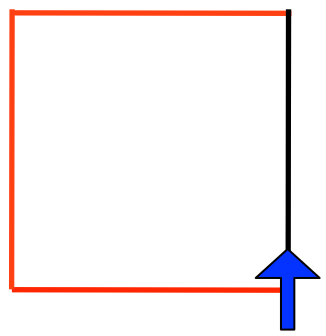
$J < 0$, antiferromagnetic

$$H[\sigma] = -\sum_{(i,j)} J_{ij} s_i s_j$$

$$s_i = \pm 1$$

J_{ij} are quenched (fixed) Gaussian random couplings with mean zero and variance one.

Frustration



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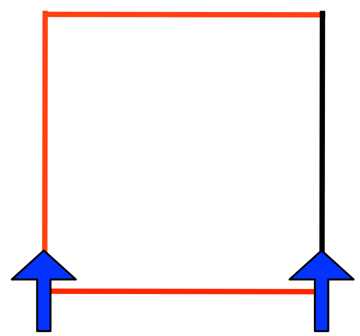

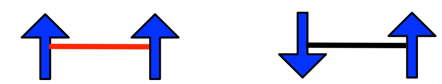

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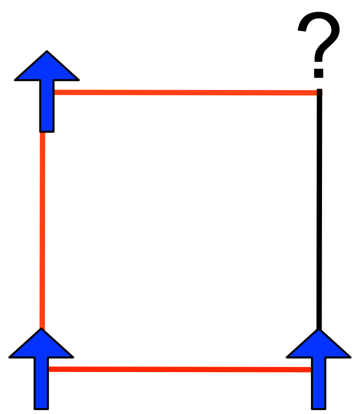

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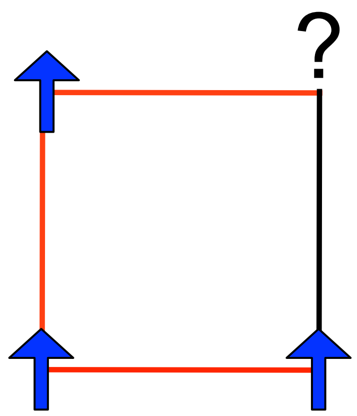
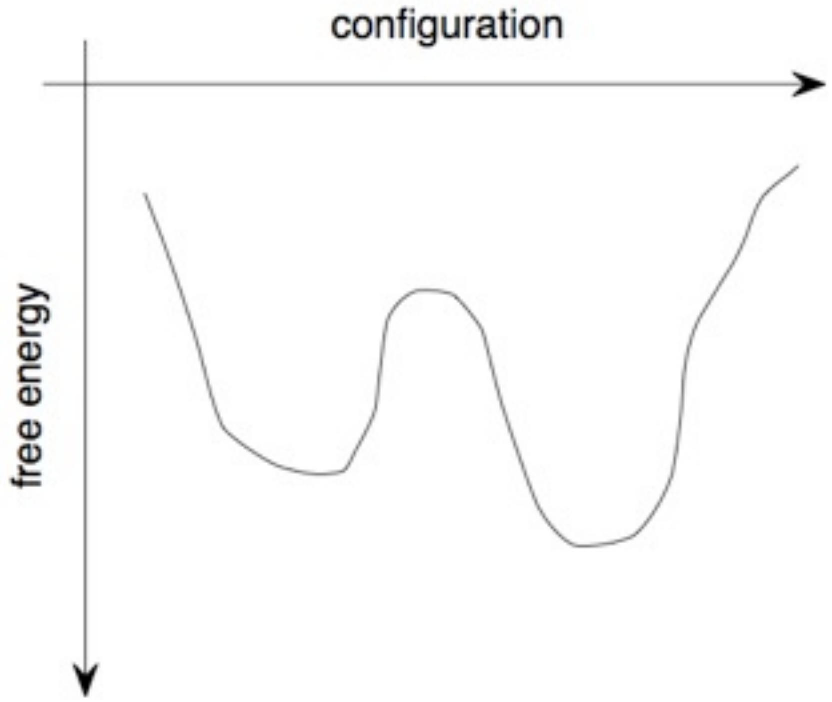


Rough free energy landscape.



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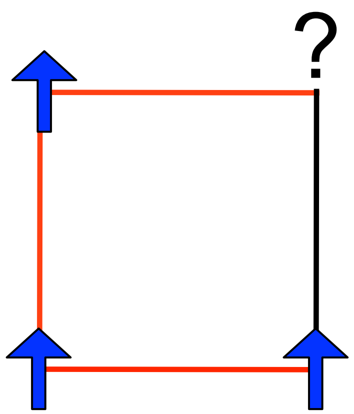

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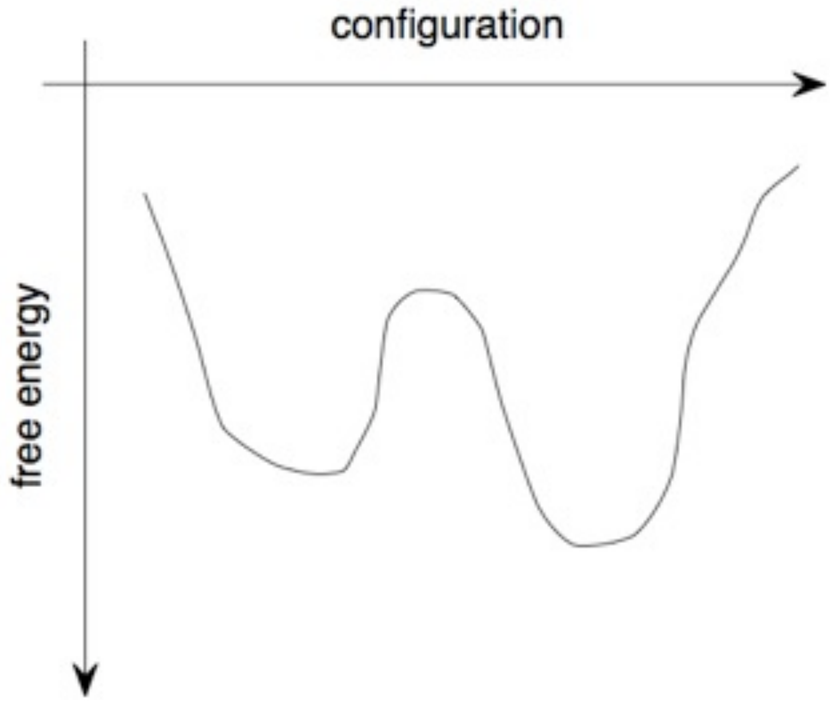

Finding ground states is NP-hard (non-planar graphs)

Spin Glass Order

- Spin overlap: $$q = \frac{1}{N} \sum_i s_i^{(1)} s_i^{(2)}$$

The superscripts refer to two independent spin configurations from the same problem instance.

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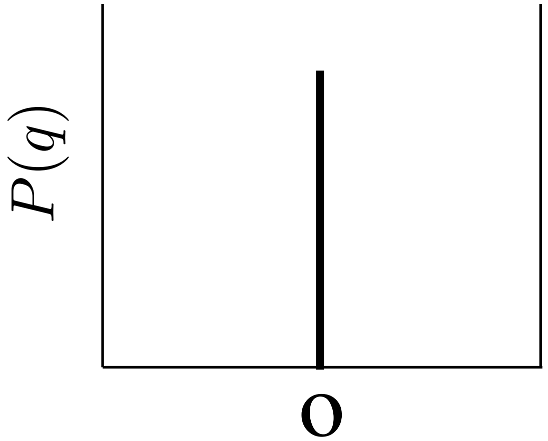
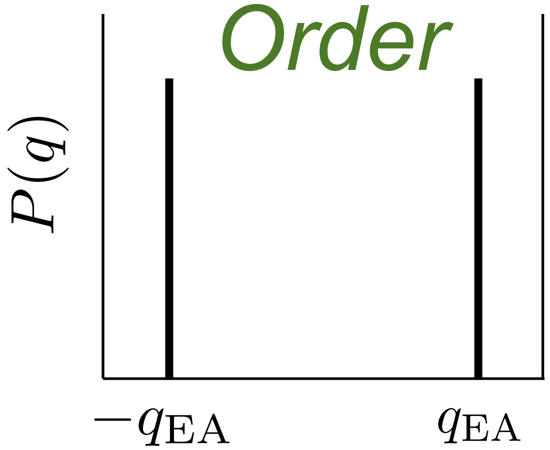
No order



Order



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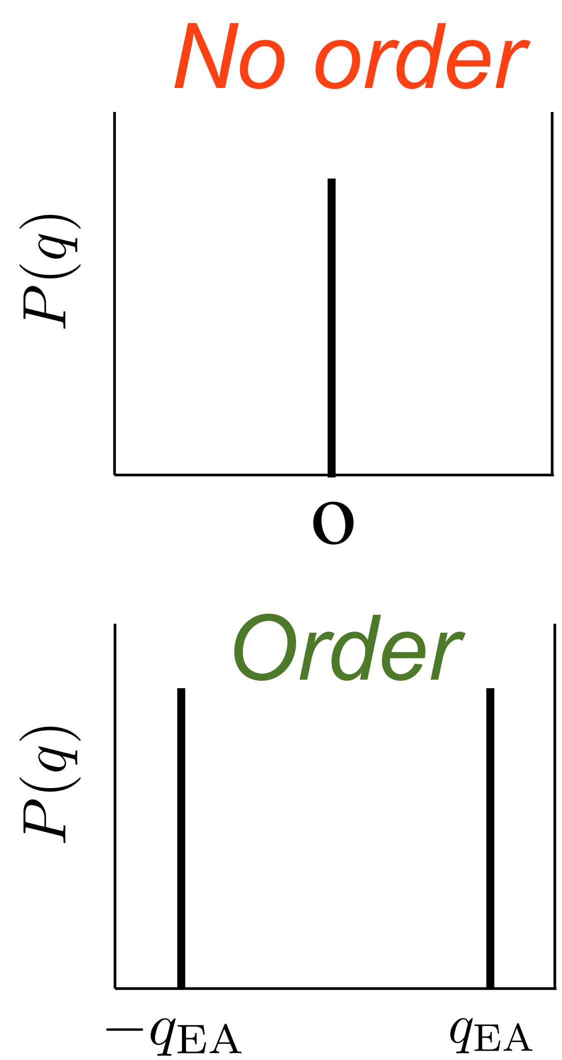
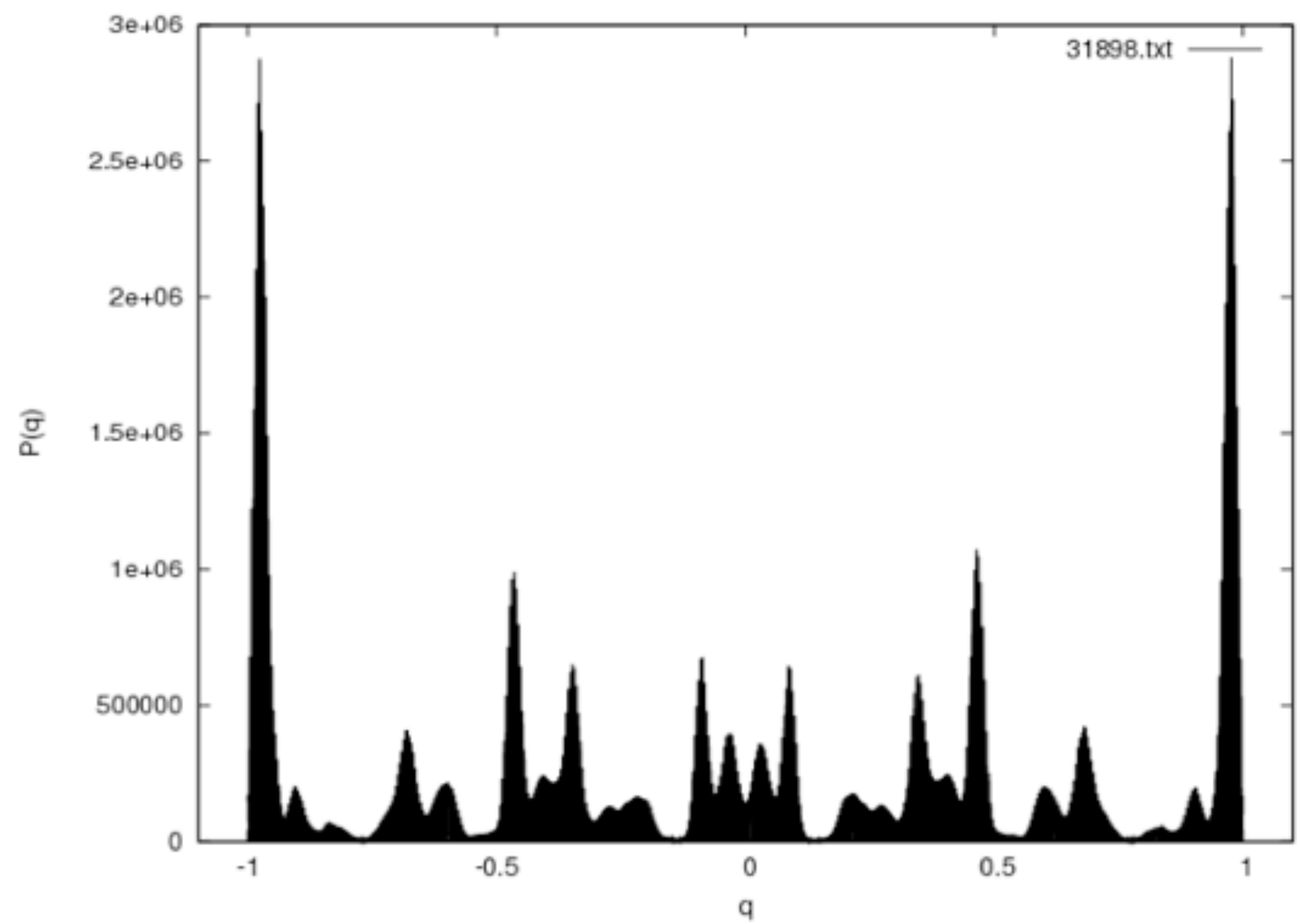


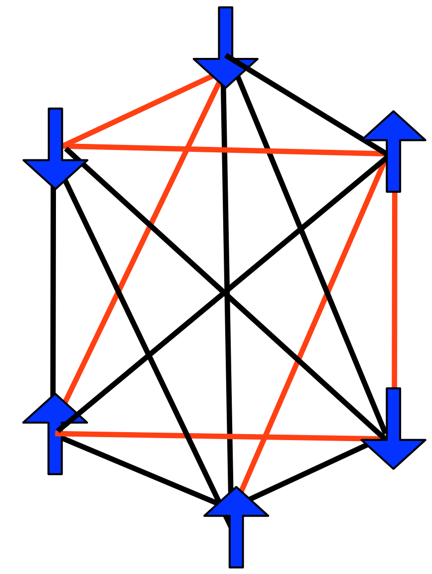


An example of an overlap histogram for a single 8x8x8 instance at low temperature.

Mean Field Theory

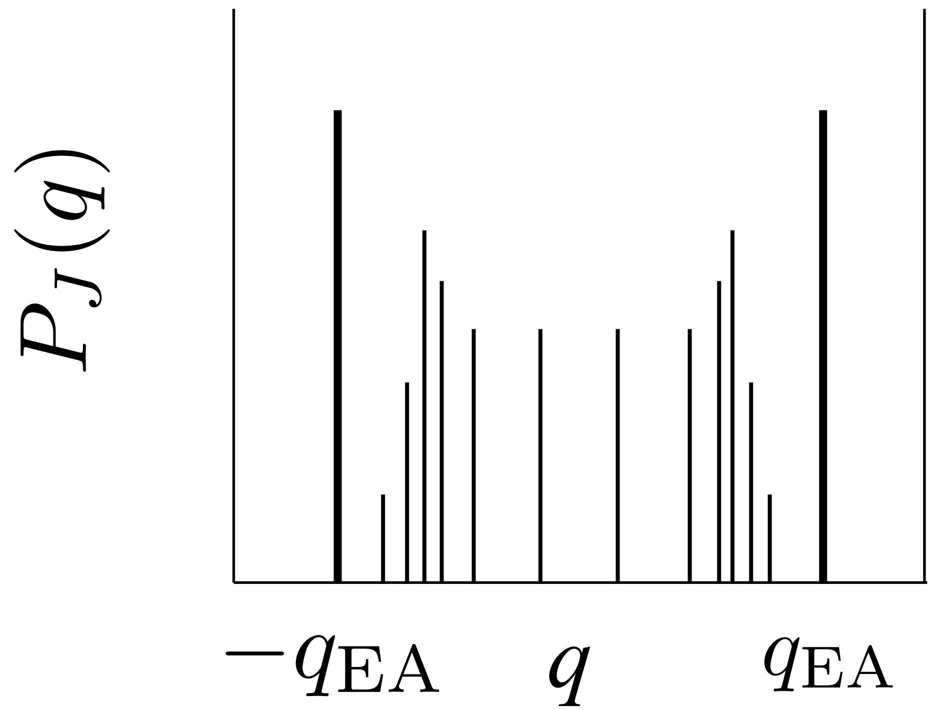
- Sherrington-Kirkpatrick model (1975)
  - –Ising spin glass on the complete graph

$$H[\sigma] = \frac{1}{\sqrt{N}} \sum_{(i,j)} J_{ij} s_i s_j$$



Parisi's solution for the SK Model (1979)

- Replica symmetry breaking (RSB)
- Overlap distribution not self-averaging
- Countable infinity of "pure states"
- Ultrametricity



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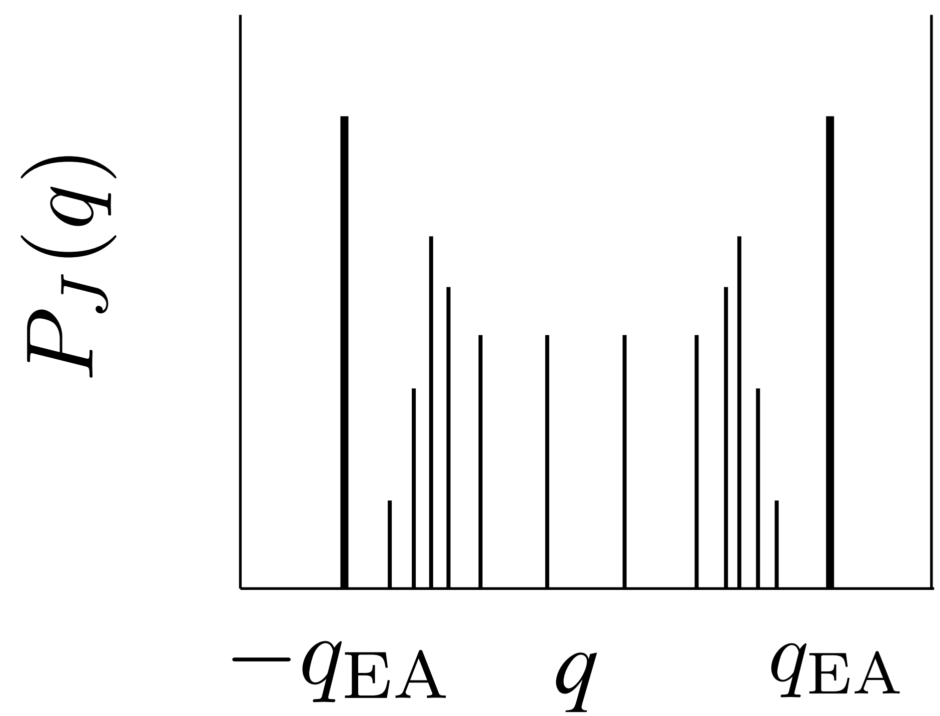

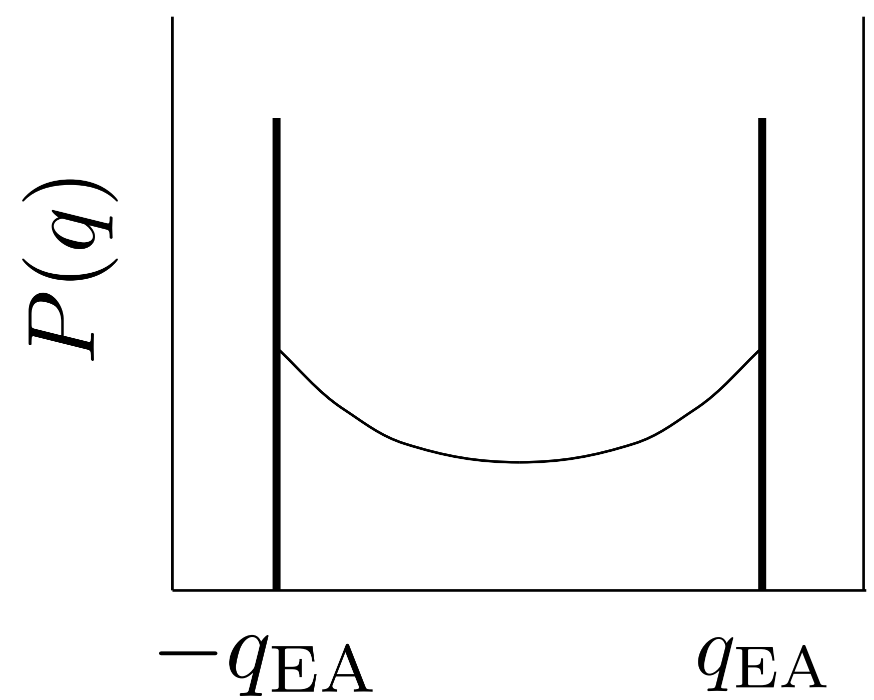

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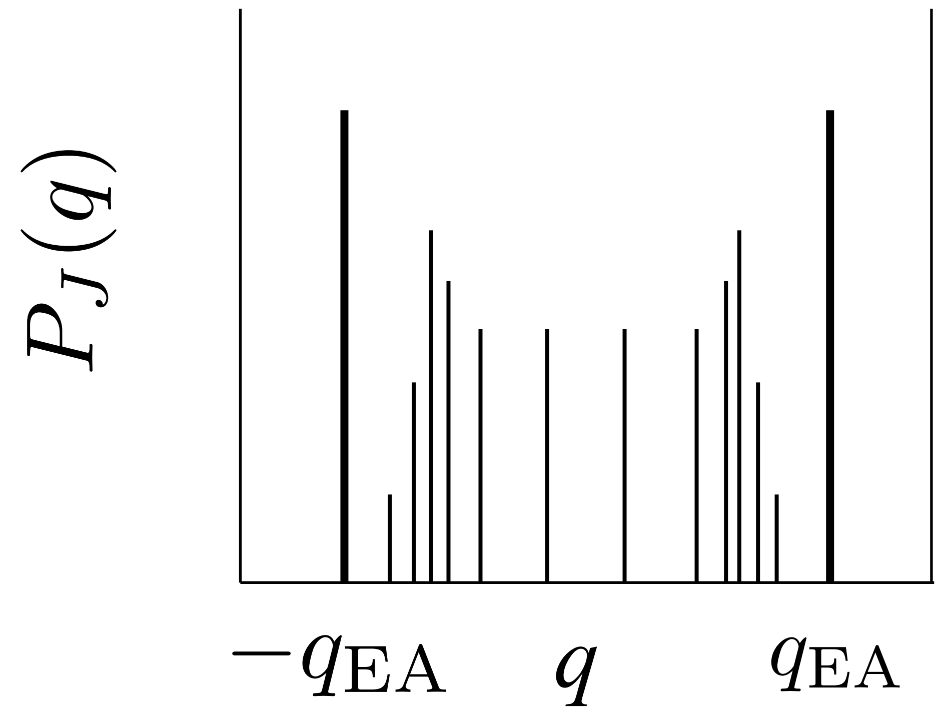
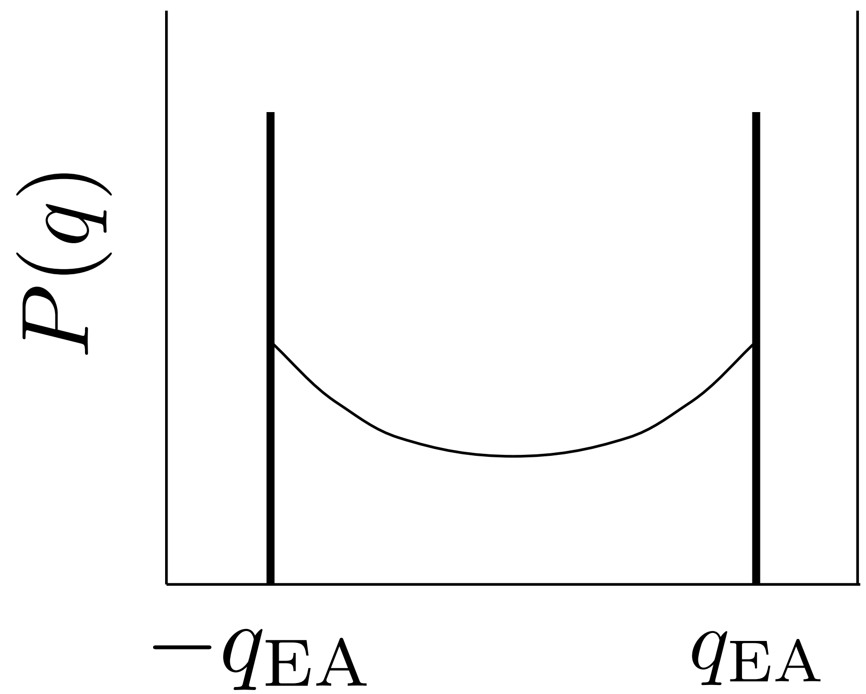
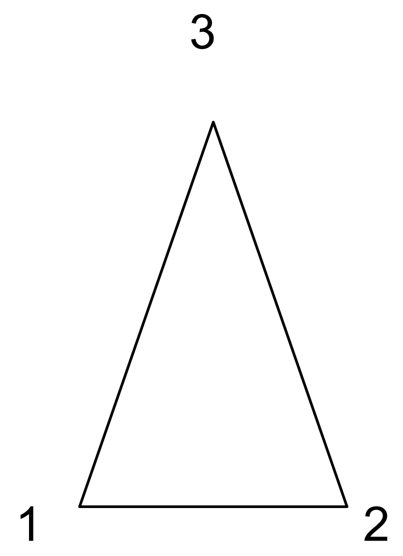






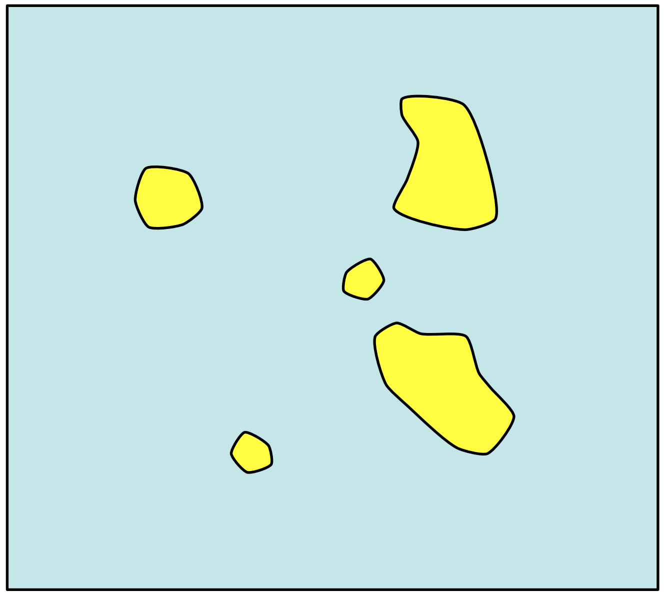
What about finite *d*?

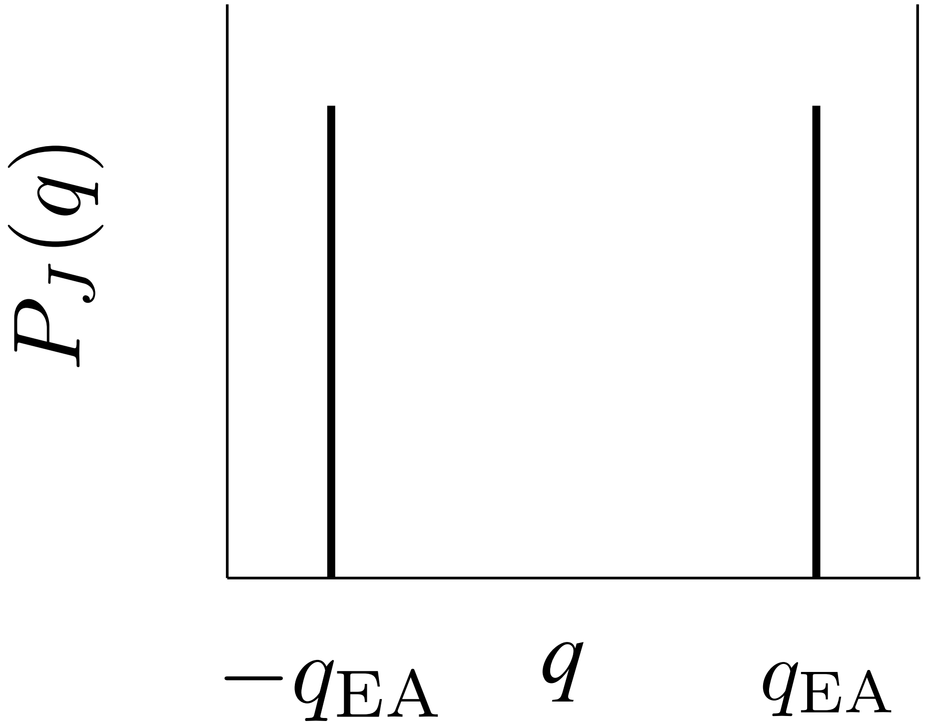
- Mean field (complete graph) results are often qualitatively correct for finite-dimensional systems.
- Does RSB apply to the three-dimensional Ising spin glass (Edwards-Anderson model)?

Droplet Picture

Fisher & Huse, Bray & Moore 1985

- Low temperature phase of 3D Ising spin glass consists of a pair of pure states related by up-down symmetry (similar to the ordinary Ising model).
- Low lying excitations are isolated compact "droplets" of flipped spins.





RSB vs Droplet

- Spin overlap: $$q = \frac{1}{N} \sum_i s_i^{(1)} s_i^{(2)}$$

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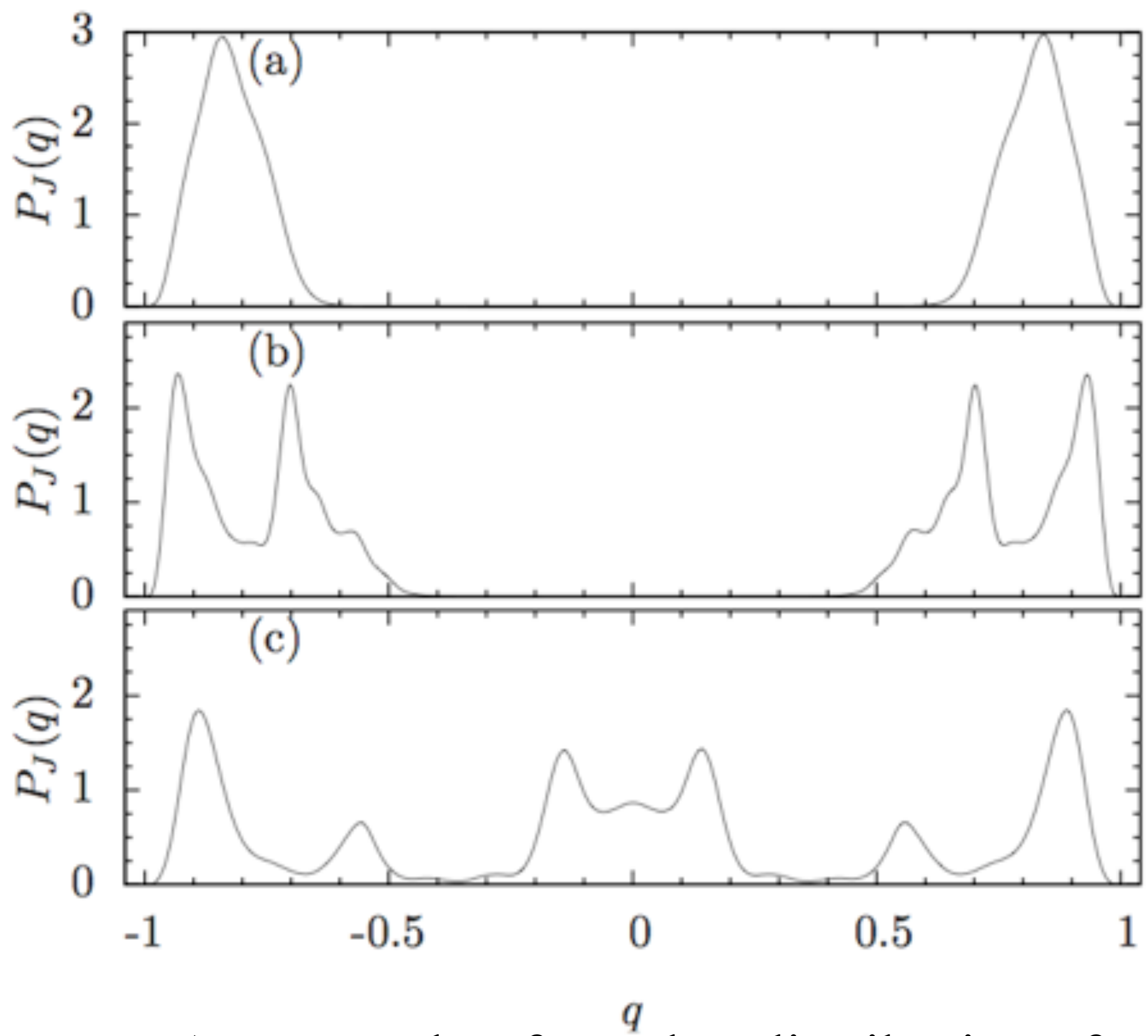
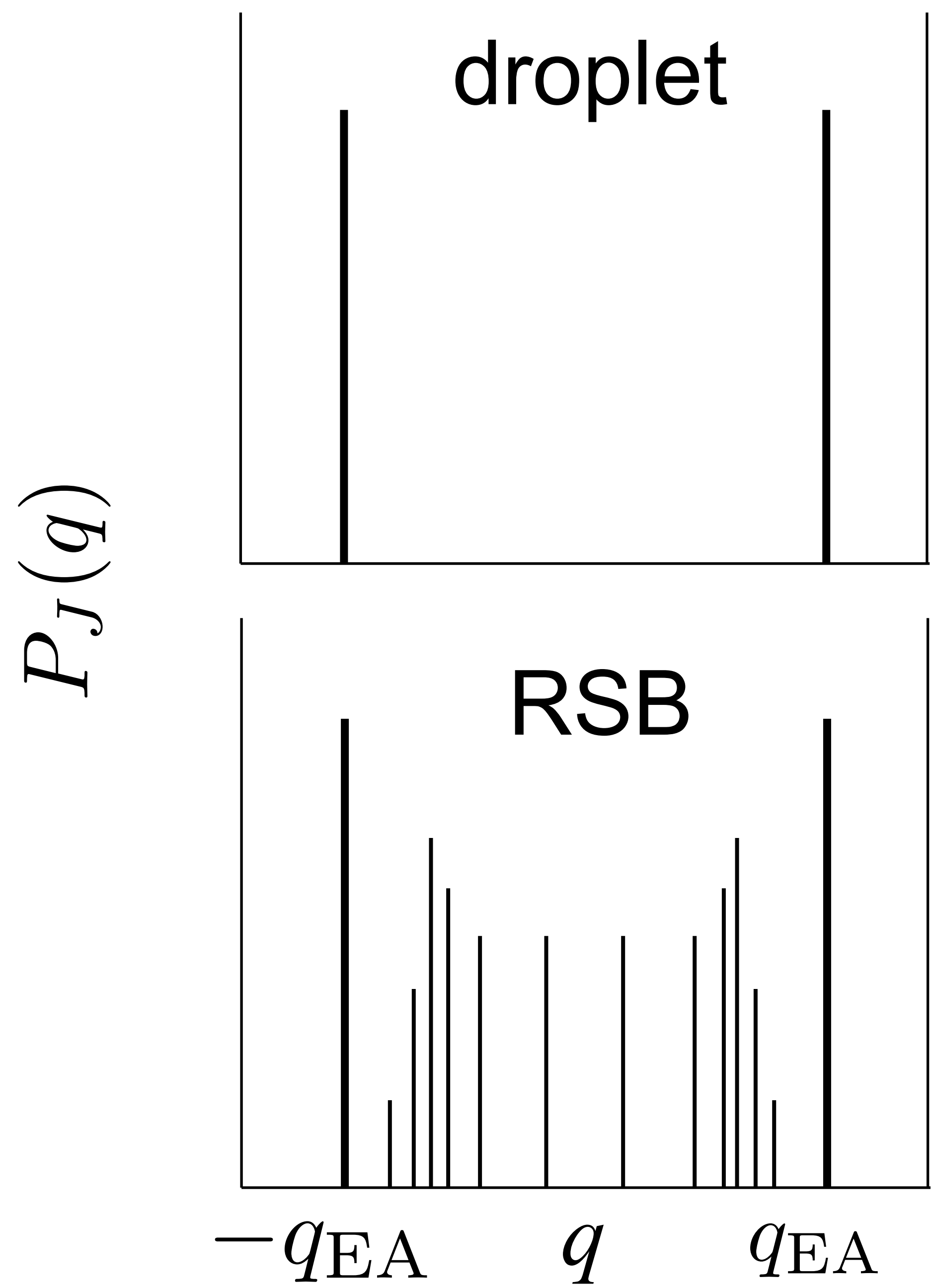


An example of overlap distributions for three disorder instances.



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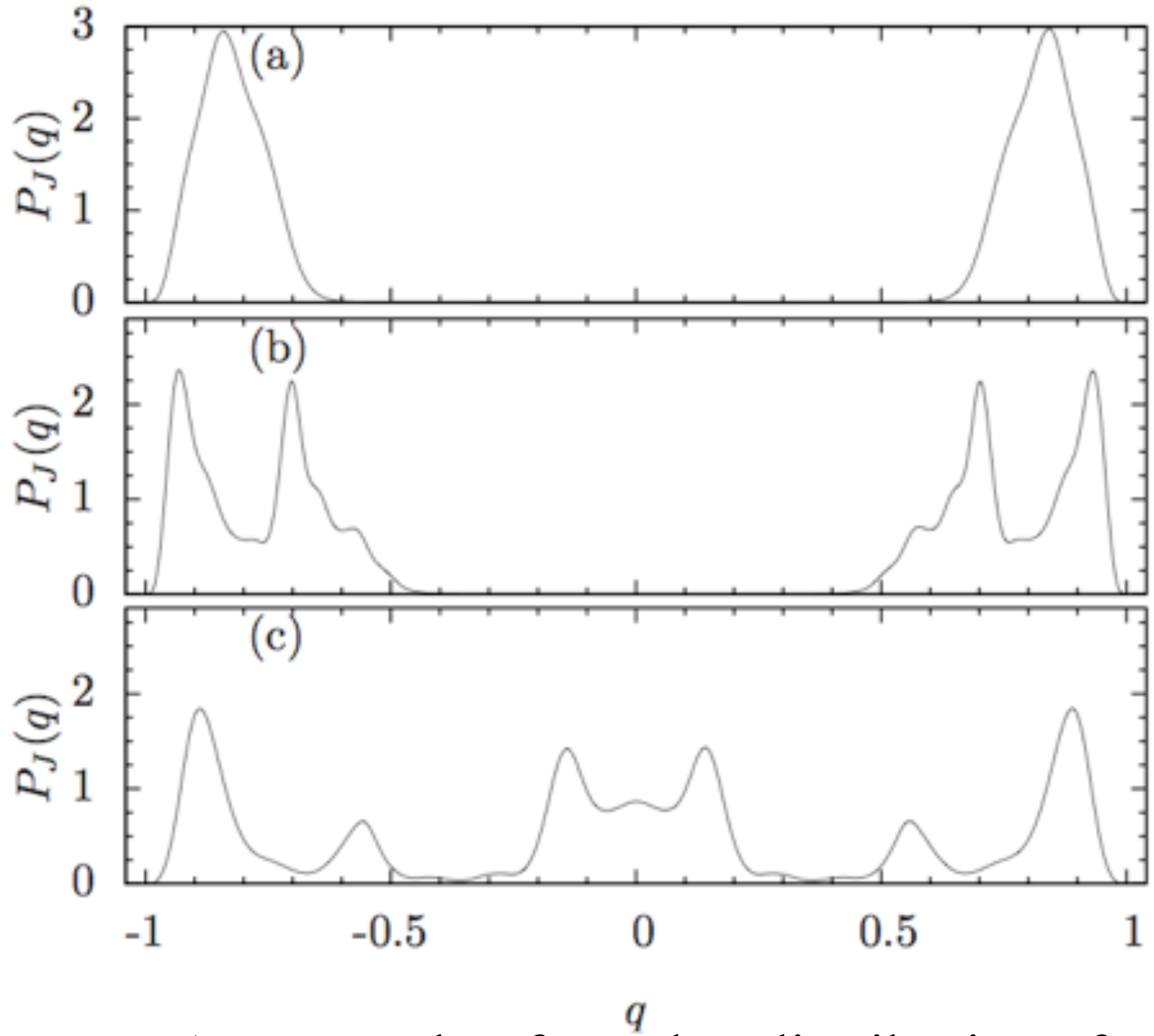

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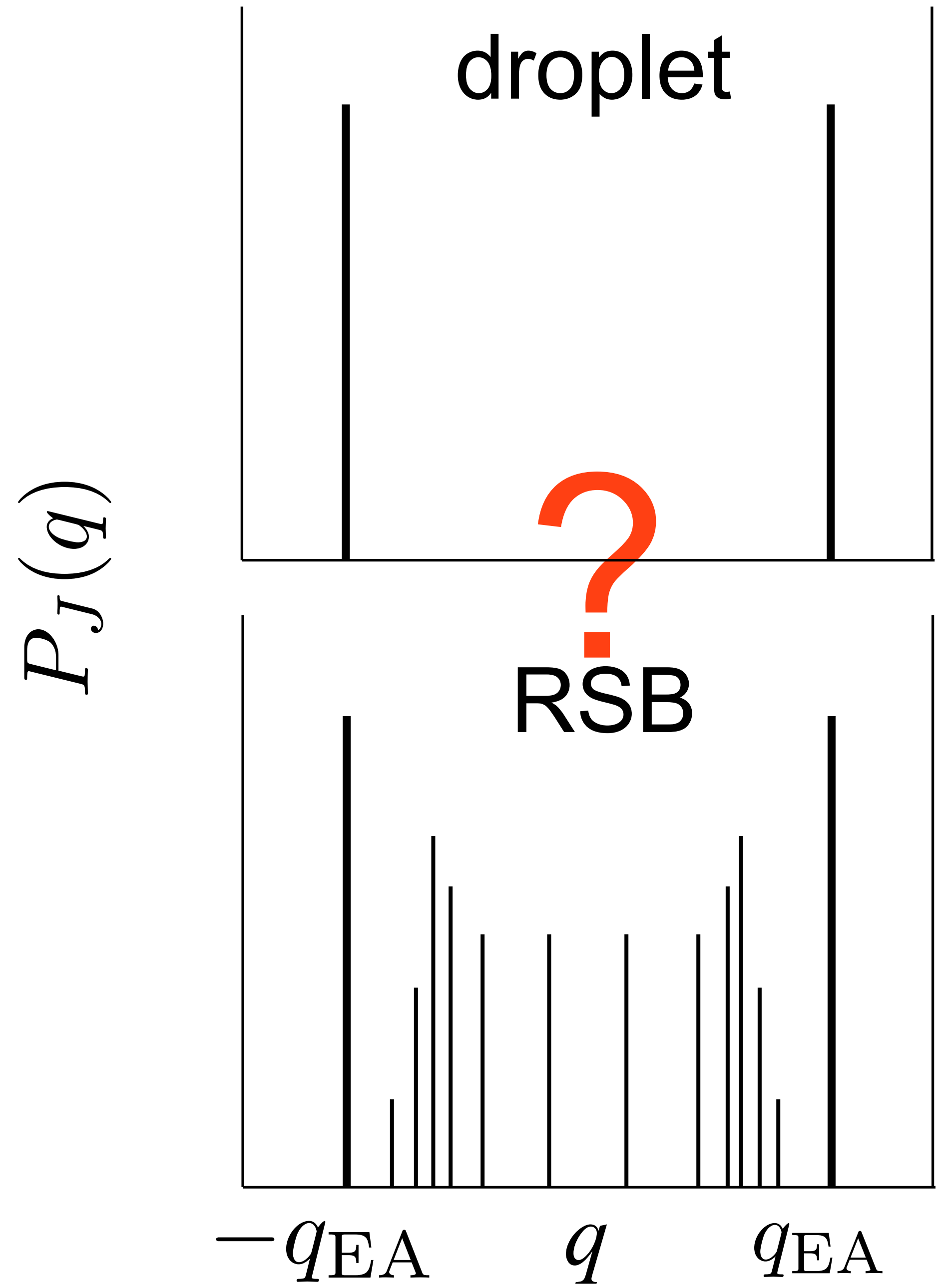
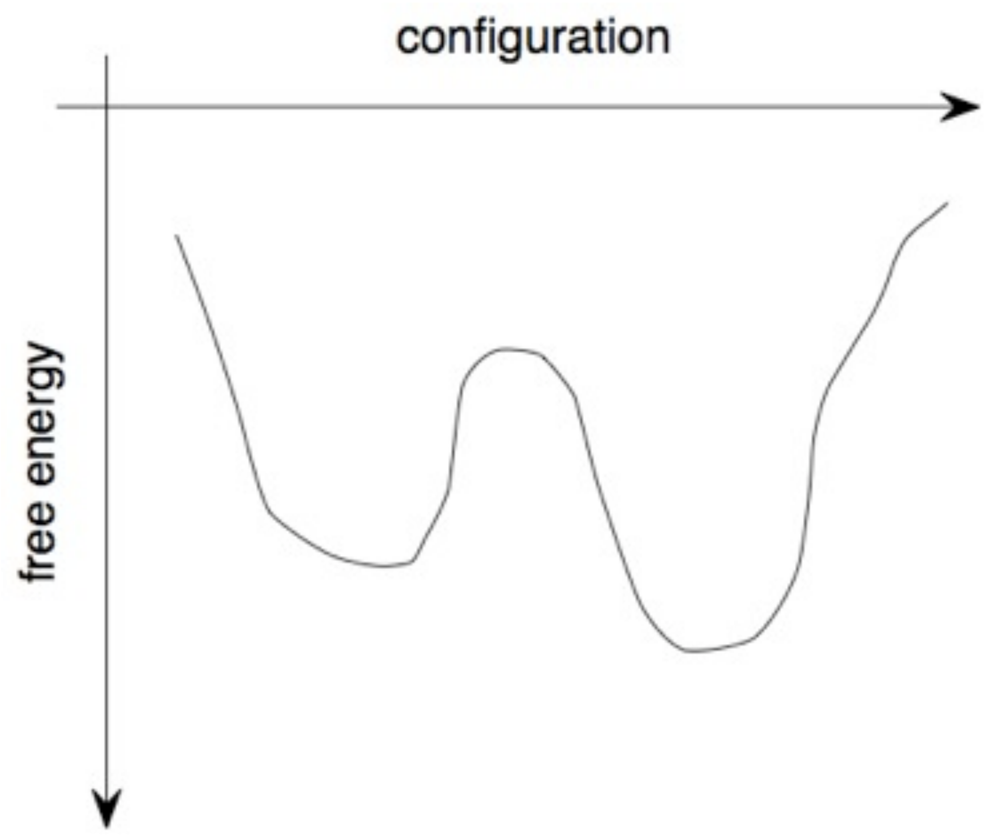


Computational Studies of Spin Glasses

- Find ground states using branch and bound or genetic algorithms.
- Find ground states, sample thermal states and compute free energies using polynomial time algorithms in 2D
- Find ground states, sample thermal states and estimate free energies using Monte Carlo methods for d>2 and the complete graph
  - Parallel tempering
  - **Population annealing**

Problem

- Markov chain Monte Carlo (MCMC) at a single temperature such as the Metropolis-Hastings algorithm gets stuck in local minima.



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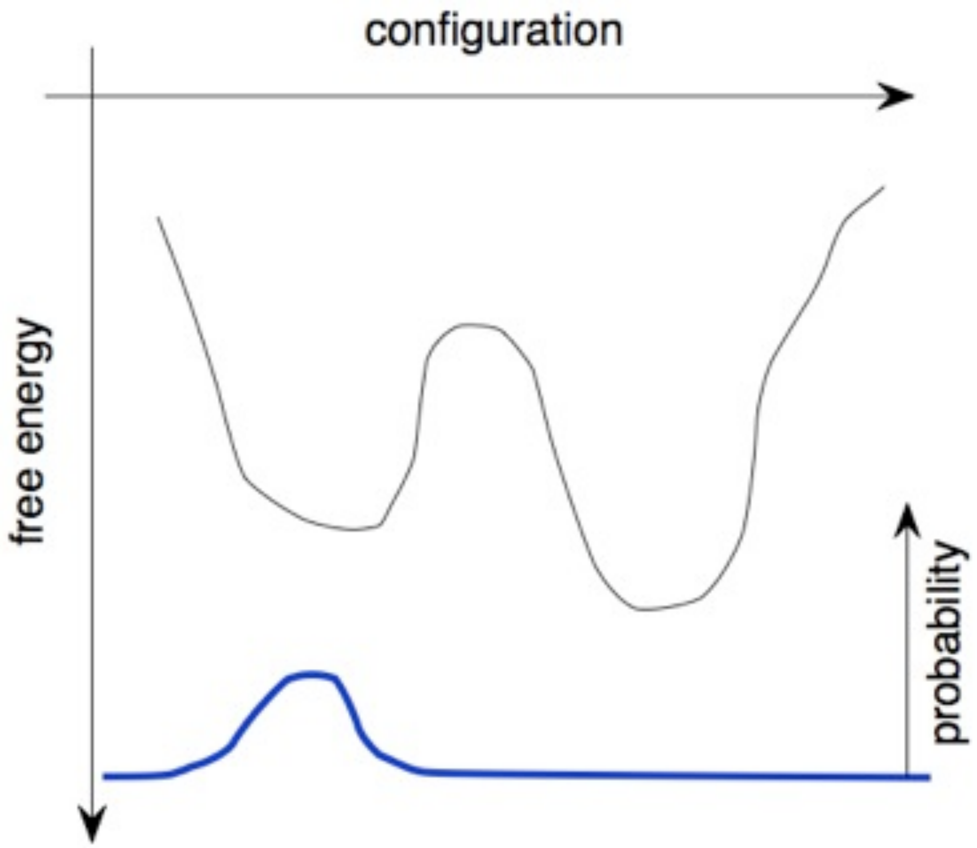
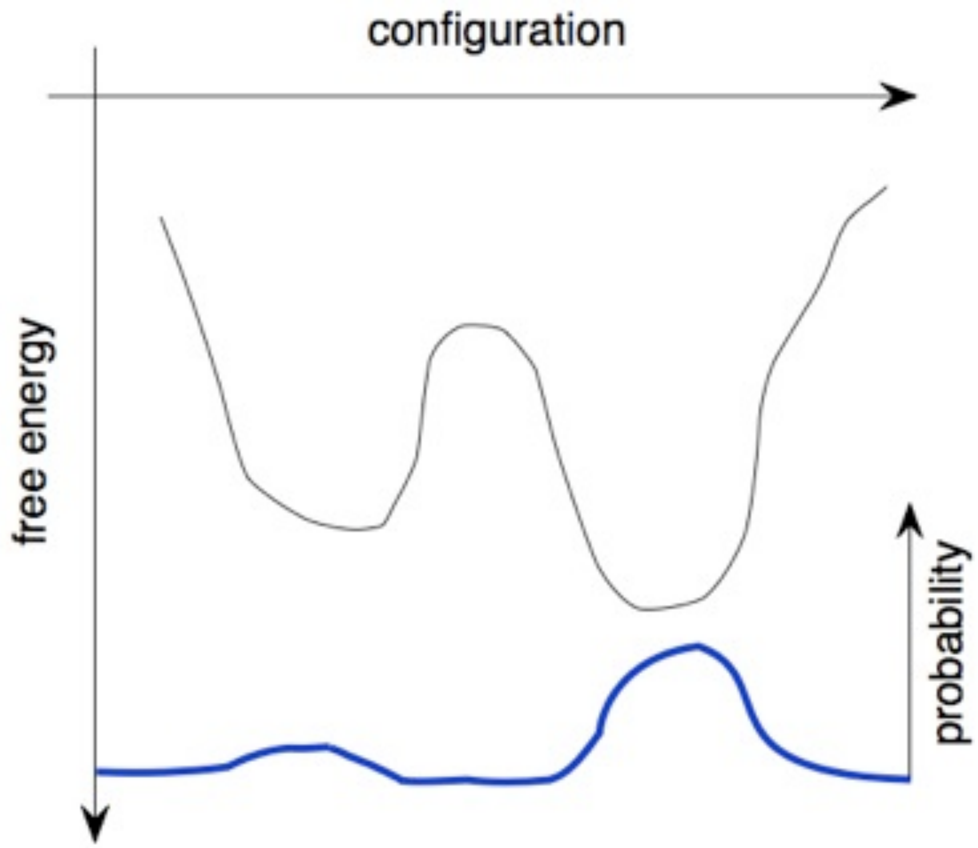
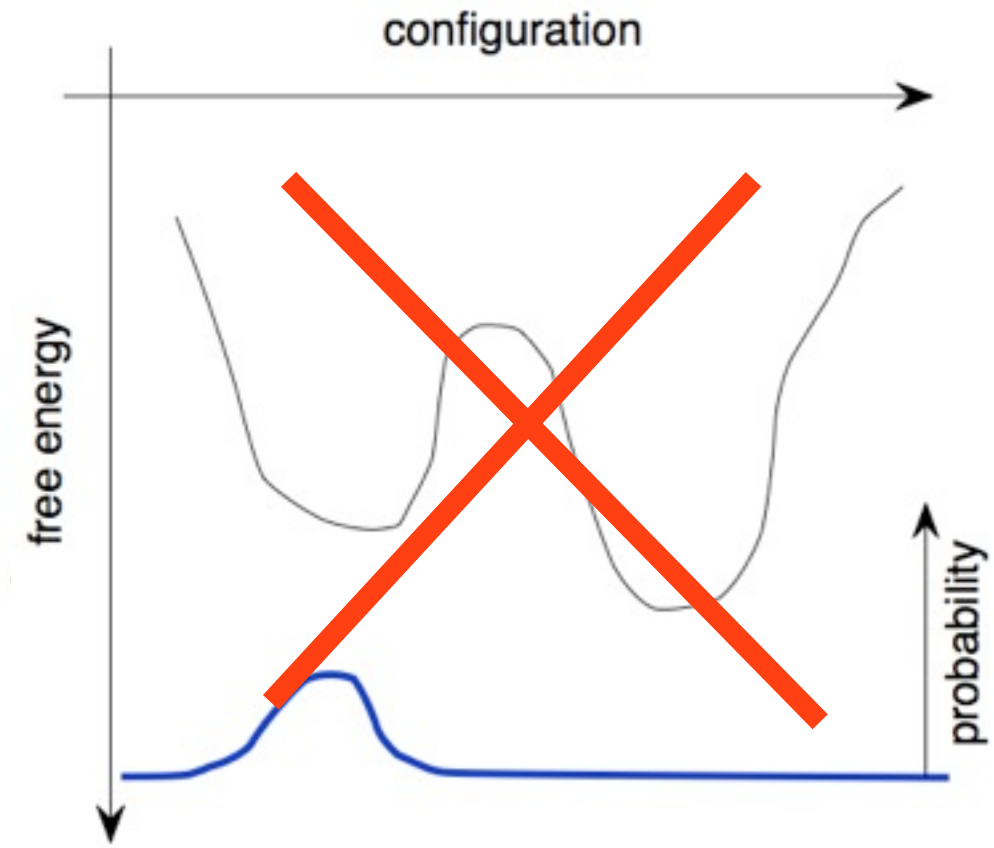



configuration
free energy
probability


configuration
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Population Annealing

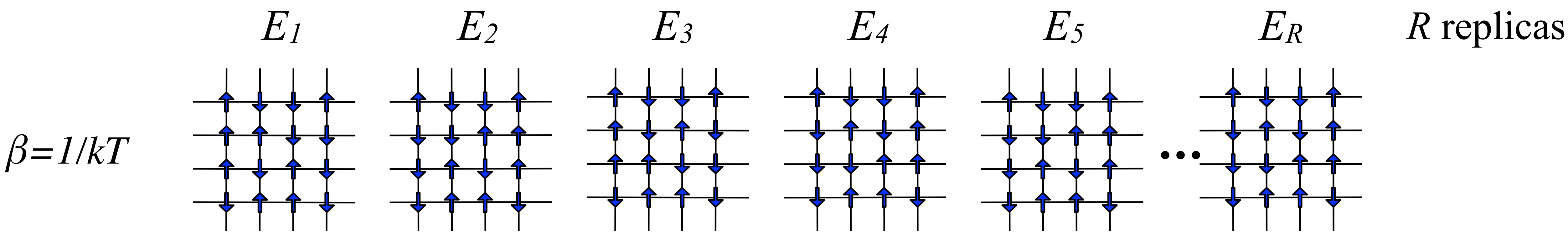
K. Hukushima and Y. Iba, in *THE MONTE CARLO METHOD IN THE PHYSICAL SCIENCES: Celebrating the 50th Anniversary of the Metropolis Algorithm*, edited by J. E. Gubernatis (AIP, 2003), vol. 690, pp. 200–206.

- Modification of *simulated annealing* for equilibrium sampling.
- A *population* of replicas is cooled according to an annealing schedule. Each replica is acted on by the Metropolis-Hastings at the current temperature.
- During each temperature step, the population is differentially reproduced (*resampled*) according to the correct Boltzmann re-weighting to maintain equilibrium.
- *See:* Phys. Rev. E 82, 026704 (2010); E 92, 063307 (2015)

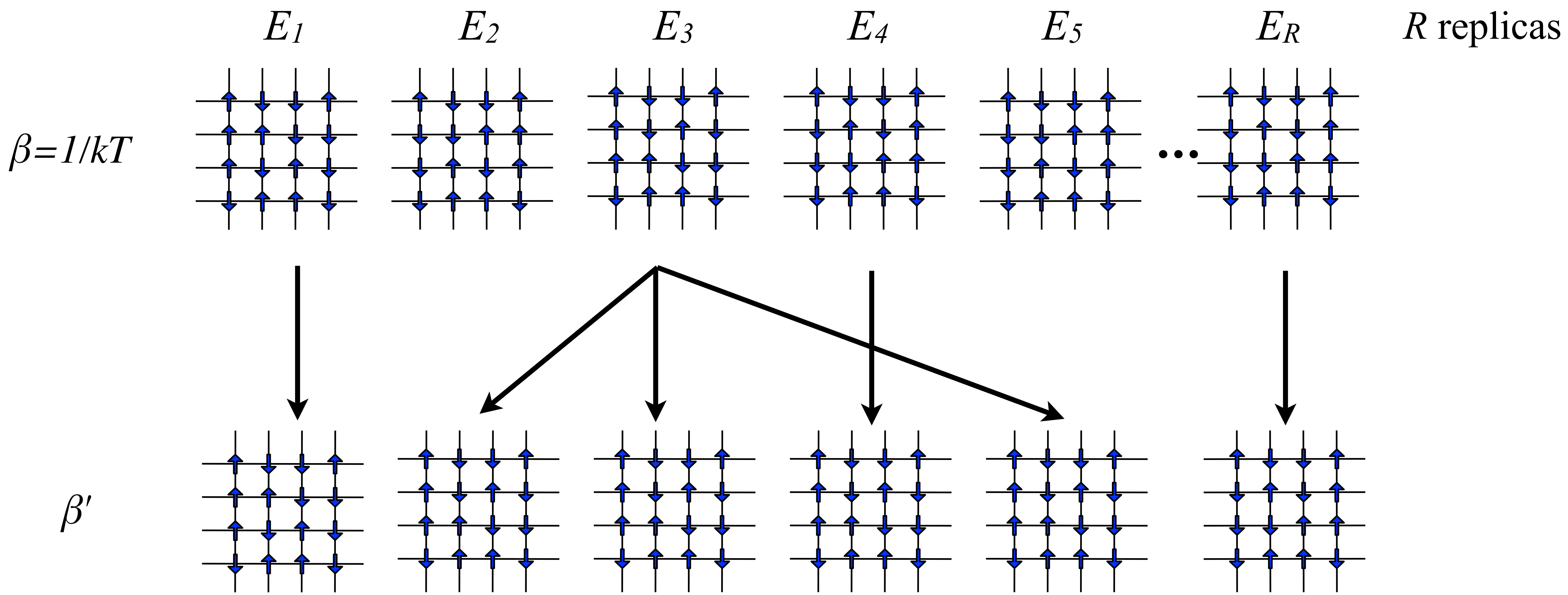
Population Annealing is related to...

- Simulated annealing
- Sequential Monte Carlo
  - See e.g. "Sequential Monte Carlo Methods in Practice", A. Doucet, et. al. (2001)
  - aka Particle Filters
  - Nested Sampling, Skilling
- Go with the Winners, Grassberger (2002)
- Diffusion (quantum) Monte Carlo
- Nonequilibrium Equality for Free Energy Differences, Jarzynski (1997)
- Histogram Re-weighting, Swendsen and Ferrenberg (1988)

Population Annealing

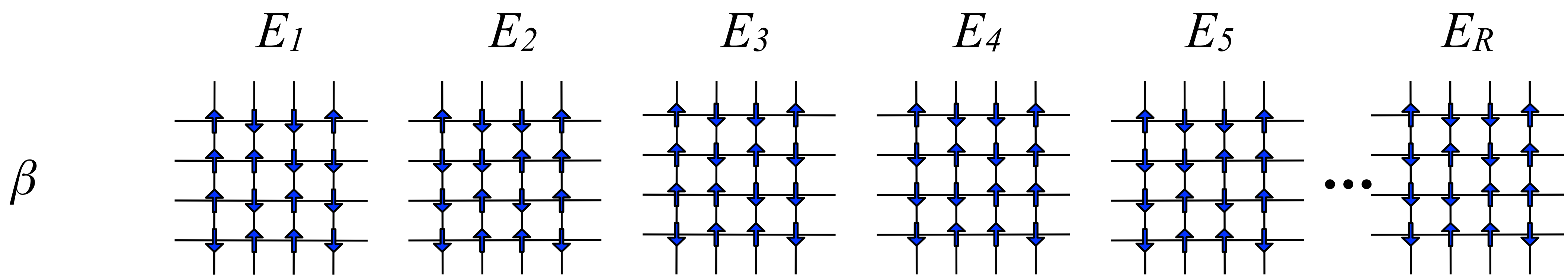


Population Annealing



Population annealing = simulated annealing with differential reproduction (resampling) of replicas

Temperature Step

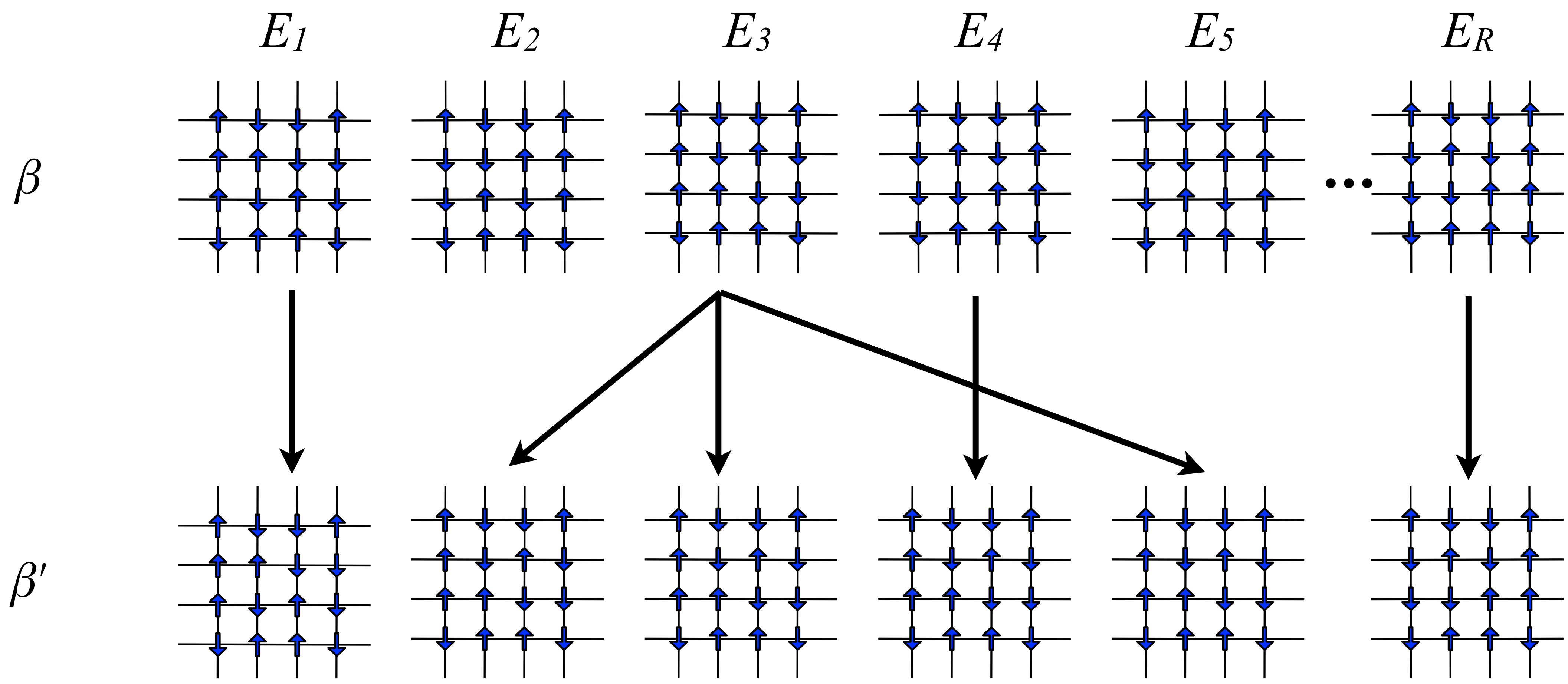


$$\tau_j(\beta, \beta') = \frac{\exp\left[-(\beta' - \beta)E_j\right]}{Q(\beta, \beta')}$$

$$Q(\beta, \beta') = \frac{\sum_{j=1}^{R} \exp\left[-(\beta' - \beta)E_j\right]}{R}$$

Replica j is reproduced n_j times where n_j is an integer random variate with mean τ_j.

Temperature Step



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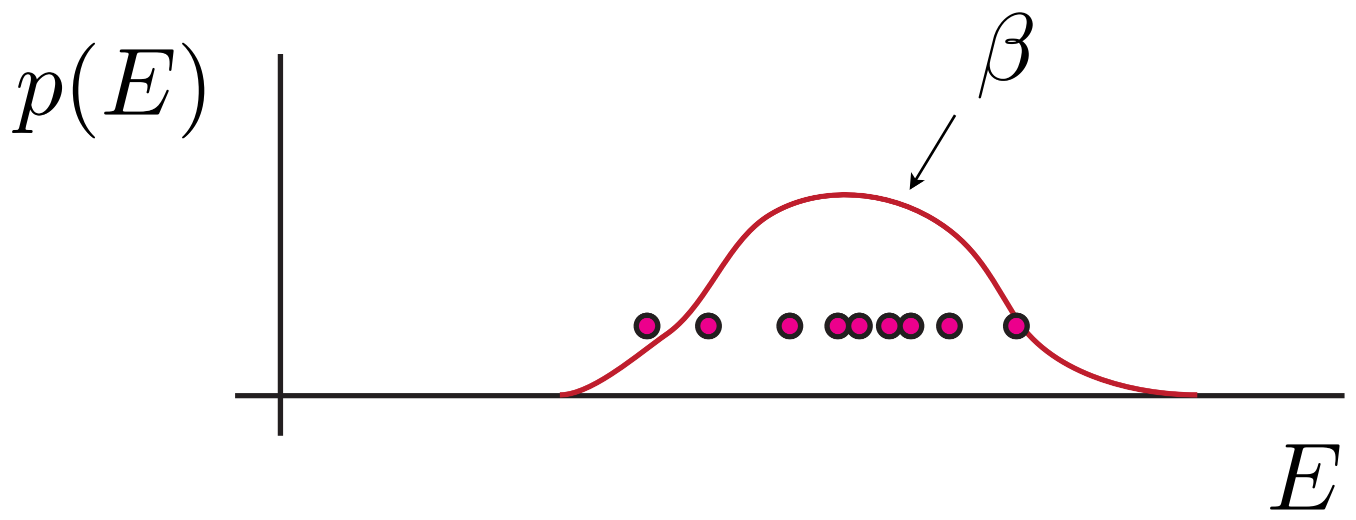
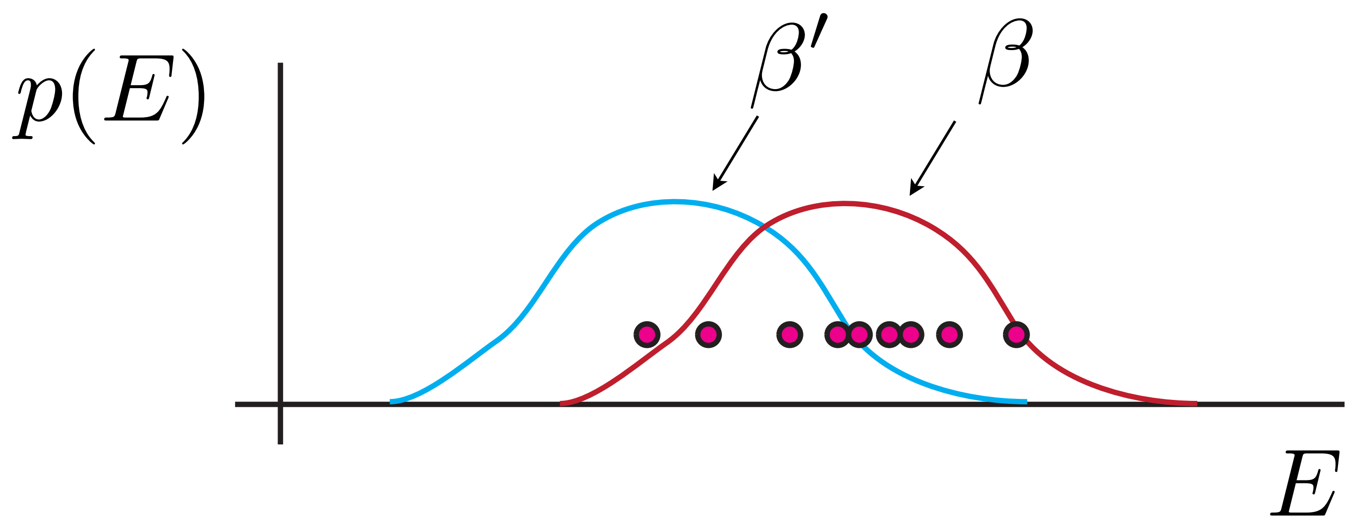
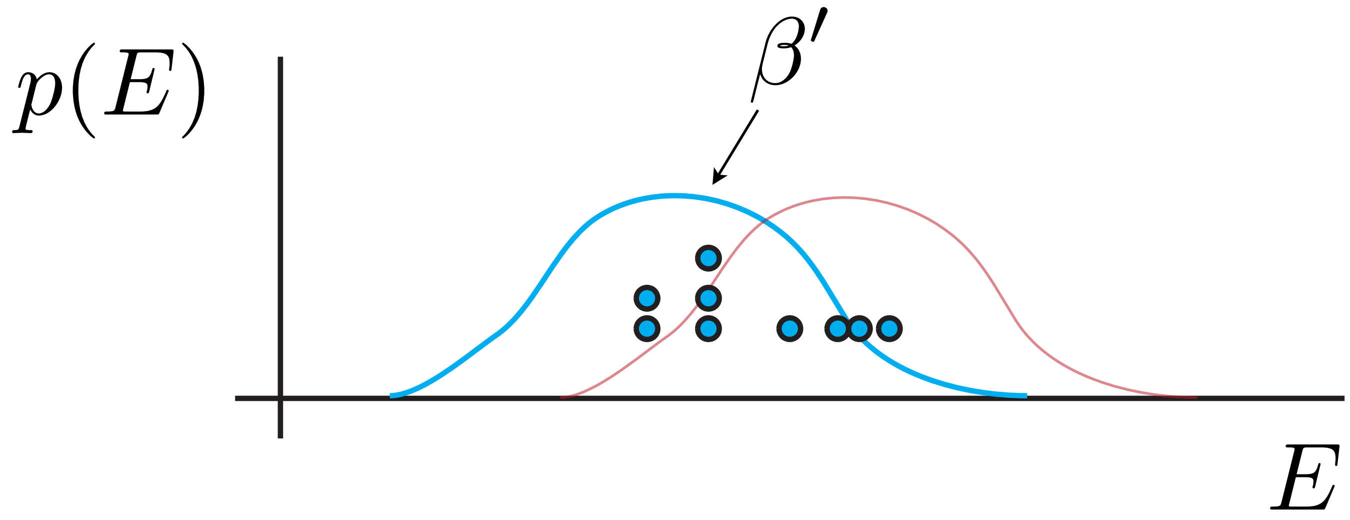


Population represents the Gibbs distribution at β

Systematic Errors



Systematic Errors



Resampled population represents the Gibbs distribution at β'

... but new population is biased toward high energy and correlated

Direct Estimate of Free Energy

$$Q(\beta, \beta') = \frac{\sum_{j=1}^{R} \exp\left[-(\beta' - \beta)E_j\right]}{R}$$

$$-\beta_k F(\beta_k) = \sum_{\ell=k}^{K} \ln Q(\beta_{\ell+1}, \beta_\ell) + \beta_K F(\beta_K)$$

Derivation:

$$\begin{aligned}
\frac{Z(\beta')}{Z(\beta)} &= \frac{\sum_\gamma e^{-\beta' E_\gamma}}{Z(\beta)} \\
&= \sum_\gamma e^{-(\beta'-\beta)E_\gamma}\left(\frac{e^{-\beta E_\gamma}}{Z(\beta)}\right) \\
&= \langle e^{-(\beta'-\beta)E_\gamma}\rangle_\beta \\
&\approx \frac{1}{R}\sum_{j=1}^{R} e^{-(\beta'-\beta)E_j} = Q(\beta, \beta').
\end{aligned}$$

Weighted Averaging

JM, PRE82,26704(2010)

- Results from small population runs are biased.
- Results from independent runs can be combined and biases reduced using *weighted* averages.
- Observables from each run weighted by the exponential of the free energy estimator for that run.

$$\overline{A}(\beta) = \sum_{m=1}^{M} \tilde{A}_m(\beta)\omega_m(\beta) \qquad \omega_m(\beta) = \frac{R_m e^{-\beta \tilde{F}_m(\beta)}}{\sum_{i=1}^{M} R_m e^{-\beta \tilde{F}_i(\beta)}}$$

Weighted Averaging

Imagine population annealing with unlimited resources and let the population in each run m grow according to unnormalized weights

$$\tau_i = \exp\left[-(\beta' - \beta)E_i\right]$$

$$\mathfrak{R}_m = R_m \prod_{\beta_k} Q_m(\beta_k) = e^{-\beta \tilde{F}_m(\beta)}$$

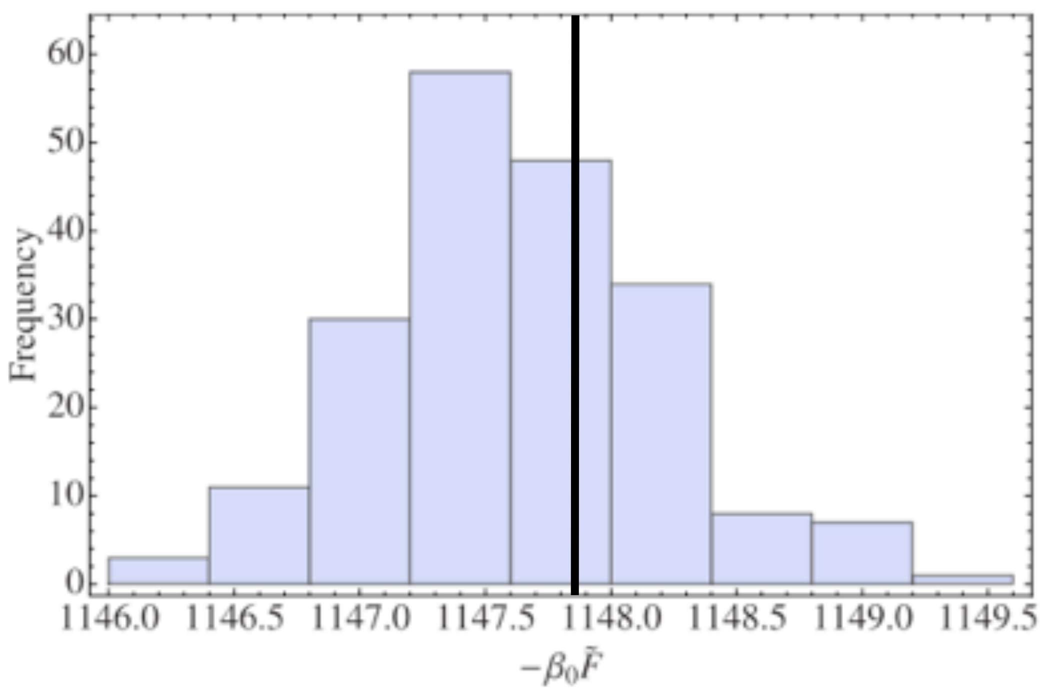
final population of run m

$$\overbrace{\cdot\cdot\cdot\cdot\cdot}^{\mathfrak{R}_1}\ \overbrace{\cdot\cdot\cdot\cdot\cdot\cdot\cdot}^{\mathfrak{R}_2}\ \overbrace{\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot\cdot}^{\mathfrak{R}_3}\qquad \overbrace{\cdot\cdot\cdot\cdot\cdot}^{\mathfrak{R}_M}$$

An ordinary average over the combined populations of unlimited PA is equivalent to a weighted average with standard PA

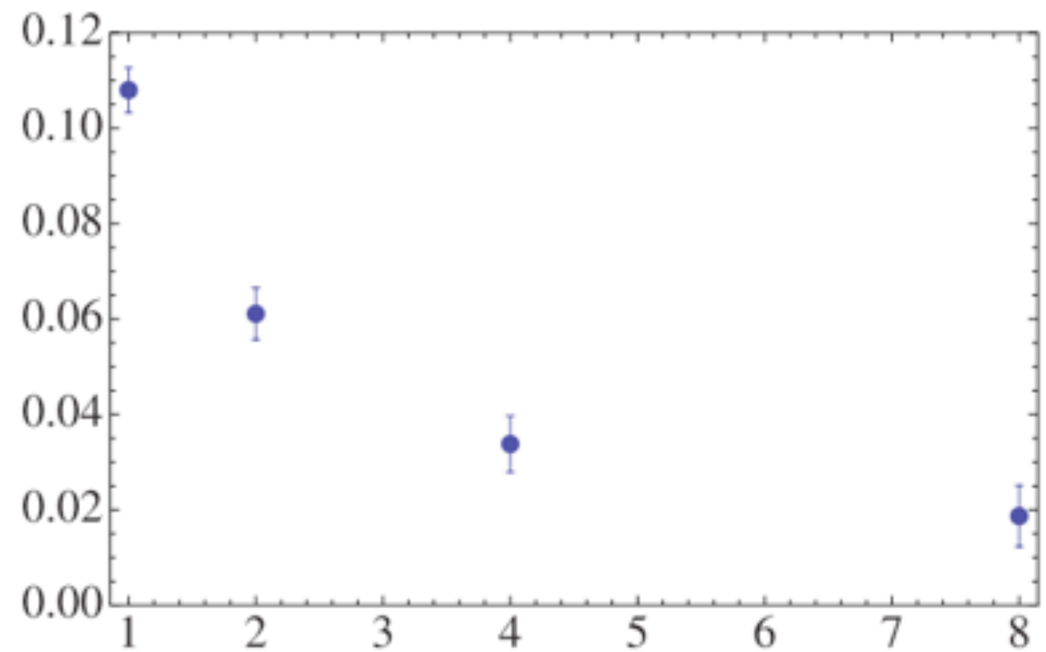
Weighted Averaging

histogram



free energy

systematic error



number of runs

Systematic Errors

If an observable is a function of the free energy estimator there will be a systematic error (bias) proportional to the variance of the free energy estimator.

$$\delta A_{\mathrm{systematic}} \approx -(\mathbf{Var}\beta\tilde{F})\frac{d\tilde{A}}{\beta d\tilde{F}} \approx -\frac{\rho_0}{R}\frac{dA}{\beta dF}$$

$$\rho_0 = \lim_{R\to\infty} R\ \mathbf{Var}\beta\tilde{F}$$

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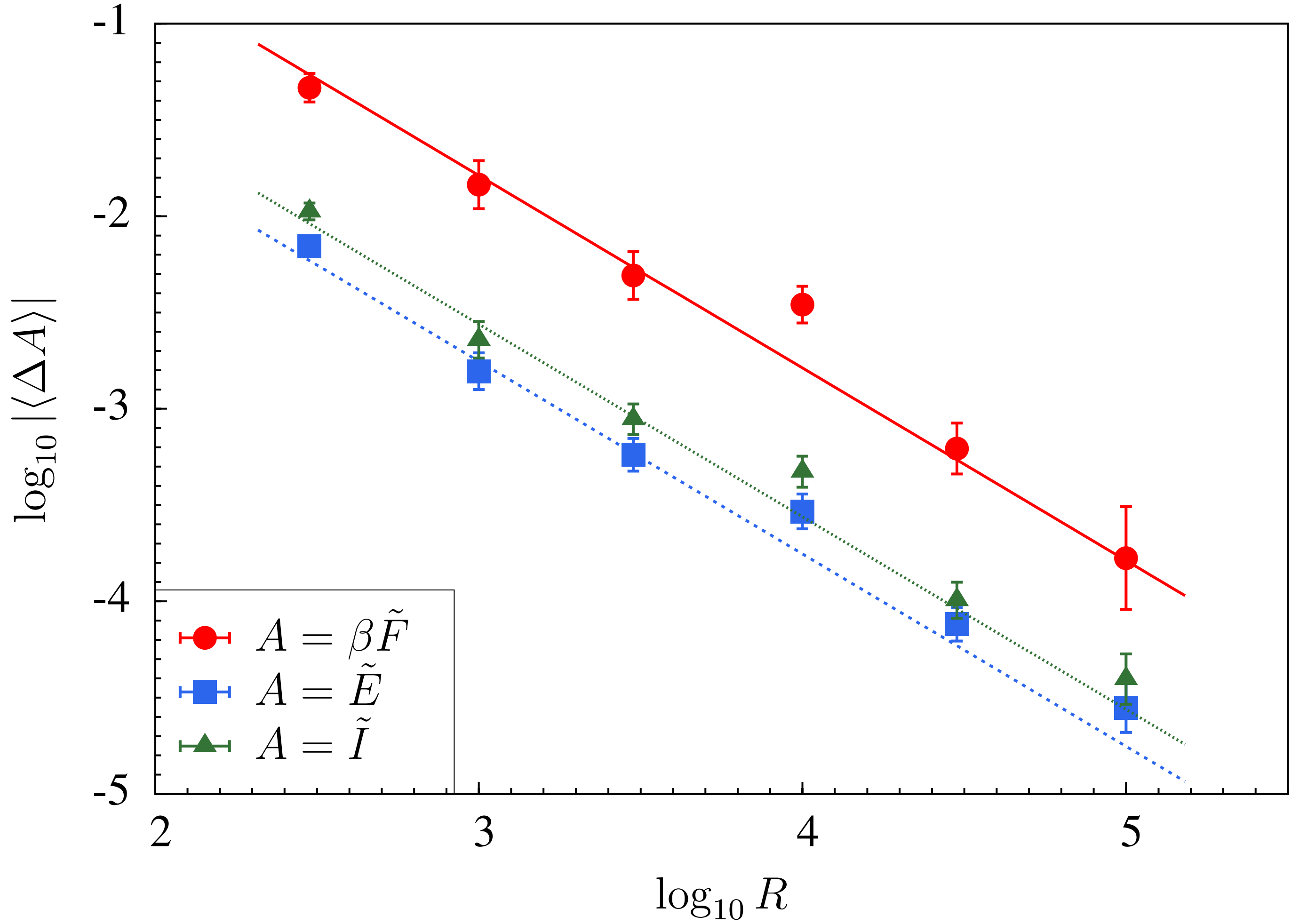
ρ_0 is the population size scale for systematic errors
(like the exponential autocorrelation time for MCMC)

Convergence in Population Size

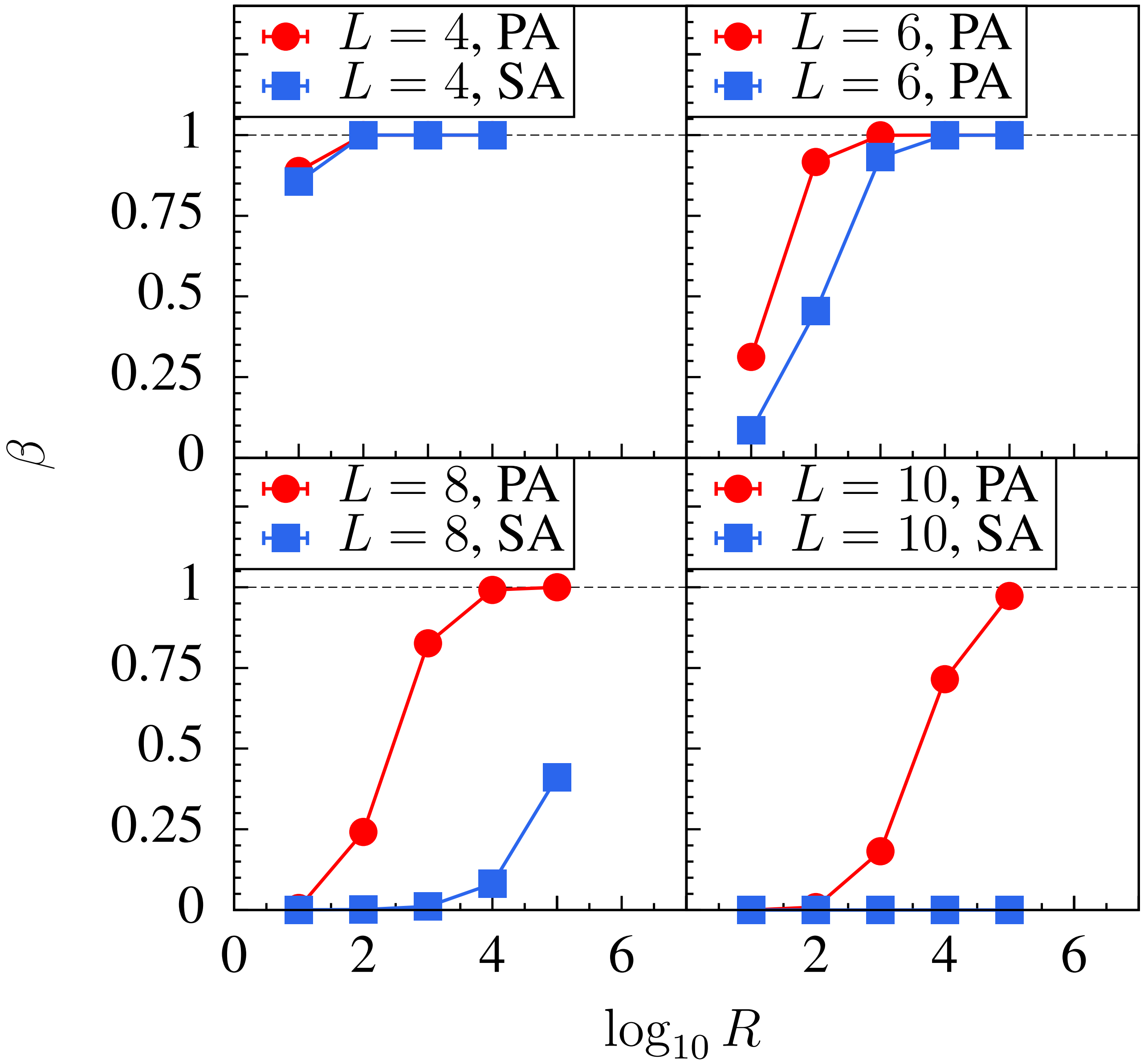
log systematic errors



log population size

Compare PA and SA for finding GS's

•Simulate a population of R replicas with resampling (PA) and without resampling (SA) holding the annealing schedule fixed.
•Do for many spin glass instances.
• The vertical axis is the disorder averaged probability of finding the true ground state.



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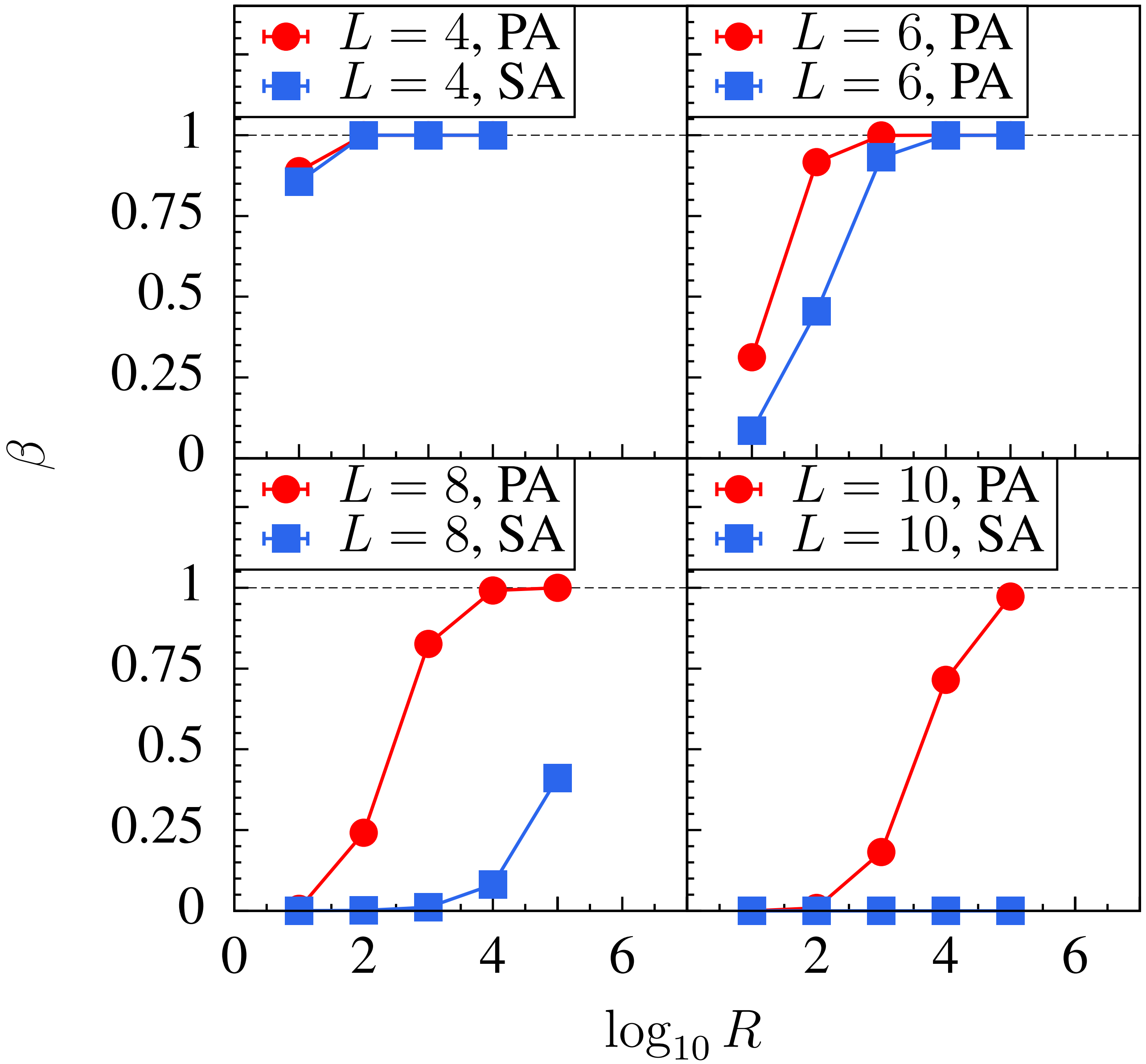

Population annealing is far more efficient than simulated annealing with almost no overhead

RSB vs Droplet

- Spin overlap: $$q = \frac{1}{N} \sum_i s_i^{(1)} s_i^{(2)}$$

RSB vs Droplet

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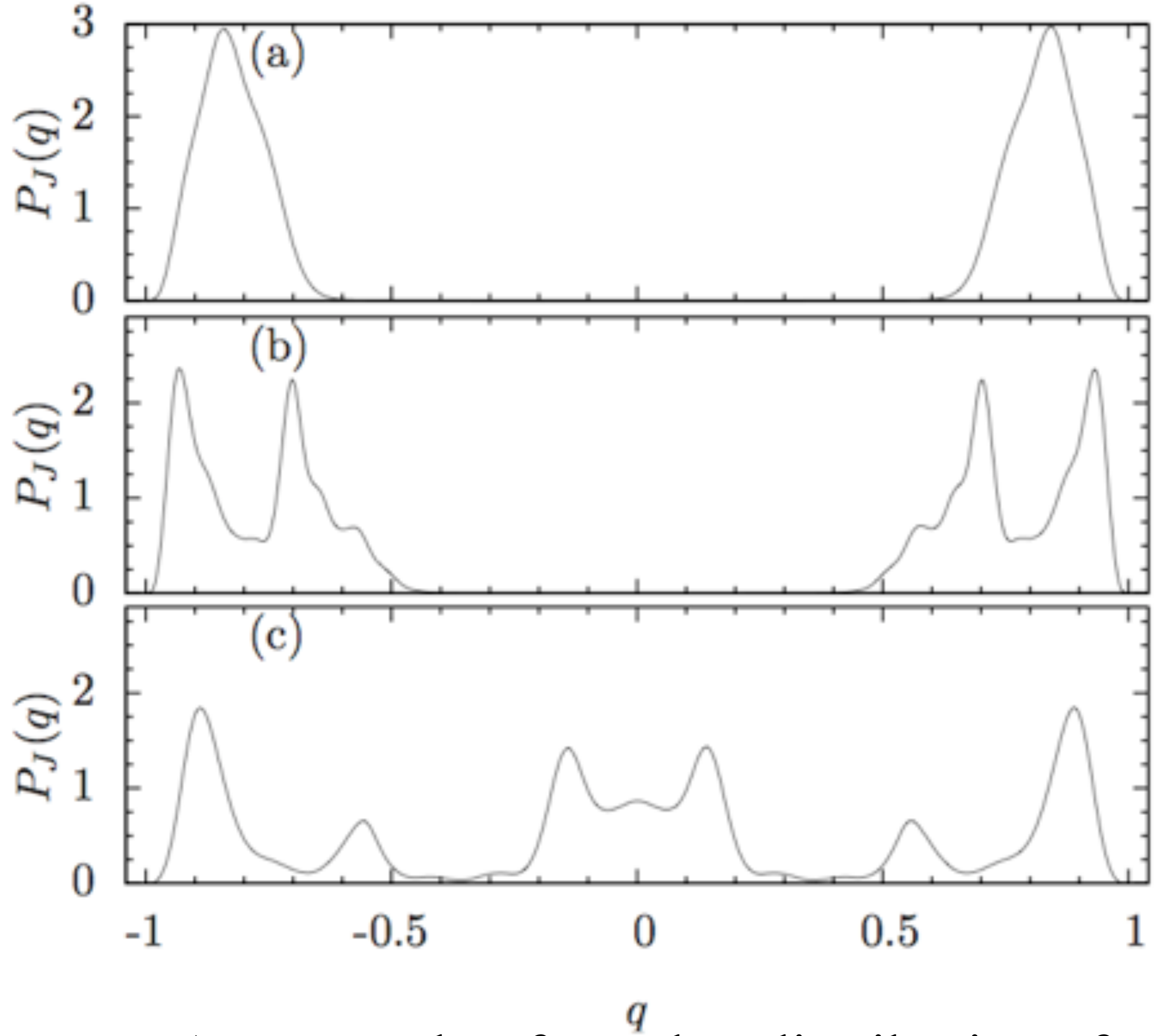
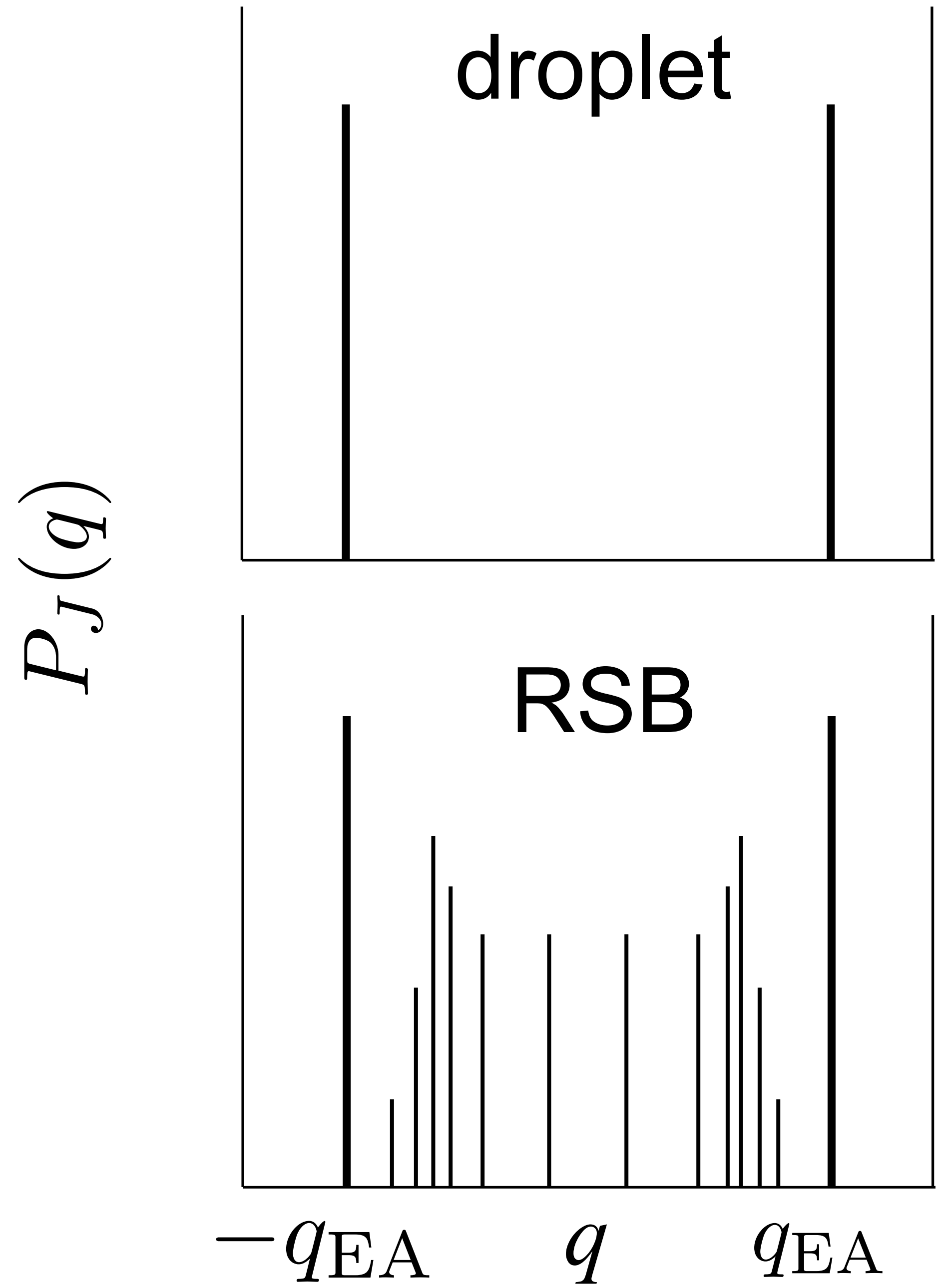


An example of overlap distributions for three disorder instances.



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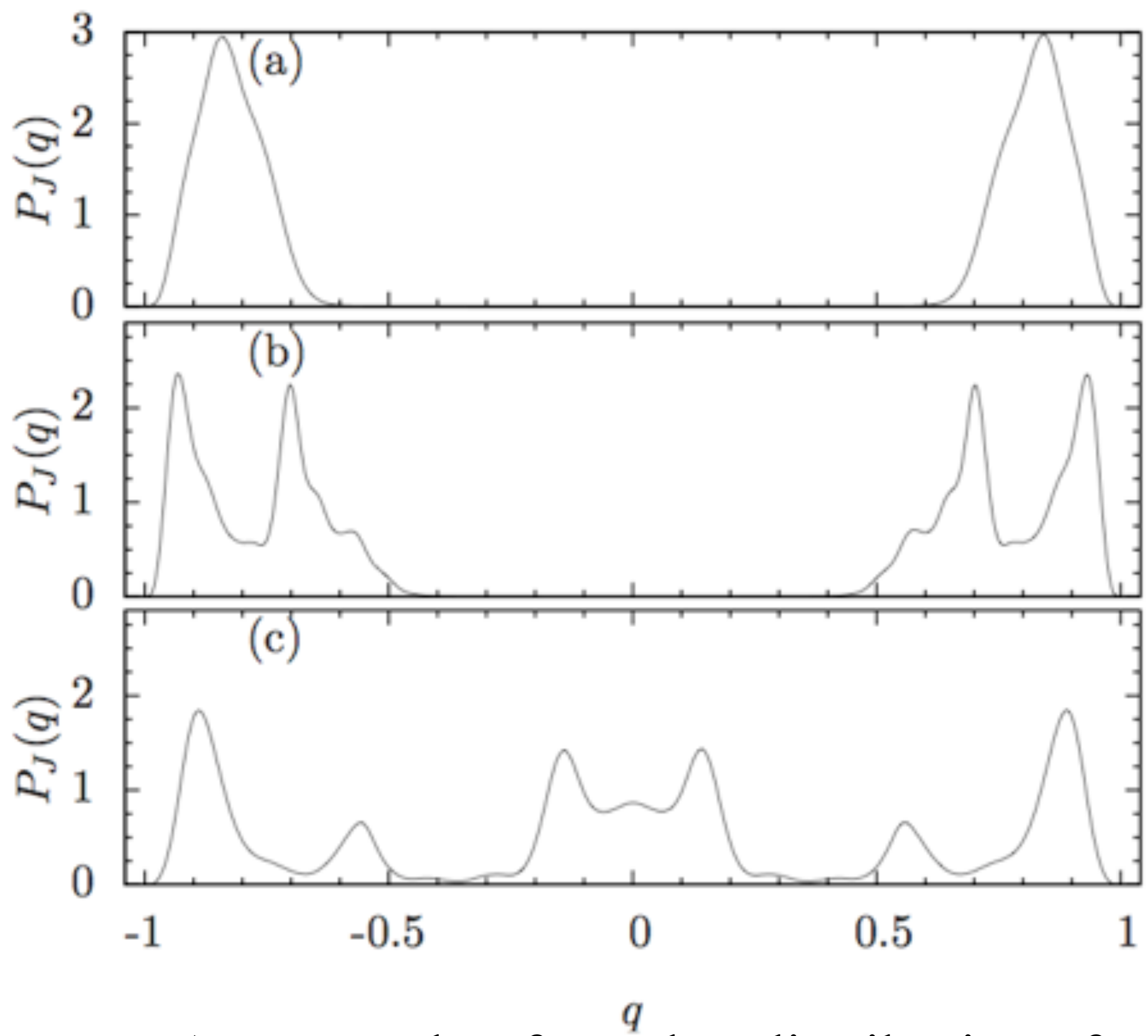

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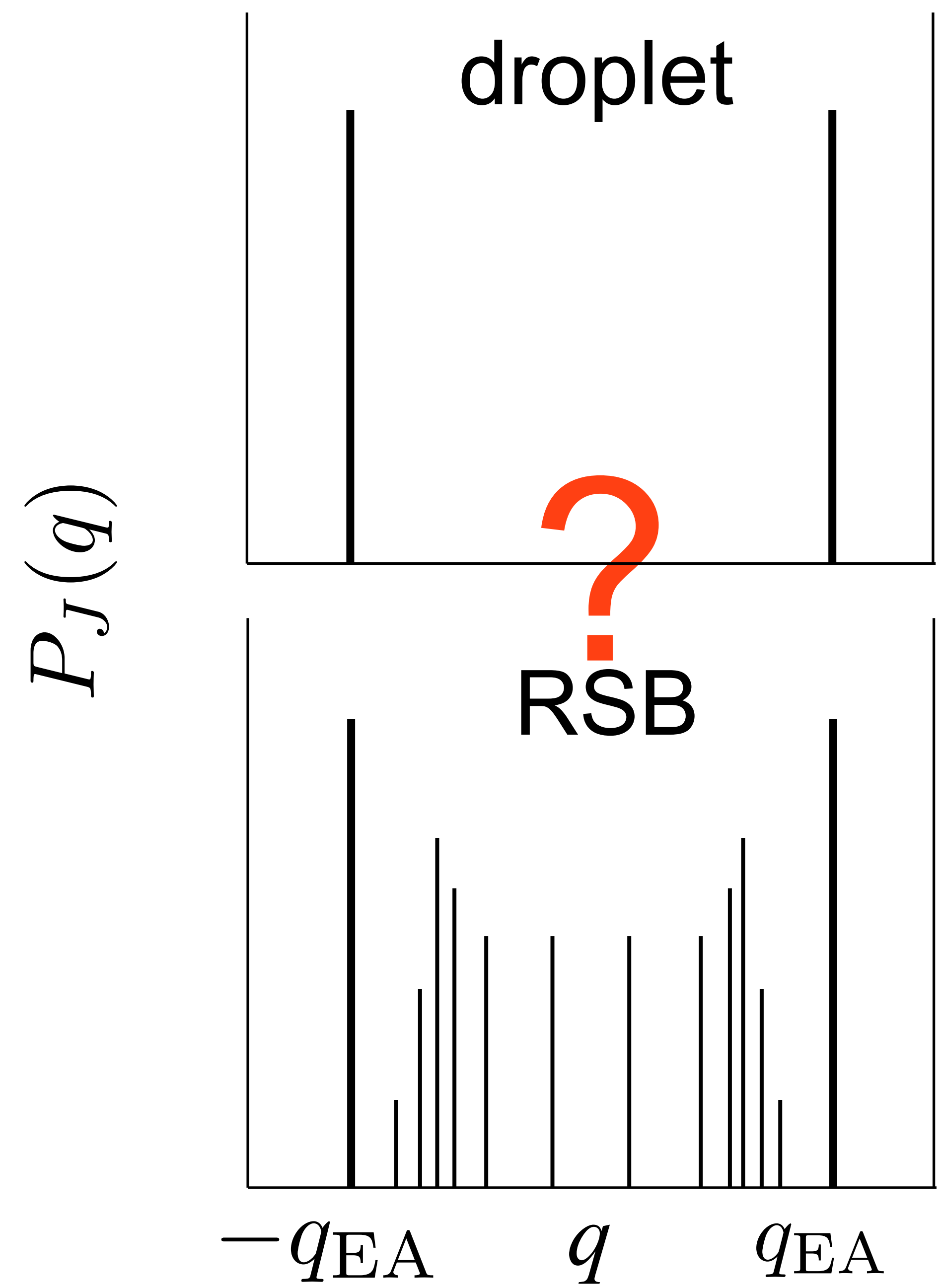
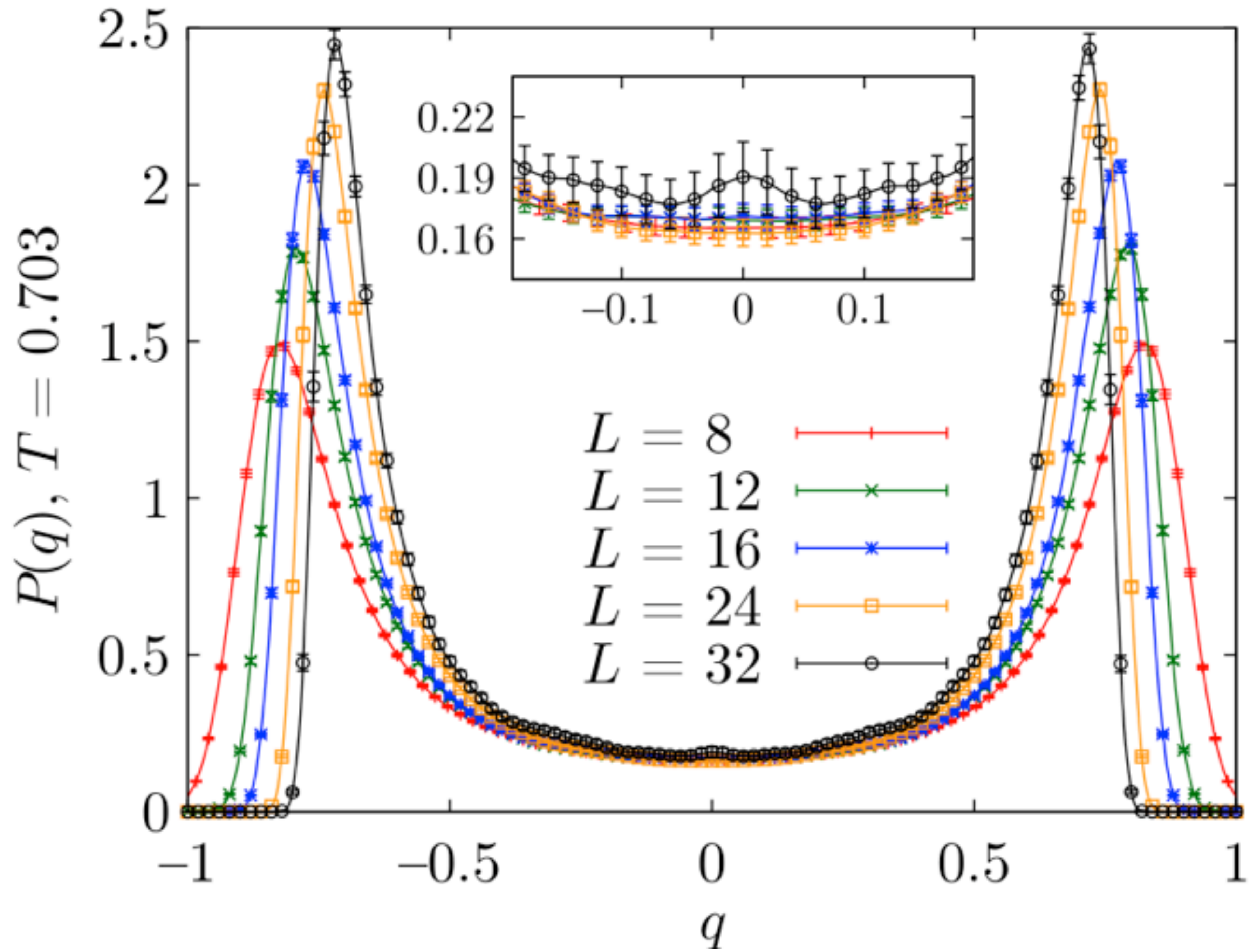


Nature of the spin-glass phase at experimental length scales

R Alvarez Baños[1,2], A Cruz[1,2], L A Fernandez[1,3], J M Gil-Narvion[1], A Gordillo-Guerrero[1,4], M Guidetti[5], A Maiorano[1,6], F Mantovani[5], E Marinari[6], V Martin-Mayor[1,3], J Monforte-Garcia[1,2], A Muñoz Sudupe[3], D Navarro[7], G Parisi[6], S Perez-Gaviro[1,6], J J Ruiz-Lorenzo[1,8], S F Schifano[5], B Seoane[1,3], A Tarancon[1,2], R Tripiccione[5] and D Yllanes[1,3]

3D Ising spin glass

J. Stat. Mech. (2010) P06026



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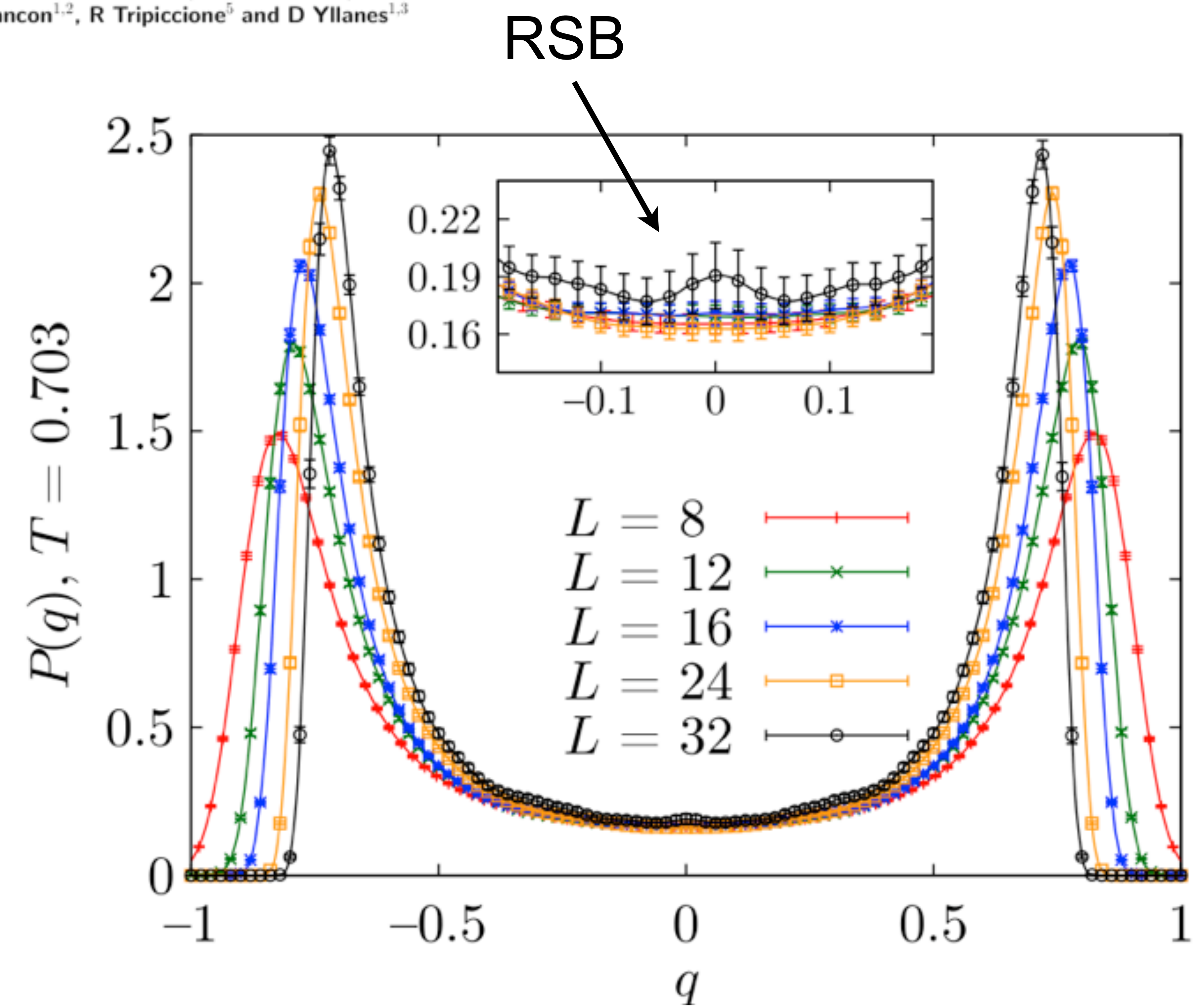
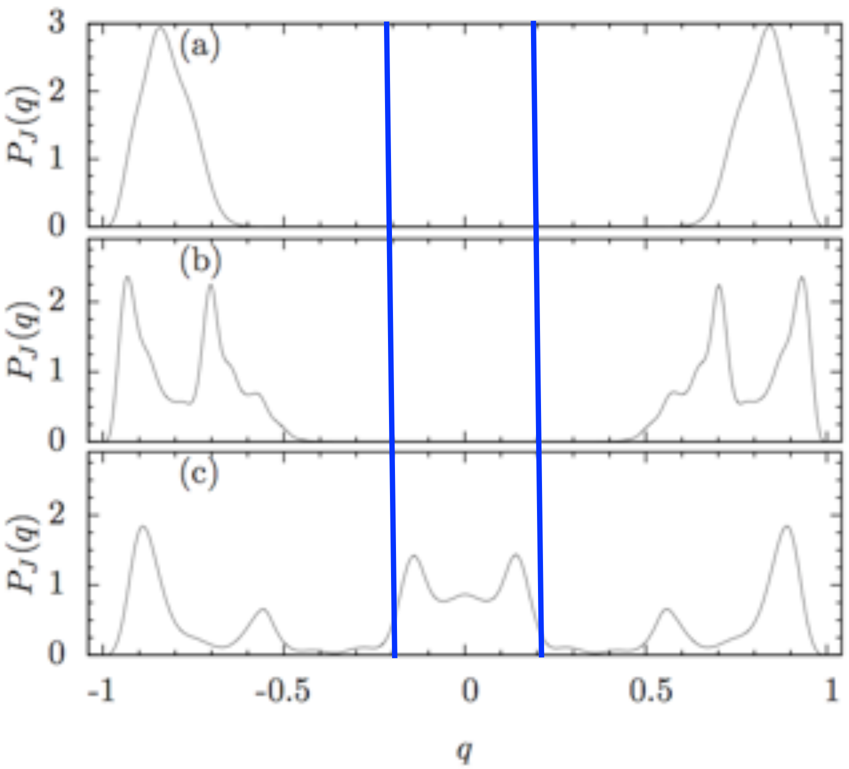


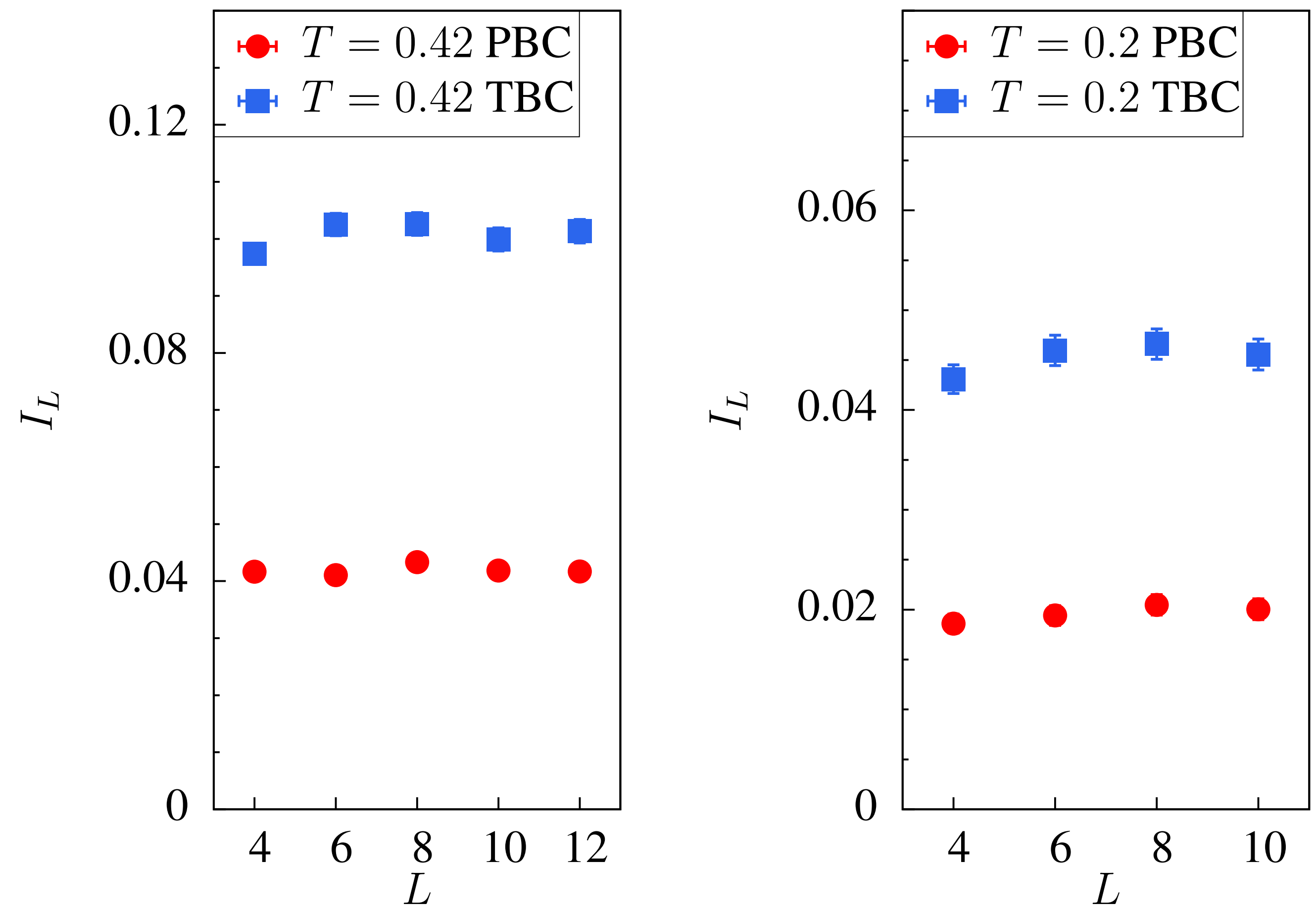
Overlap Near the Origin

$$I_J = \int_{-0.2}^{0.2} P_J(q)dq$$

Overlap near the origin



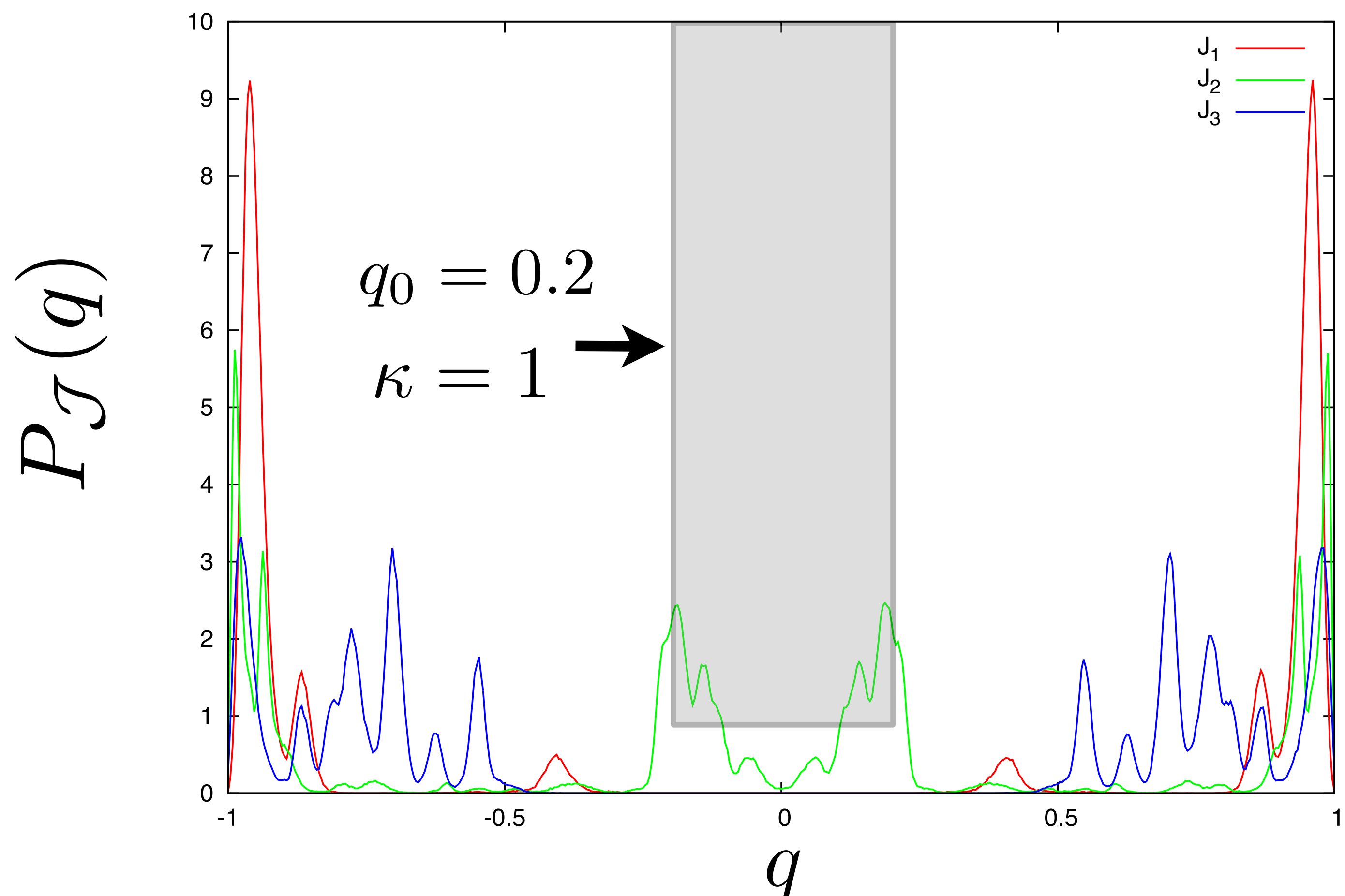
Disorder averaged overlap near the origin



$I > 0$ as $L \rightarrow \infty$ implies the RSB picture

RSB vs Droplet II

$$\Delta(q_0,\kappa) = \mathrm{Prob}\left[\max_{|q|<q_0}\left\{\frac{1}{2}\left(P_{\mathcal{J}}(q)+P_{\mathcal{J}}(-q)\right)\right\} > \kappa\right]$$

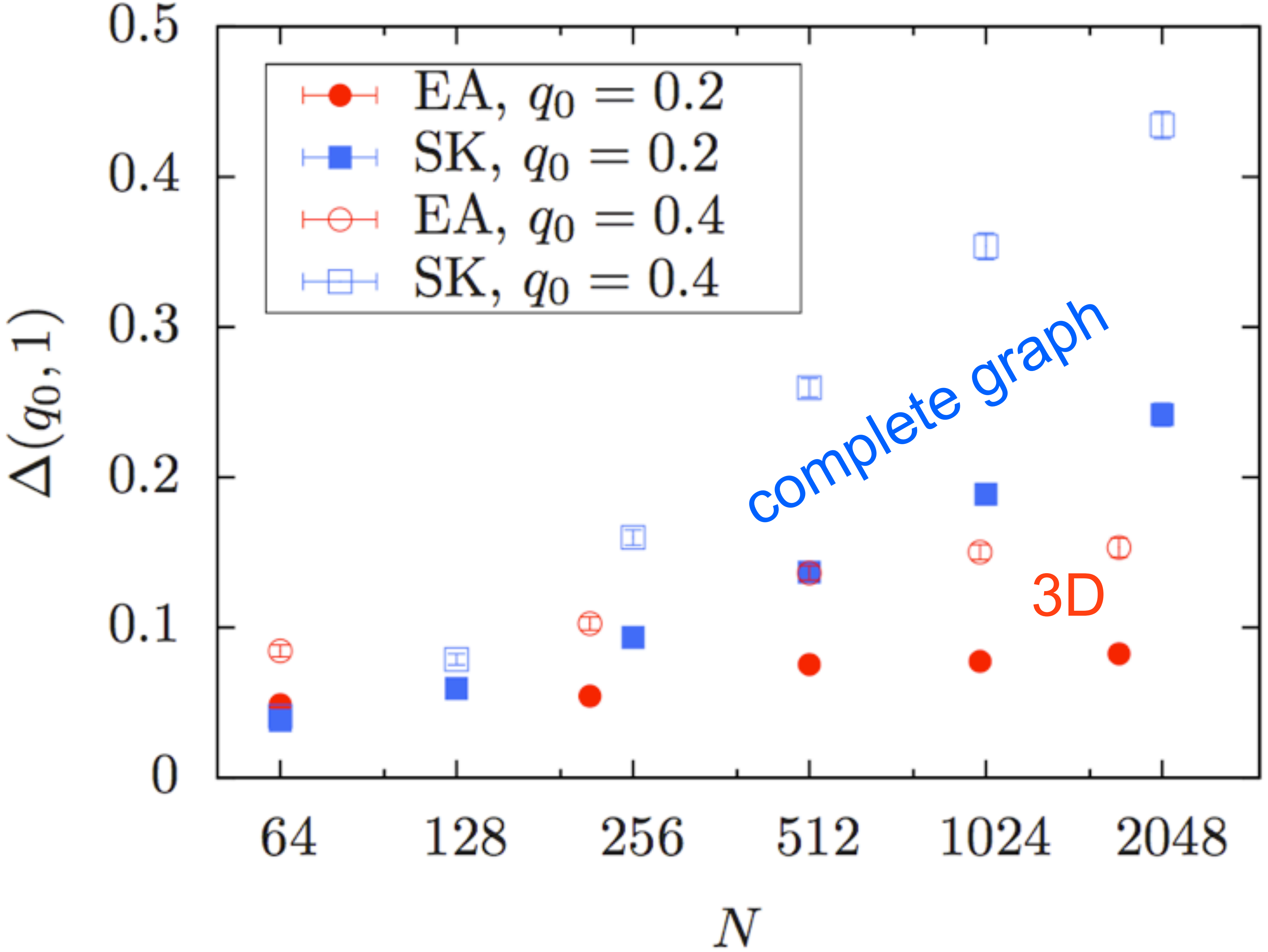


$\Delta(q_0,\kappa) \to 0$

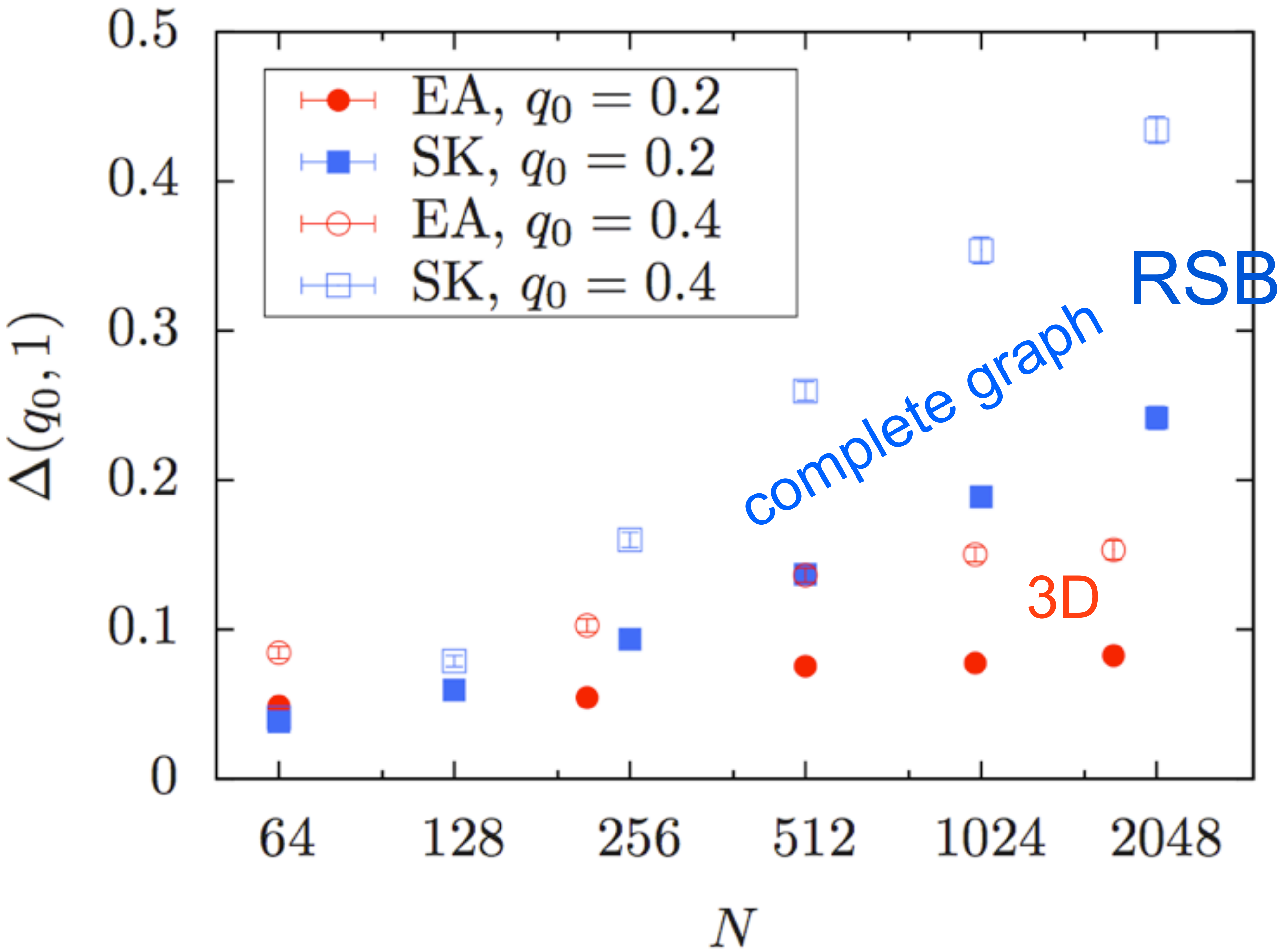
single pair of pure states

$\Delta(q_0,\kappa) \to 1$

many pairs of pure states



EA, $q_0 = 0.2$
SK, $q_0 = 0.2$
EA, $q_0 = 0.4$
SK, $q_0 = 0.4$
complete graph
3D
$\Delta(q_0, 1)$
N
0
0.1
0.2
0.3
0.4
0.5
64
128
256
512
1024
2048



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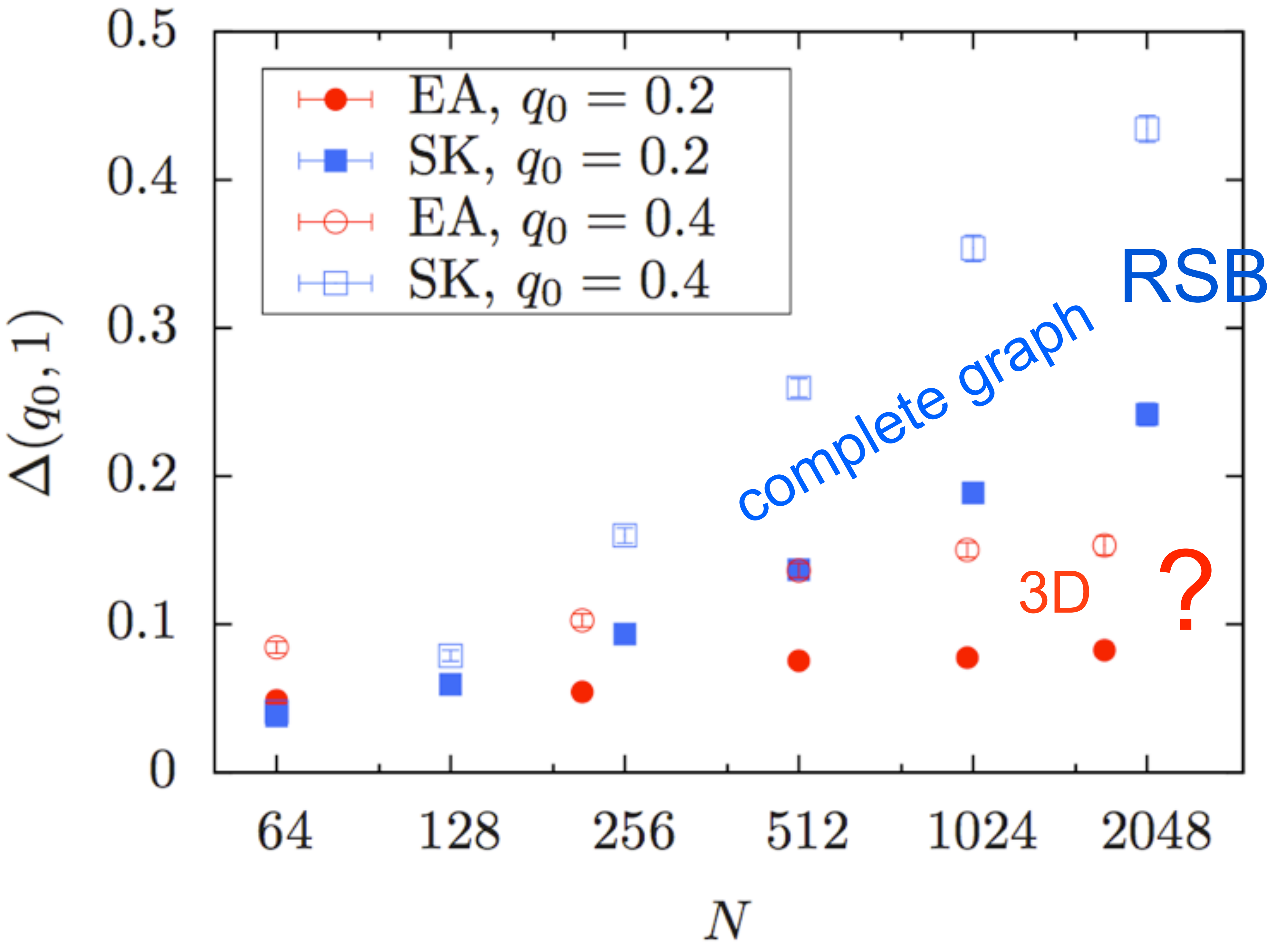

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complete graph
RSB
3D
?

Chaos

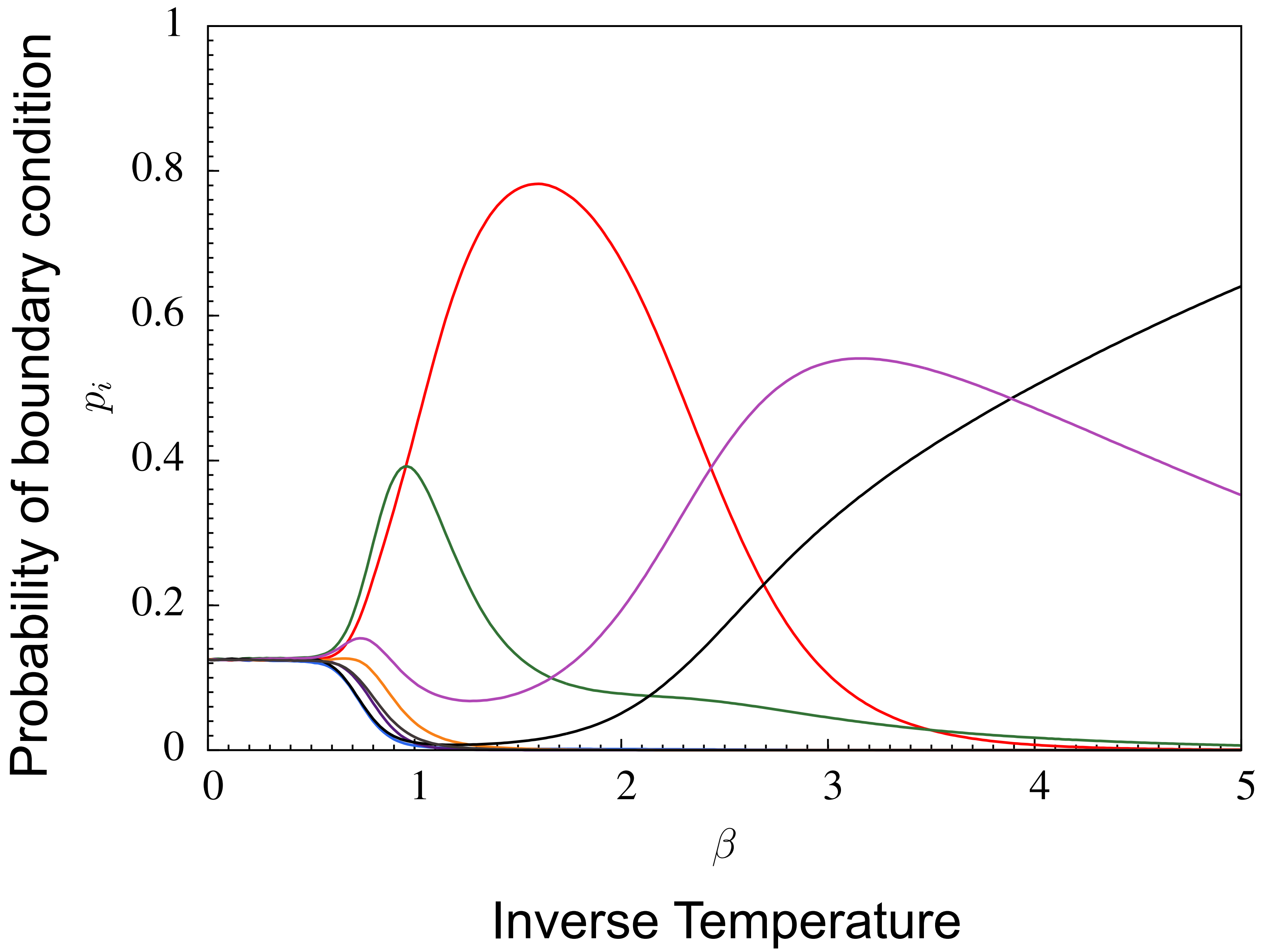
- A small change in the parameters (temperature, bond strengths,...) induces a large change in the spin configuration.

Thermal Boundary Conditions

- *What:* TBC ensemble includes the 2^d possible combinations of periodic and anti-periodic boundary conditions in the d spatial directions each with the correct Gibbs weight.
- *Why:*
  - Suppression of BC's that induce domain walls may lead to milder finite size corrections.
  - Access to a new measures of **chaos**, spin stiffness and other quantities.
- *See also:*
  - Thomas and Middleton, PRB 76, 220406(R) (2007)
  - Hasenbusch, Physica A 197, 423 (1993)

Temperature Chaos

- For many (but not all) disorder realizations the dominant boundary condition changes chaotically with temperature.



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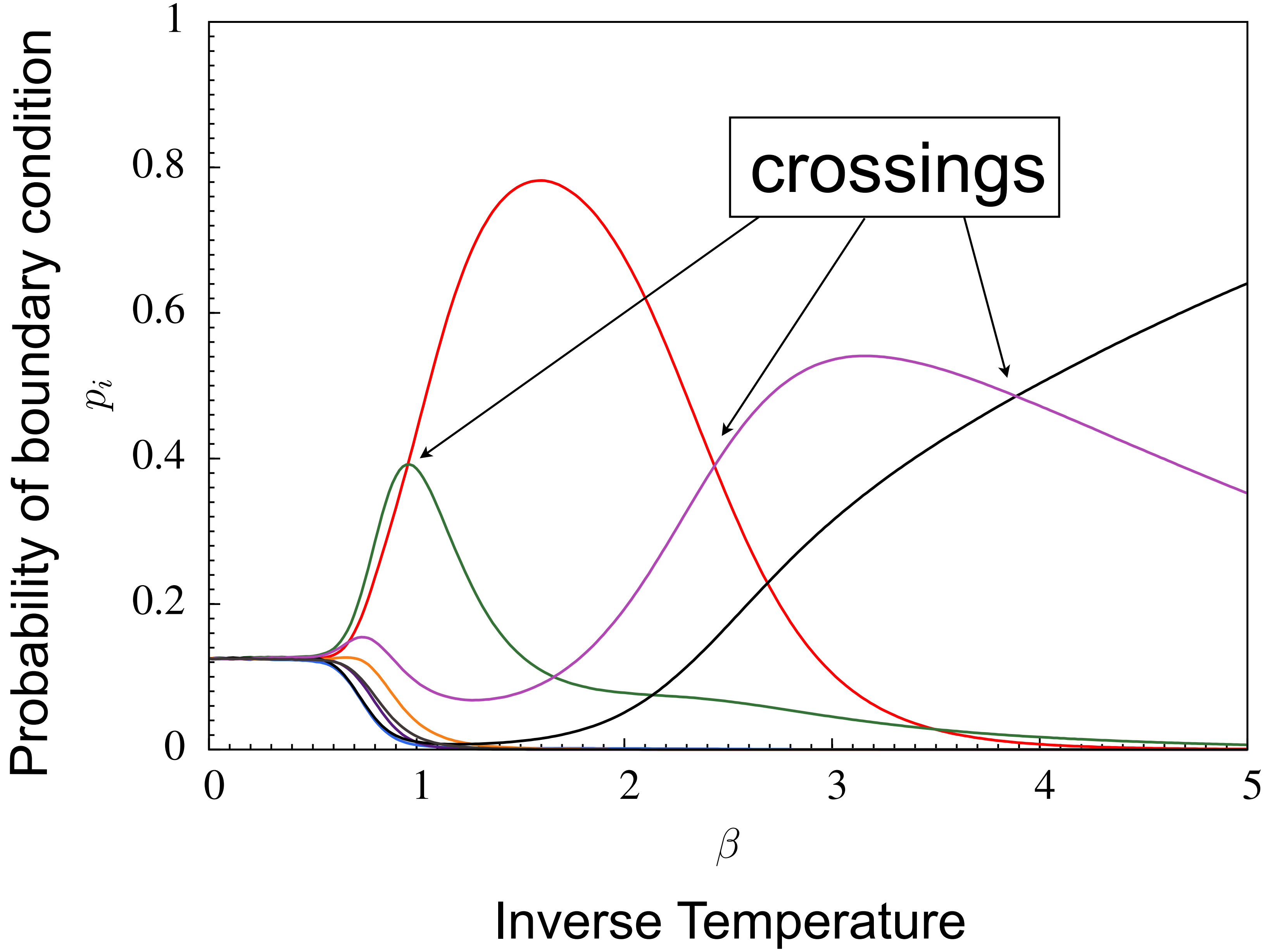
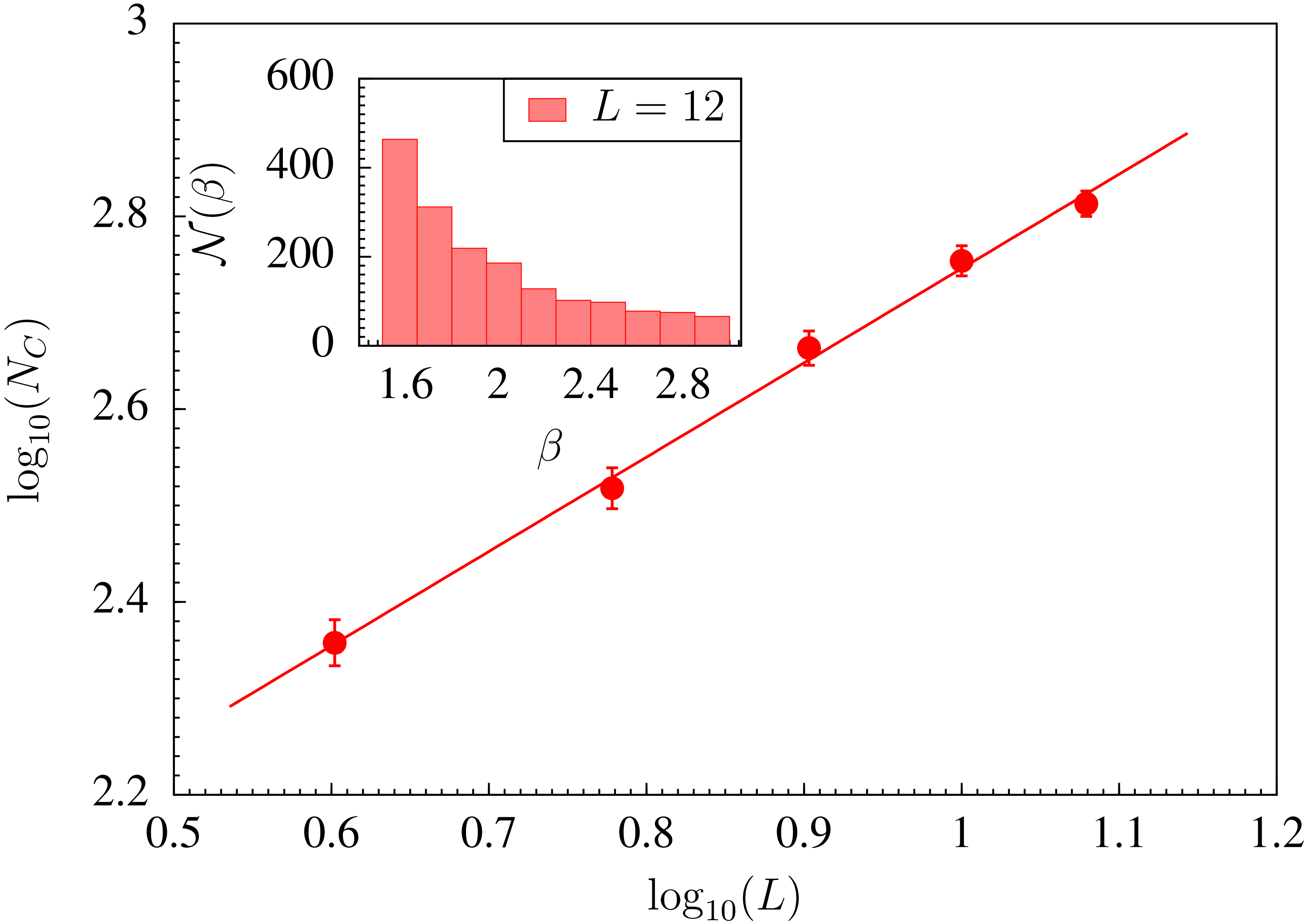


log number of crossings

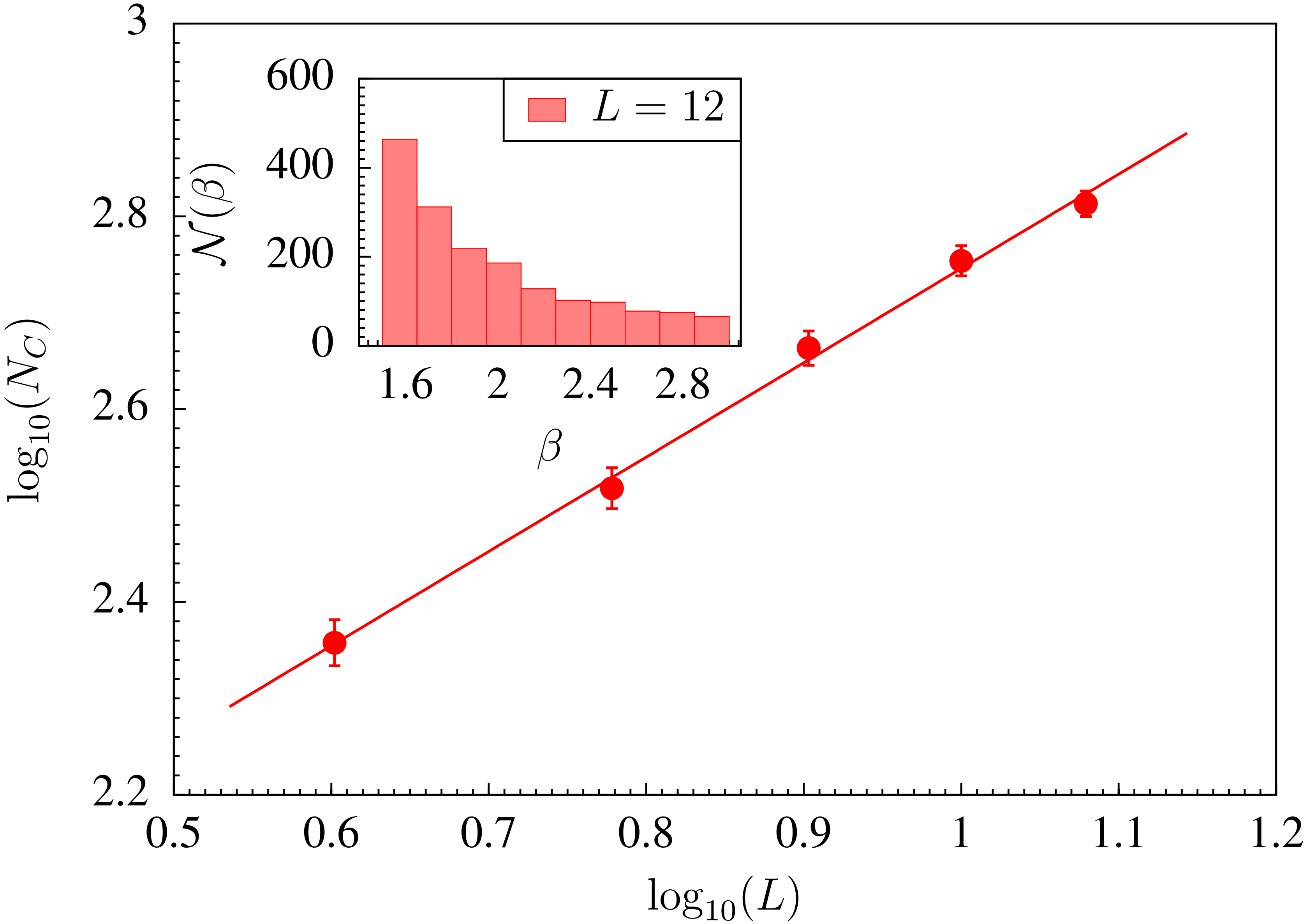


log size

$$N_C \sim L^{\zeta}$$

$$\zeta \sim 0.96(5)$$

log number of crossings



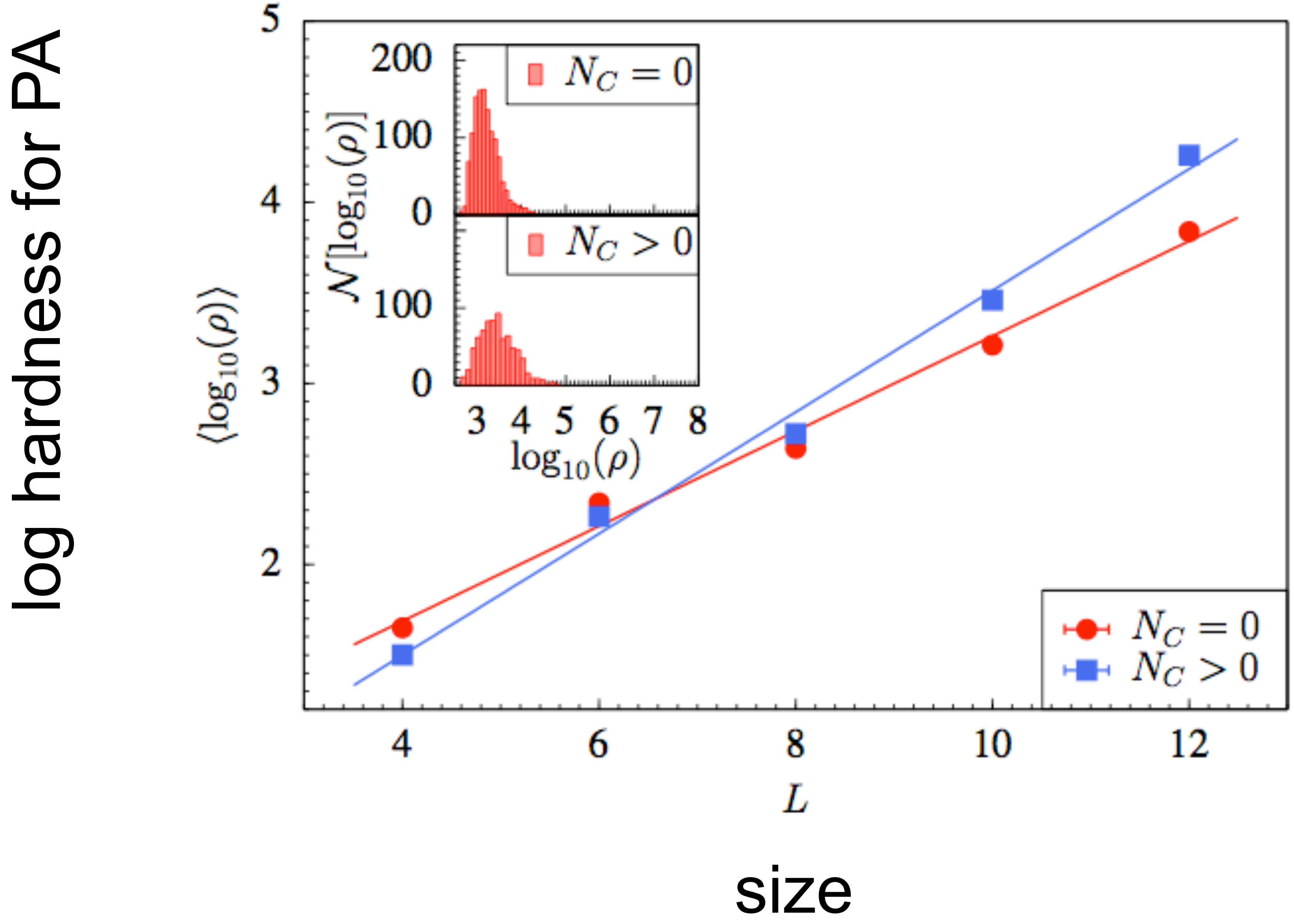
$$N_C \sim L^{\zeta}$$

$$\zeta \sim 0.96(5)$$

log size

Chaos increases roughly linearly with size

Temperature Chaos and Hardness



Questions

- Other ideas from CS about what makes an instance hard?
- Is sampling from the joint instance/solution distribution easier than first choosing a problem and then solving it?

Conclusions

- The spin glass is an example of an NP-hard problem relevant to physics.
- Population annealing is an effective algorithm for sampling thermal states and finding ground states of spin glasses.
- It is not known yet whether ordering occurs in the 3D spin glass via the many-state RSB picture or the simpler droplet picture with a single pair of pure states.
- Temperature chaos in spin glasses is associated with the hardness of an instance (for population annealing).