Probing the nature of the spin-glass state with Monte Carlo simulations

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Why Study 1D Spin Glasses at Low Temperatures?

• The ground-state structure is poorly understood. (Few analytical calculations).

• Simulations of higher-dimensional systems can only be done for moderate system sizes (e.g. in 3D $L_{\text{max}} \approx 10$).

• So far, simulations have been done at too high temperatures. (Effects of critical fluctuations?).

$\longrightarrow$ Test if droplet-like excitations are similar to domain-wall excitations for large systems at low temperatures.

• Spin glasses are challenging (NP-hard) and have many applications:

computer design, pattern recognition, neural networks, biological species evolution, vortex glass transition, hysteresis modeling, . . .

Outline

• What are spin glasses?

• Two standard models: RSB vs. Droplet Picture

• Preceding work

• Numerical method: parallel tempering Monte Carlo

• Results for short-range spin glasses

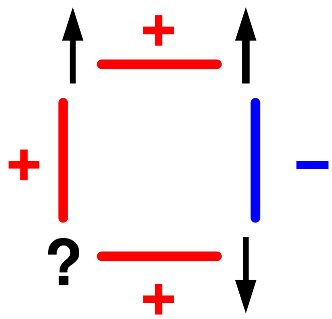
• The 1D disordered Ising spin chain

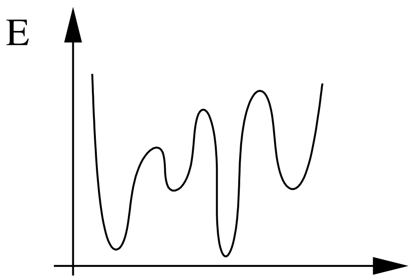
What is a spin glass?

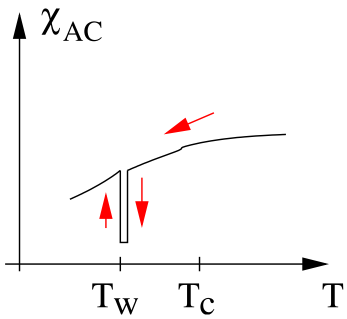
Spin glasses are magnetic systems in which the interactions between the magnetic moments are in conflict with each order due to some frozen structural disorder.

Besides disorder, frustration is a necessary ingredient found to give rise to the following behavior:

• The Hamiltonian of the system can only be minimized locally (complex energy landscape with deep valleys).







• There is a phase transition at $T = T_c$ with a divergence in a non-linear response function: The system orders with no apparent "spatial" order.

• Slow dynamics: The system is never really in equilibrium for $T < T_c$.

• Hysteresis when an external field is applied.

• Unexpected effects, e.g. the memory effect (Jonason et al.) when measuring the AC susceptibility below T_c.

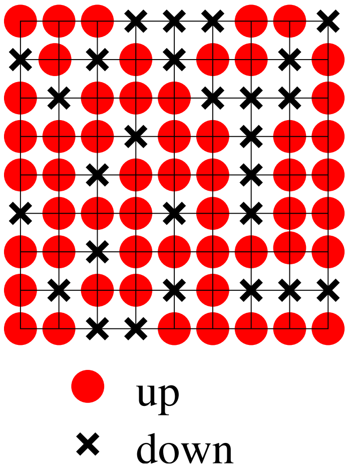
Experiments: dope gold (non-magnetic) with iron (magnetic). Fe_xAu_{1-x} then exhibits spin-glass behavior (Cannella & Mydosh 72).

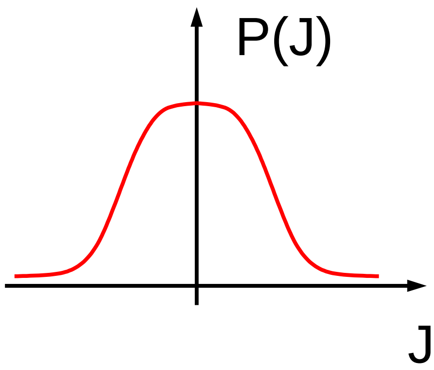
Simple Model: EA Ising spin glass

The Edwards-Anderson Ising spin glass Hamiltonian is given by:

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j \qquad\qquad S_i \in \{\pm 1\}$$

The sum ranges over the nearest neighbors on a hyper-cubic lattice in d dimensions.





- $J_{ij} = 1 \ \forall\, i,j \quad \longrightarrow$ Ferromagnetic order
- $J_{ij} = -1 \ \forall\, i,j \ \longrightarrow$ Antiferromagnetic order
- J_{ij} random $\quad \longrightarrow$ Spin Glass

For example:

$$\mathcal{P}(J_{ij}) \sim e^{-J_{ij}^2/2J^2}$$

Here $[J_{ij}] = 0$ and $[J_{ij}^2] = 1$, where

$$[\mathcal{F}(J_{ij})] = \int \mathcal{D}\{J_{ij}\} \mathcal{F}(J_{ij}) \mathcal{P}(J_{ij})$$

We obtain a frustrated system with a finite transition temperature in 3D ($T_c \approx 0.95$) and 4D ($T_c \approx 1.8$).

What are we interested in?

There are two main models describing scaling and geometry of excitations in spin glasses:

•Replica Symmetry Breaking (RSB) (Parisi 79): exact solution of the mean-field Sherrington-Kirkpatrick (SK) model.

•Droplet Picture (DP) (Fisher, Huse 86), (Bray, Moore 86): phenomenological approach.

•Krzakala & Martin (99) and Palassini & Young (99) suggest an intermediate picture for realistic spin-glass models that combines results from both models above.

The differences between both models can be quantified by studying:

•Edwards-Anderson order parameter q:

$$q = \frac{1}{N}\sum_{i=1}^{N} S_i^{\alpha} S_i^{\beta} \quad \sim \text{Volume of cluster}$$

S^{α}, S^{β} are two spin copies of the system with the same disorder. q can be seen as a “magnetization”.

•Link Overlap q_l:

$$q_l = \frac{1}{N_b}\sum_{i,j} S_i^{\alpha} S_j^{\alpha} S_i^{\beta} S_j^{\beta} \quad \sim \text{Surface of cluster}$$

$N_b = Nd$ is the number of bonds.

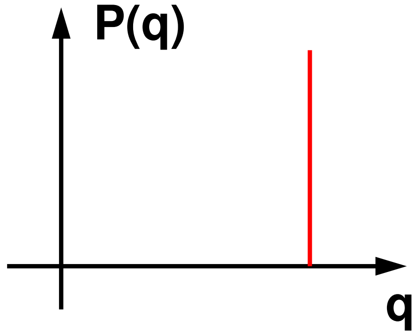
RSB vs. DP

DP

- System-size excitations cost $E \sim L^{\theta}$, $\theta > 0$ stiffness exponent. $E \to \infty$ for $L \to \infty$.

- Excitations are fractal: $d - d_s > 0$.

- Trivial ground-state structure: The distribution of q has zero weight in the thermodynamic limit, i.e. $P(0) \sim L^{-\theta}$.



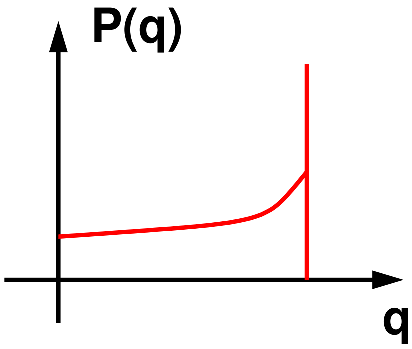
- The distribution of q_l is trivial, i.e. $\mathrm{Var}(q_l) \sim b/L^{\mu_l}$, $\mu_l = \theta' + 2(d - d_s)$.

RSB

- System-size excitations cost a finite energy in the thermodynamic limit: $E \sim L^{\theta}$ with $\theta = 0$.

- Excitations are space filling: $d = d_s$.

- Non-trivial ground-state structure: The distribution of q has a finite weight at $q = 0$ in the thermodynamic limit, i.e. $P(0) \sim L^{0}$.



- The distribution of q_l is non-trivial, i.e. $\mathrm{Var}(q_l) \sim a + b/L^{c}$.

NOTE: Long-range models (e.g. SK model) follow RSB.

NOTE: DP claims that $\theta = \theta'$, where θ describes domain-wall excitations and θ' thermal droplet-like excitations.

$\longrightarrow$ We want to test this here!

What has been done so far?

$T = 0$:

•Simulations changing BC in 2D find $\theta \approx -0.28$ and $T_c = 0$ (Bray, Moore 00, Hartmann et al. 02, ...).

•Simulations changing BC in 3D predict $\theta \approx 0.2$ (Bray, Moore 00) $\longrightarrow$ θ very small,but positive, hence $T_c > 0$.

•Simulations changing BC in 4D find $\theta \approx 0.7$ (Hartmann 99, Hukushima 99) $\longrightarrow$ θ large and positive.

•Simulations exciting droplets predict $\theta' = 0$, but $d - d_s > 0$ (Palassini 99)

$\longrightarrow$ Easiest to distinguish RSB and DP in 4D.

$T > 0$:

•Simulations at $T \approx 0.67 T_c$ of the 4D EA SG (Reger et. al. 90) find $\theta' \approx 0$. Problem: T too close to T_c, critical fluctuations might be relevant (as criticized by Drossel et. al. 00).

•Simulations at $T \approx 0.7 T_c$ in 3D (Marinari 94), same problem as above.

Previous simulations at finite temperatures were done too close to T_c.

Problem: it is very hard to equilibrate a spin glass at such low temperatures.

Solution: Parallel tempering Monte Carlo.

Introduction to Monte Carlo

In statistical mechanics we calculate the average of an observable $\mathcal{O}$ as follows

$$\langle \mathcal{O} \rangle = \sum_n P_n^{\text{eq}} \mathcal{O}_n \qquad\qquad P_n^{\text{eq}} = \frac{e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}$$

Problem: the number of states is exponentially large.

Solution: statistically sample a few states to obtain an estimate of $\langle \mathcal{O} \rangle$ but with a statistical error.

If we choose the states according to P_n^{eq} and ensure detailed balance then we obtain a Markov chain for $\langle \mathcal{O} \rangle_{\text{est}}$:

$$\langle \mathcal{O} \rangle_{\text{est}} = \frac{1}{M} \sum_{i=1}^{M} \mathcal{O}_i$$

where M is the number of samples chosen.

Implementation: we chose a spin S_i at random and flip it. We accept the new configuration according to the following rule:

$$P(S_i \leftrightarrow -S_i) = \begin{cases} e^{-\Delta} & : \quad \Delta > 0 \\ 1 & : \quad \Delta \leq 0 \end{cases}$$

with $\Delta = E_{\text{new}} - E_{\text{old}}$.

Metropolis Algorithm:

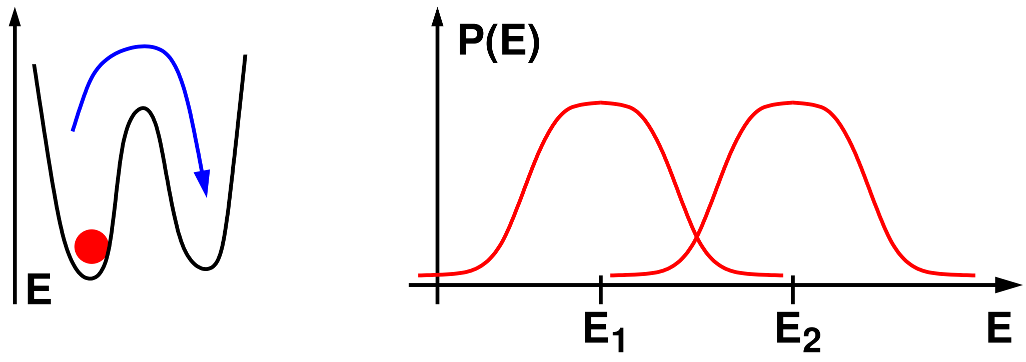
$$\text{if } (e^{-\Delta} < \text{rand}())\{S_i \to -S_i\}$$

Parallel Tempering MC

Simulate M copies of the system at different temperatures with $T_{max} \gg T_c$ and allow swapping of neighboring temperatures.

The temperature of a given set of spins varies during the simulation allowing for an easy crossing of barriers when the temperatures are high.

This speeds up equilibration.



To ensure detailed balance we use the following probability for interchanging the temperatures:

$$P(S_{m+1} \leftrightarrow S_m; \beta_{m+1} \leftrightarrow \beta_m) = \begin{cases} e^{-\Delta} & : \quad \Delta > 0 \\ 1 & : \quad \Delta \leq 0 \end{cases}$$

$$\Delta = (\beta_{m+1} - \beta_m)(E_m - E_{m+1})$$

if $(e^{-\Delta} <$ rand()){FLIP COPIES}

Pick # of copies so that the energy distributions of the different copies overlap and the acceptance ratios are not too small, i.e. $\Delta T_{m,m+1} \sim c_V T_m / \sqrt{N}$.

Equilibration Test

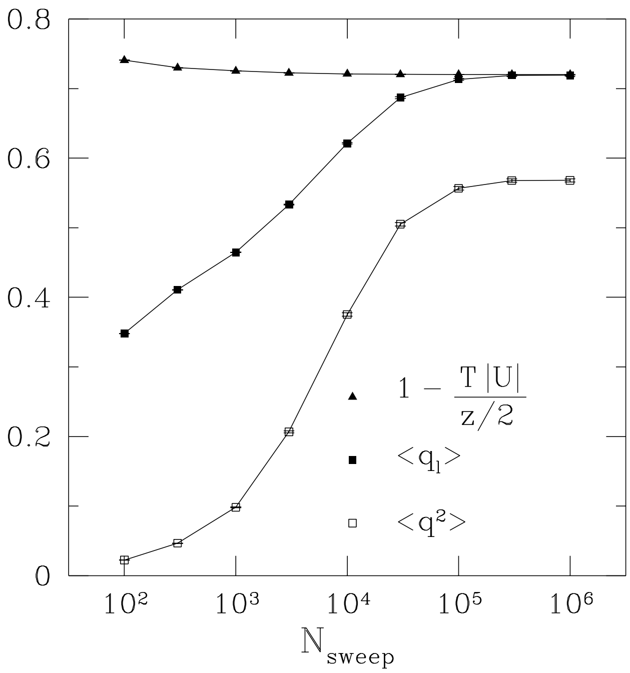
So far: wait until observable saturates as a function of Monte Carlo steps. This does not work well with parallel tempering.

Since we simulate a spin glass with Gaussian bonds, we can use the following relation as an equilibration test (Bray, Moore 80 for SK model):

$$q_l = 1 - \frac{T|U|N}{J^2 N_b}$$

where N_b is the number of bonds and U the energy per spin (thermal and disorder averages are implied).

LHS and RHS will approach from different sides and agree when system is equilibrated.



(Data for 3D EA Ising spin glass, L = 8, T = 0.50)

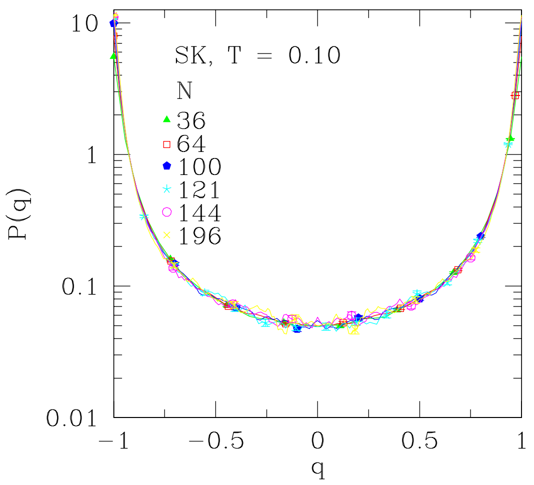
Reminder: long-range Spin Glasses

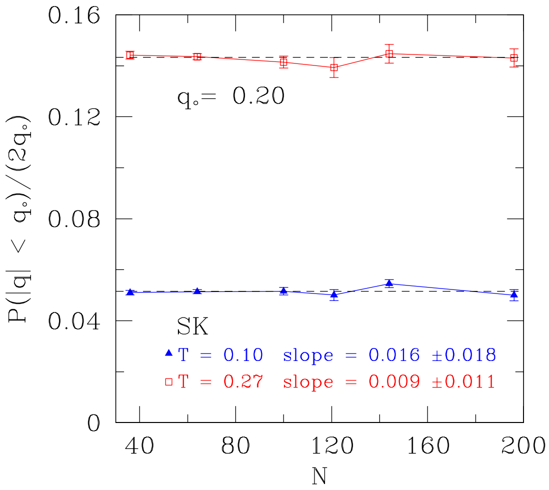
The SK (mean-field) model is given by

$$\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j \qquad \text{(sum over all spins)}$$

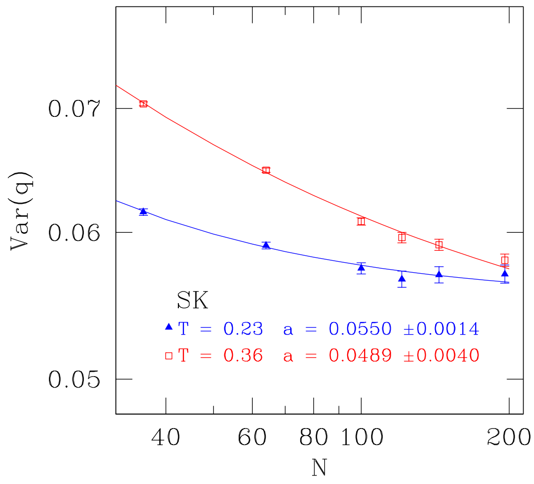
The sum ranges over all spins in the system ($T_c = 1.0$). J_{ij} Gaussian distributed with $[J_{ij}] = 0$, $[J_{ij}^2] = 1/(N-1)$.

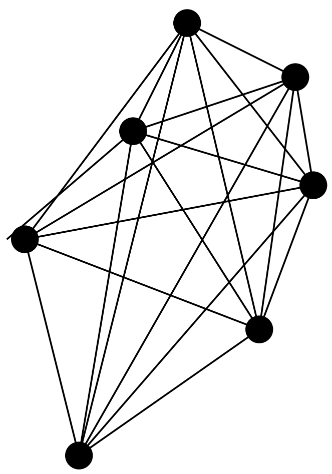
We expect $P(0) \sim L^0$ . . .





. . . and Var$(q_l) \sim a + bL^c$ . . .





$\longrightarrow$ **RSB BEHAVIOR!**

Reminder: short-range Models

From zero-temperature calculations (Palassini 99), we expect the short-range EA Ising spin glass to follow the intermediate picture, i.e.

- The energy cost of large-scale excitations is finite in the thermodynamic limit:

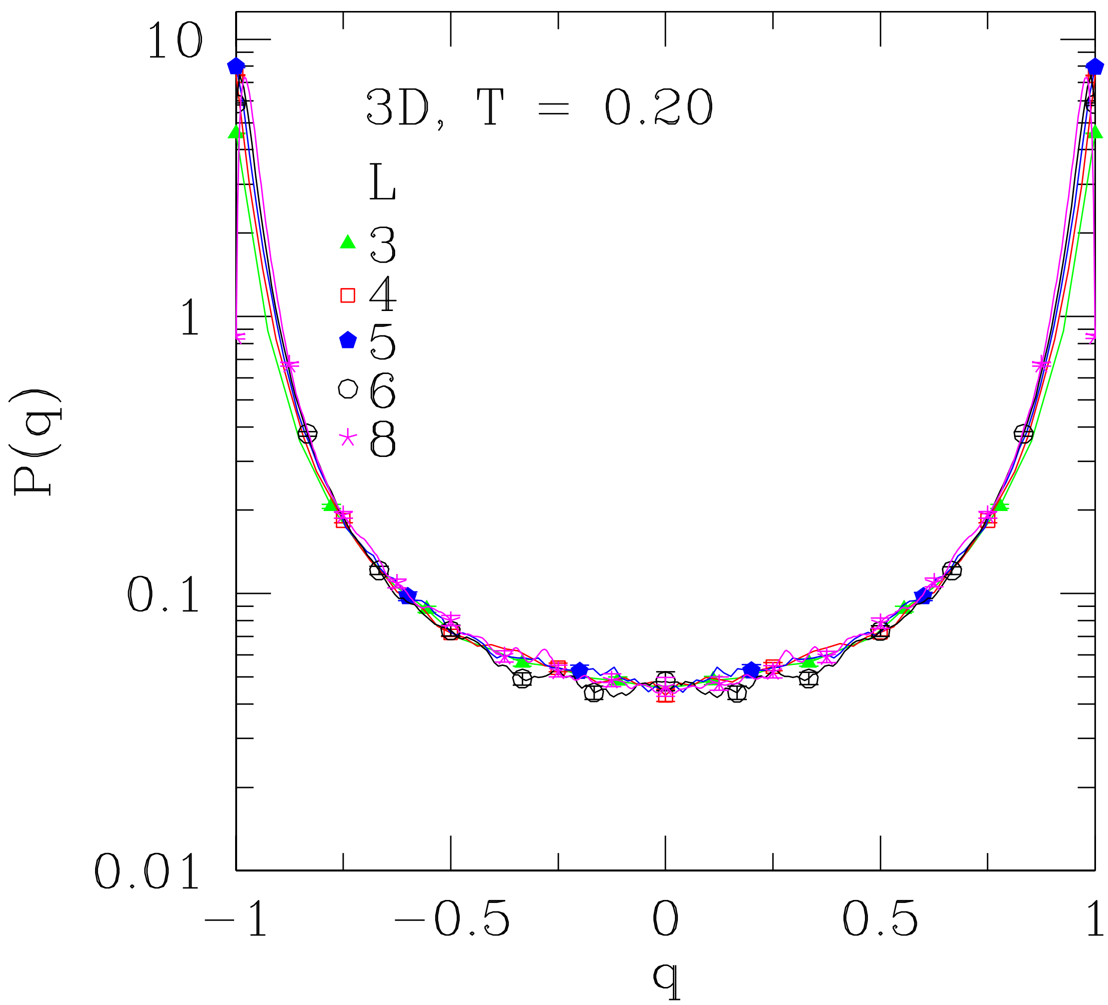
$$P(0) \sim L^0 \quad \longleftrightarrow \quad E \sim L^0$$

- The surface of these excitations is fractal:

$$\text{Var}(q_l) \sim L^{-\mu_l} \qquad \mu_l = \theta' + 2(d - d_s)$$

Remember: Droplet model predicts $\theta = 0.20$ in 3D and $\theta = 0.70$ in 4D; also $\theta = \theta'$.

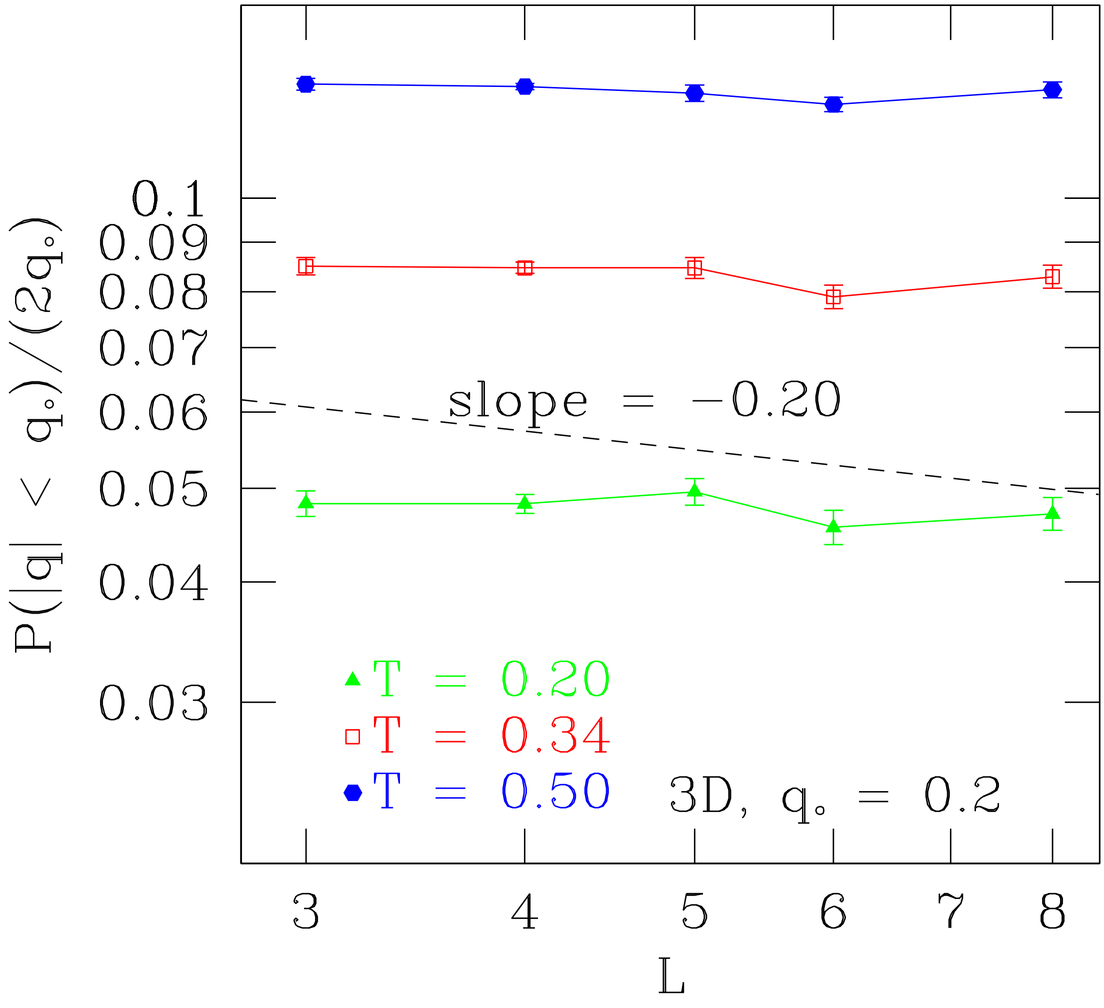
$P(q)$ at $T = 0.20$ - 3D EA Model



Note that $P(q)$ does not seem to decrease with increasing system size L, indicating that $\theta' \approx 0$.

Thermal system-size excitations have $E \sim$ const., at least for the (moderate) sizes studied.

$P(0)$ - 3D EA Model

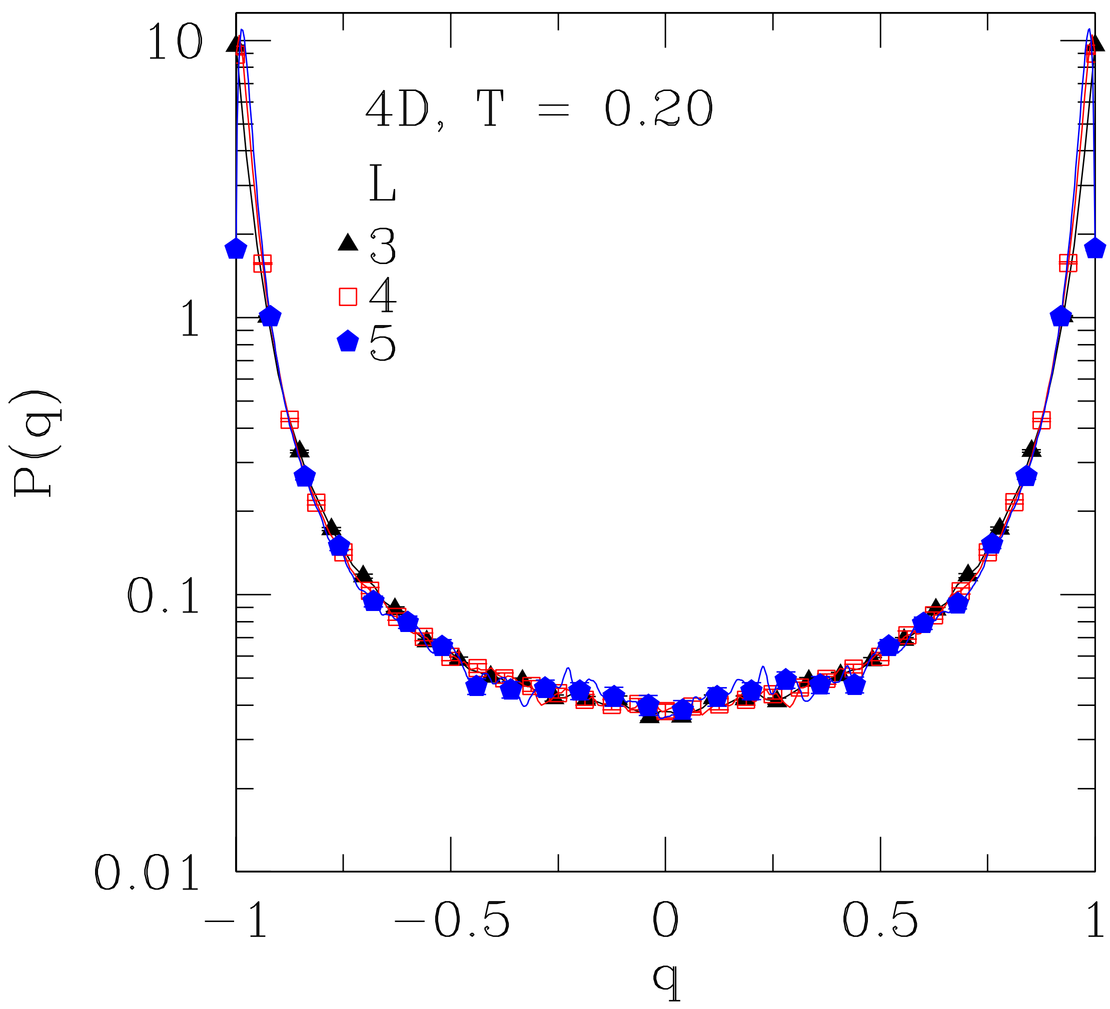


The data do not depend significantly on system size and fit well to $P(0) \sim L^{-\theta'}$ with $\theta' = 0$. (We average over a region around $q = 0$ to improve the statistics).

The dashed line has slope of −0.20 as predicted by the Droplet Picture. Problem: 0.20 is a small slope and hard to distinguish from zero.

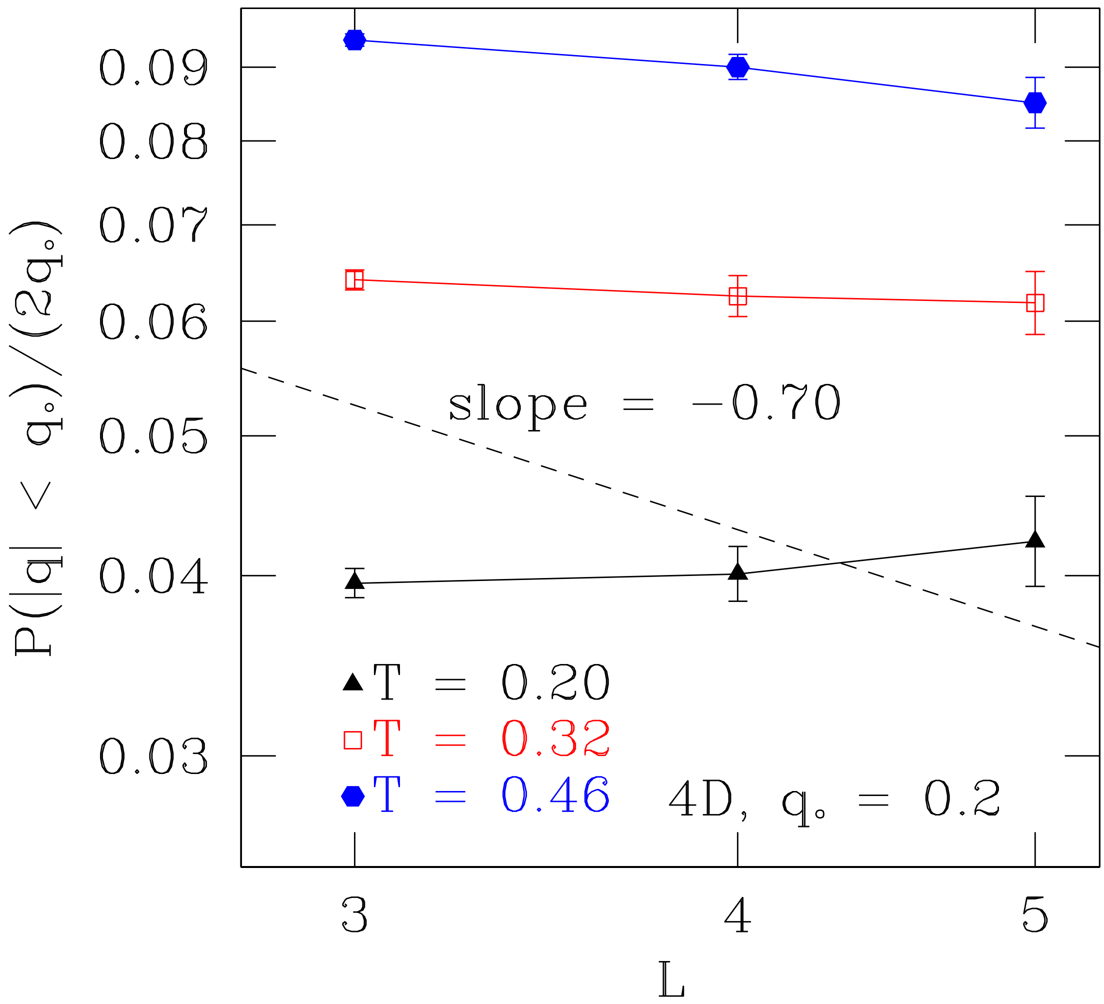
Solution: Look at 4D!

$P(q)$ at $T = 0.20$ - 4D EA Model



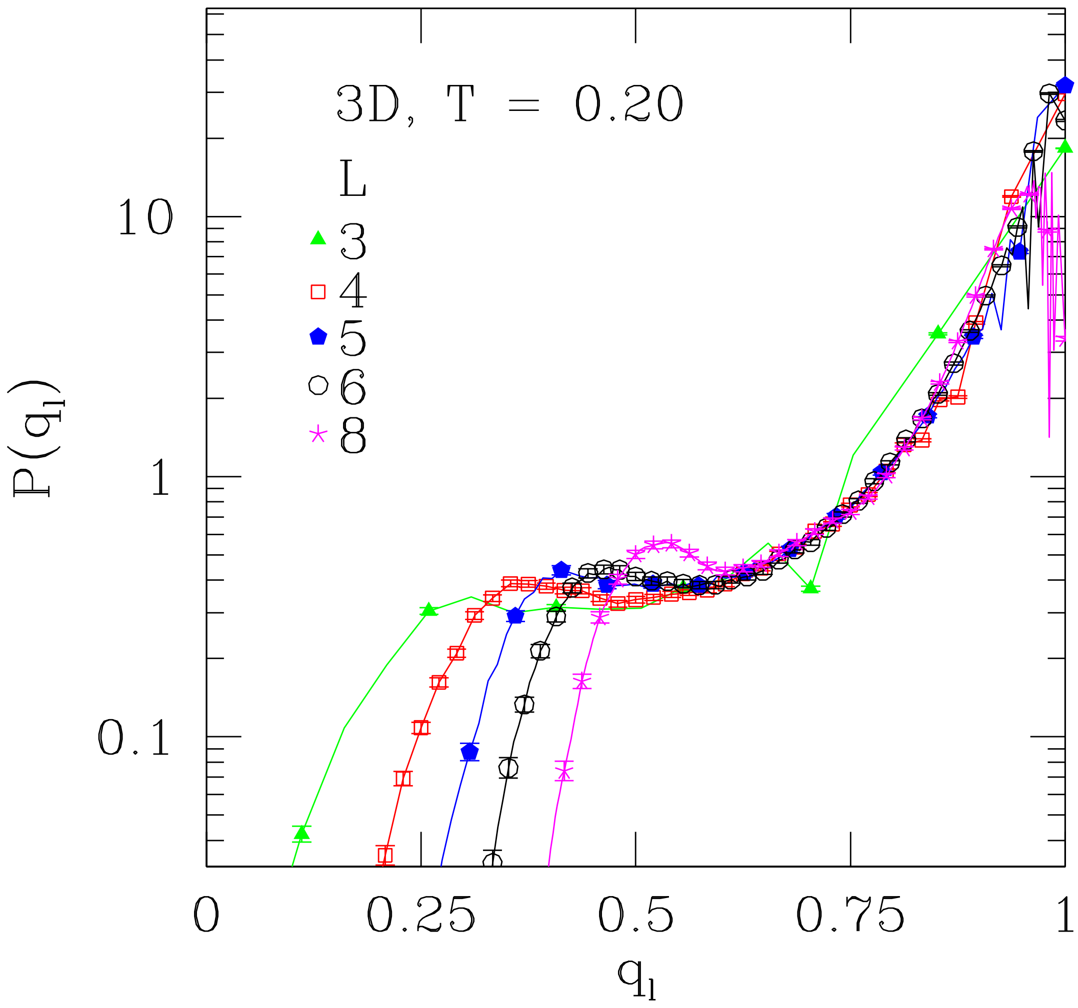
Note that $P(q)$ does not seem to decrease with increasing system size L, indicating that $\theta' \approx 0$.

$P(0)$ - 4D EA Model



The dashed line represents a slope of -0.70 as predicted by the Droplet Picture. $\theta' = 0$ is consistent with the data at $T = 0.20$.

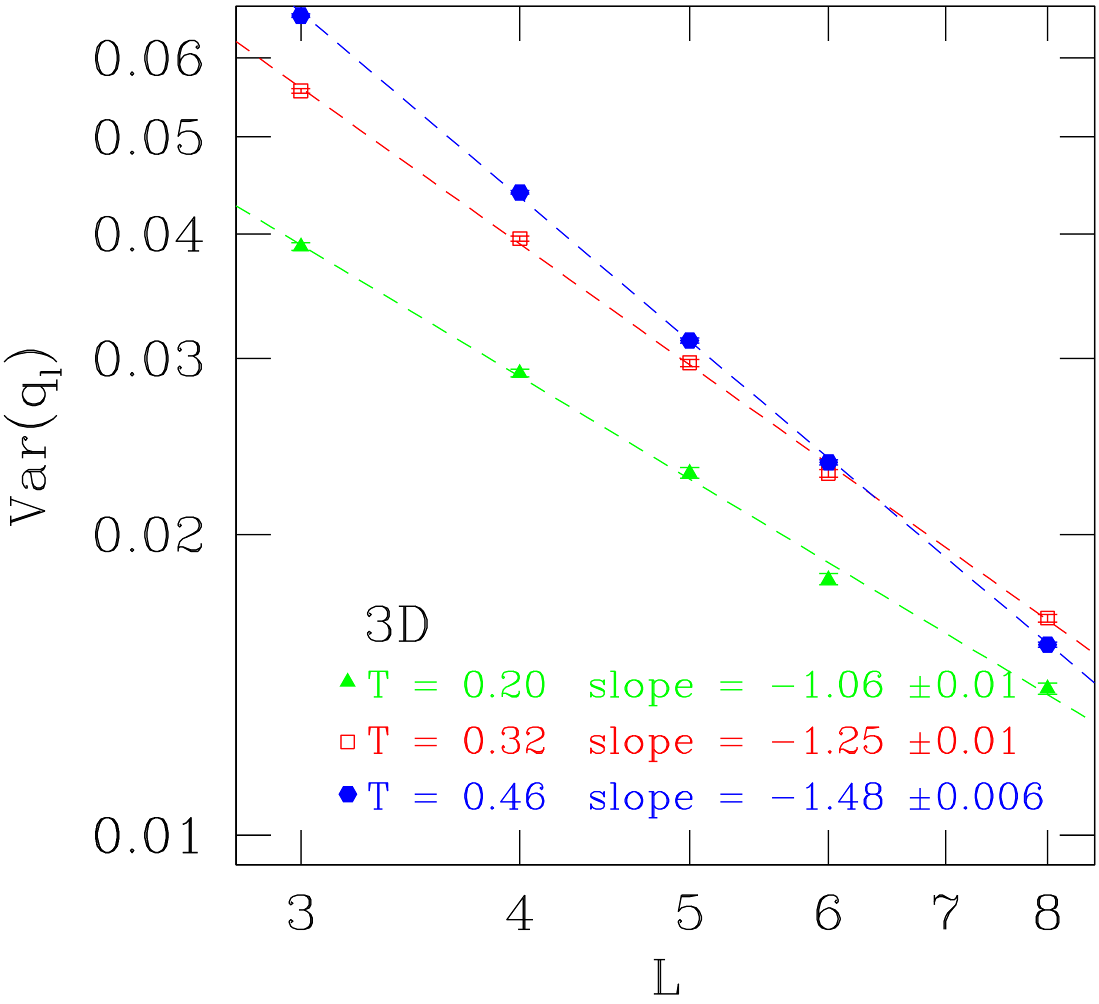
$P(q_l)$ at $T = 0.20$ - 3D EA Model



Note the double-peak structure with a tail. (Similar data in 4D).

How does the surface of the excitations scale? Look at the Variance of q_l!

Var(q_l) - 3D EA Model



Remember: Var(q_l) $\sim L^{-(\theta' + 2(d-d_s))}$. Assuming $\theta' = 0$ we obtain

$$d - d_s = 0.38 \pm 0.02$$

This agrees with previous $T = 0$ calculations by Palassini.

For 4D we have similar results with $d - d_s = 0.17 \pm 0.03$.

Summary for the EA spin glass

Our results for short-range Ising spin glasses in three and four dimensions agree qualitatively with an intermediate picture:

- Excitations cost a finite amount of energy in the thermodynamic limit ($\theta' = 0$).
- The surface of these excitations is fractal ($d - d_s < 0$).

We also have similar results for the $3D$ gauge glass and the $4D$ XY spin glass which support the intermediate scenario.

Problems

- When calculating $d - d_s$ we make a large extrapolation to $L = \infty$ as well as $T = 0$.
- Modest range of sizes: Possible crossover effects at large L.

It has been claimed (Moore 02) that $\theta \neq \theta'$ is an artifact of small sizes or that corrections have to be applied (Hartmann and Moore 02) – 2D EA SG with $L \leq 160$.

Solution

Study a model which allows for a larger range of sizes L, e.g. in one dimension.

The $1D$ Ising spin chain

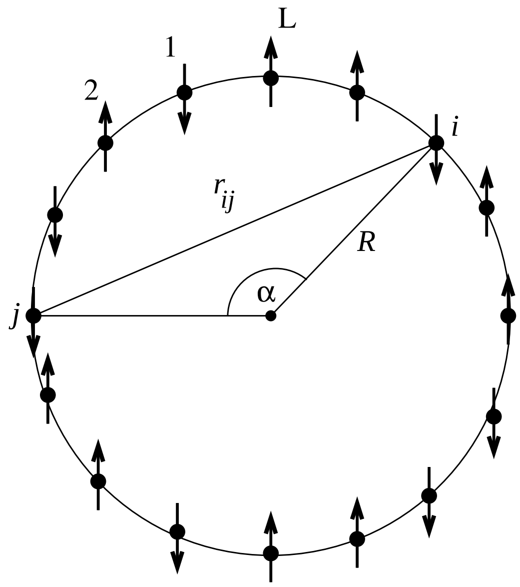
$$\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j \qquad S_i \in \{\pm 1\}$$

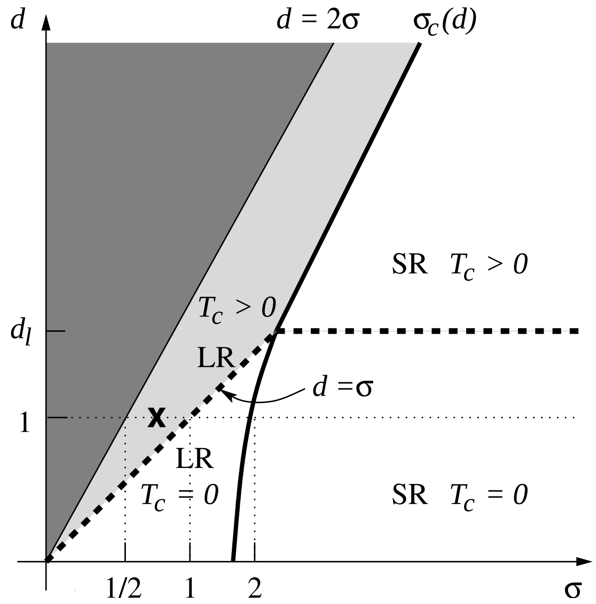
The sum ranges over all spins on the chain. The interactions J_{ij} are given by

$$J_{ij} = c(\sigma)\frac{\epsilon_{ij}}{r_{ij}^{\sigma}} \qquad \mathcal{P}(\epsilon_{ij}) = \frac{1}{\sqrt{2\pi}}\exp(-\epsilon_{ij}^2/2)\ .$$

$c(\sigma)$ is chosen to give a mean-field transition temperature of 1. r_{ij} represents the distance between the spins.

The model has a very rich phase diagram in the d–σ plane (Bray et al. 86, Fisher and Huse 88):





The "**X**" marks the location of the finite-T simulations.

(Not all bonds shown in figure for clarity).

The $1D$ Ising spin chain cont.

In the long range phase the droplet model predicts (Fisher & Huse 88)

$$\theta = d - \sigma \ .$$

For $d = 1$ we have for $\sigma > \sigma_c = 2$, $\theta = -1$.

To test if $\theta = \theta'$ we perform the following simulations:

•$T > 0$ (Thermal droplet excitation): $\sigma = 0.75$ ($T_c = 0.62 \pm 0.03$) – the system is in the LR phase. We expect from DP $\theta' \approx 0.25$ ($T \ll T_c$).

•$T = 0$ (Boundary condition twist excitation): We perform ground-state calculations for a range of σ-values and calculate the domain-wall energies and θ when changing boundary conditions (DP recipe).

$\rightarrow$ If DP is right, we should find $\theta = \theta' > 0$.

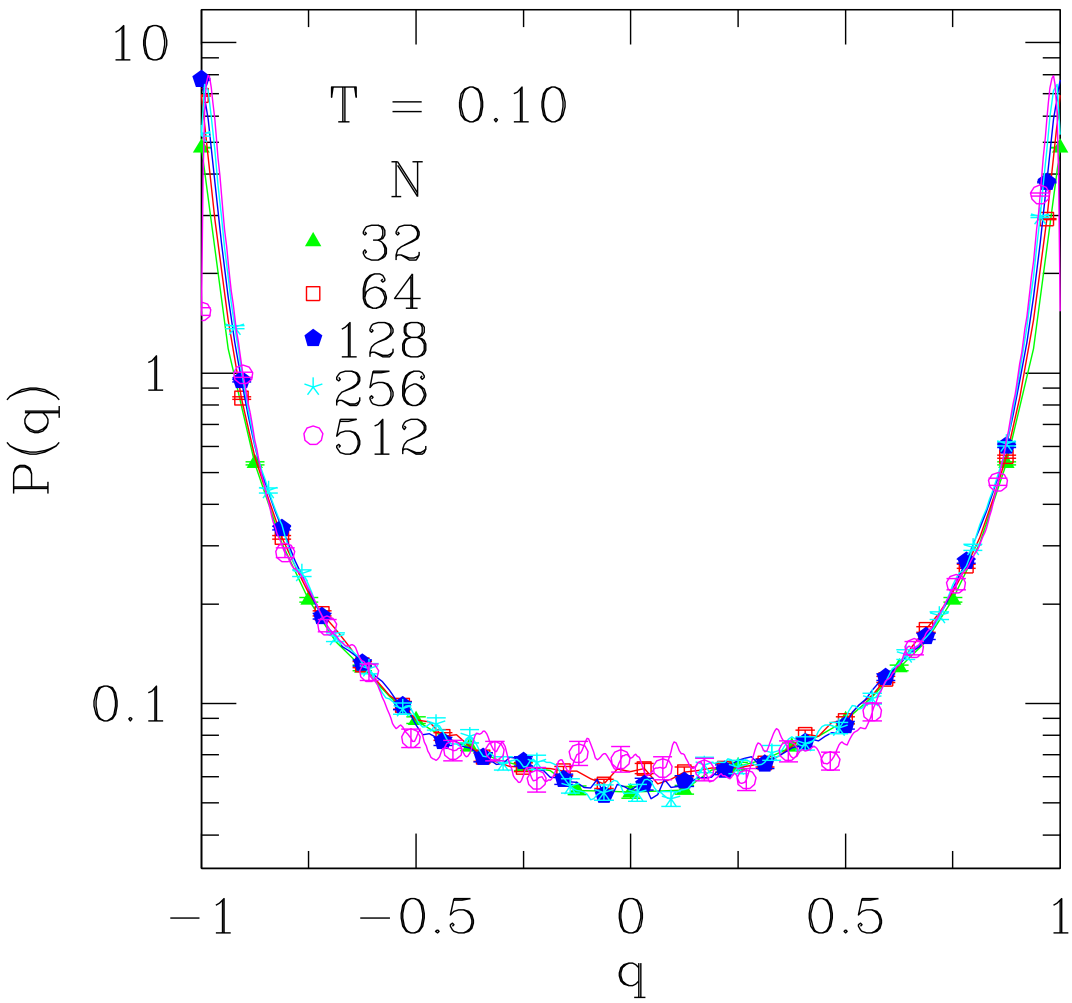
Why is this model interesting?

•Finite T_c in $D = 1$ (usually not the case in common spin-glass models).

•Large range of system sizes L as $d = 1$.

•Analytic predictions of the DP which can be tested.

$P(q)$ at $T = 0.10$ - LR chain



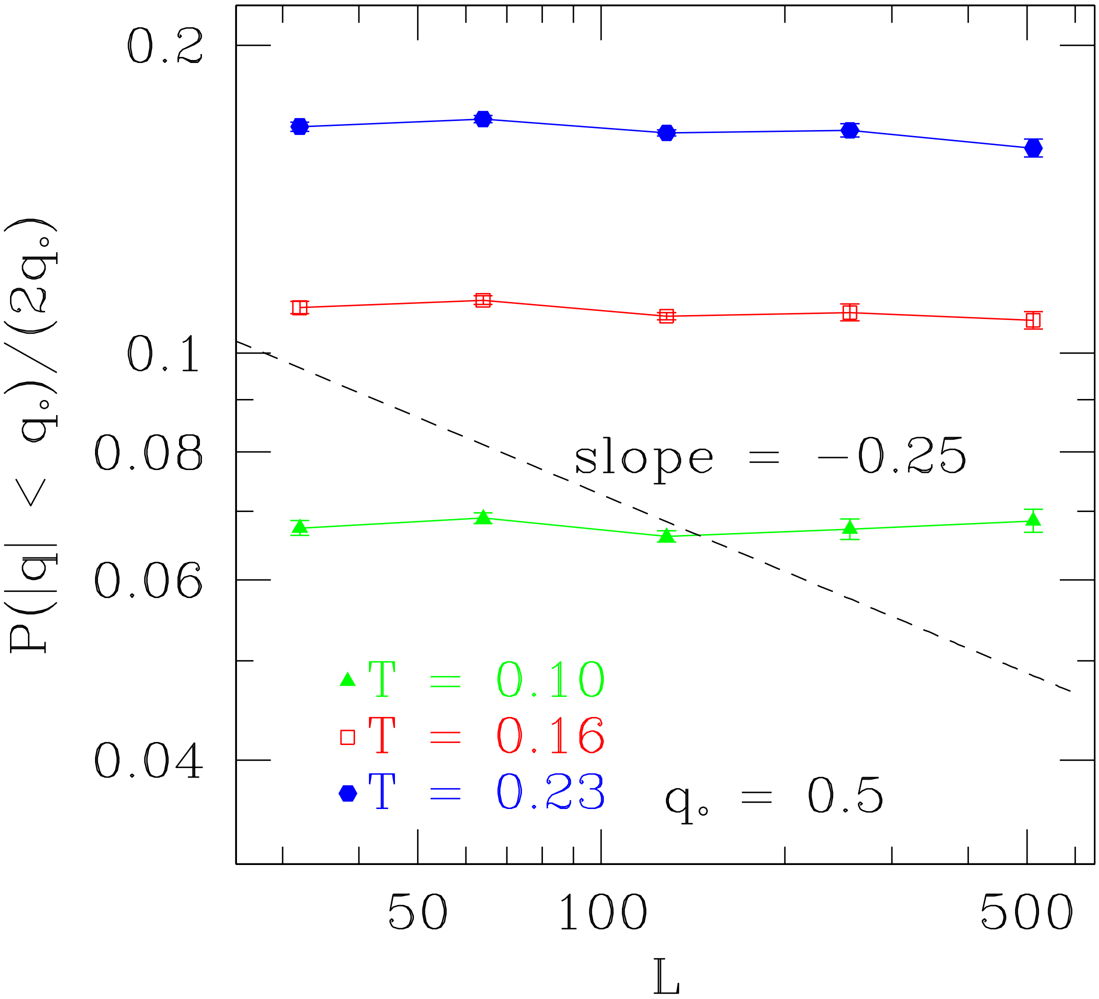
Remember

$$P(0) \sim L^{-\theta'} \qquad \longleftrightarrow \qquad E \sim L^{\theta'}$$

Note that $P(q)$ does not seem to decrease with increasing system size L, indicating that $\theta' \approx 0$.

Thermal system-size excitations have $E \sim$ const., at least for the sizes studied.

$P(0)$ **LR chain at** $T > 0$



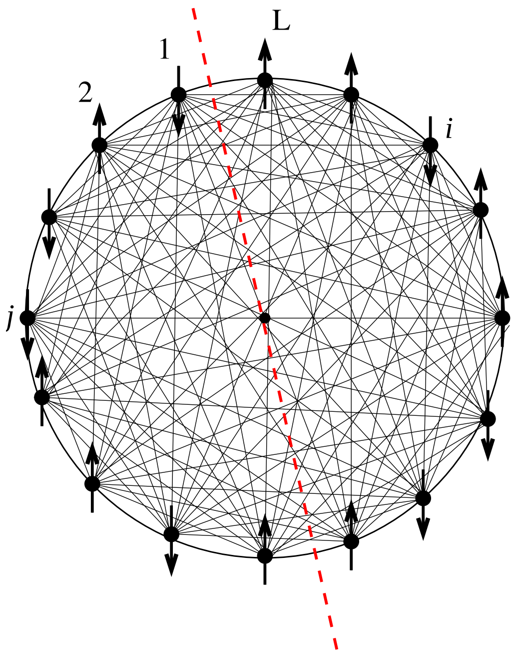
The data do not depend significantly on system size and fit well to $P(0) \sim aL^{\theta'}$, $\theta' = 0$. The dashed line has slope 0.25, the theoretical prediction from DP.

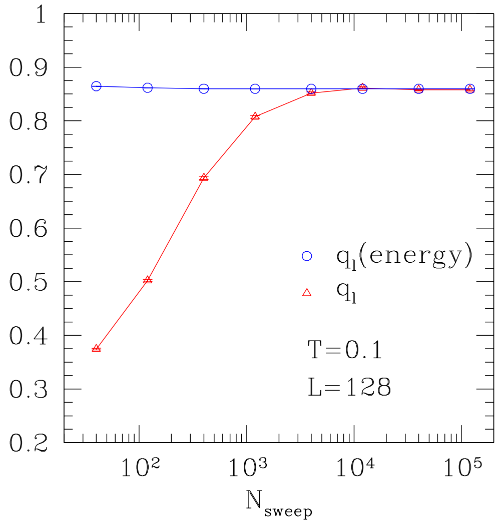
Finding ground states with PT

The droplet model states that the domain-wall energy when changing from periodic (P) to antiperiodic (AP) boundary conditions at the ground state, should scale as

$$\Delta E = [|E_{AP} - E_P|] \sim L^{\theta}$$

This forces a domain wall (excitation) into the system.





Calculation of ground states with parallel tempering: Simulate two replicas with $T_{min} = 0.05 \ll T_c$ and

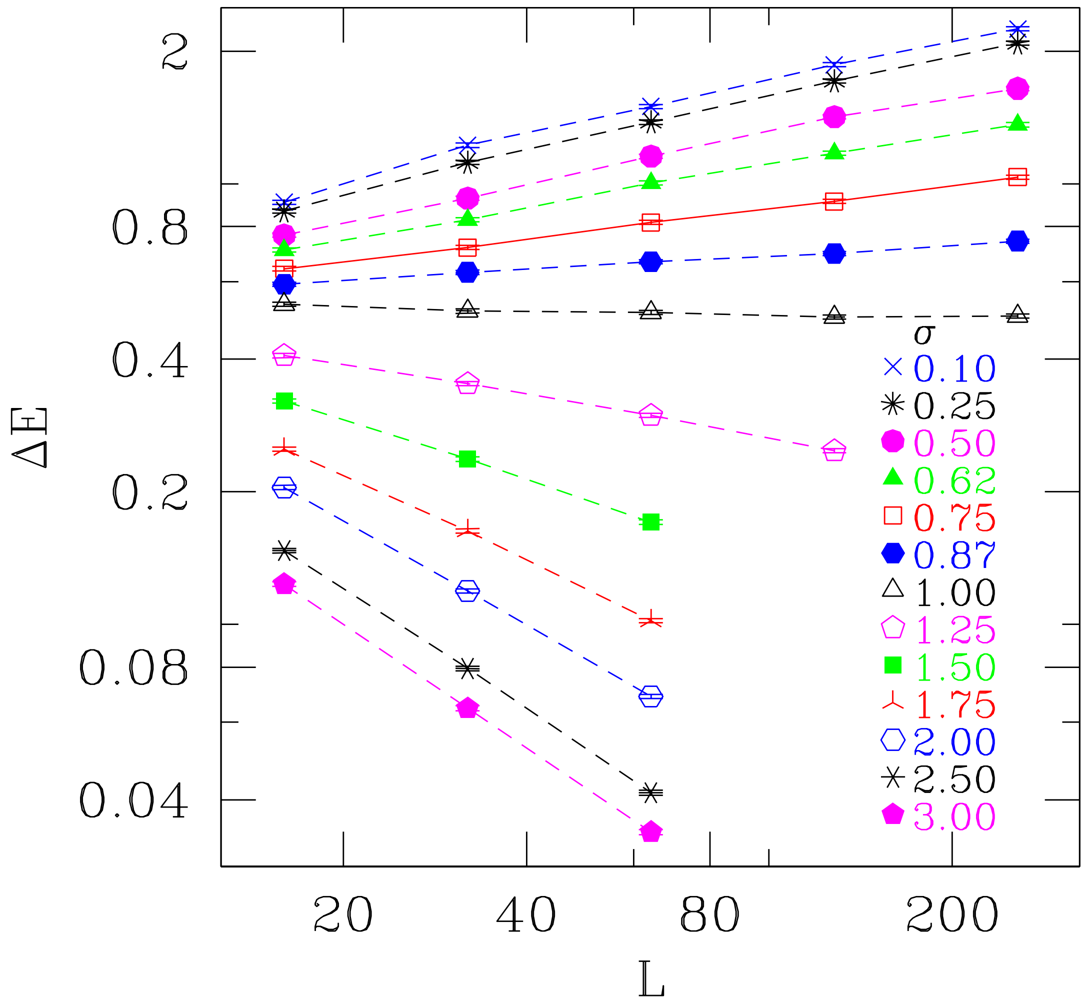
- check that after 1/4 of the MCS the energy of the system does not change

- and the energies of the replicas match after the other 3/4 of the MCS.

- Make sure that $q_l = q_L(E)$, i.e. the system is equilibrated!

Why do we use parallel tempering? Because there is no better algorithm for calculating the GS energy for this system!

ΔE for different σ at $T = 0$



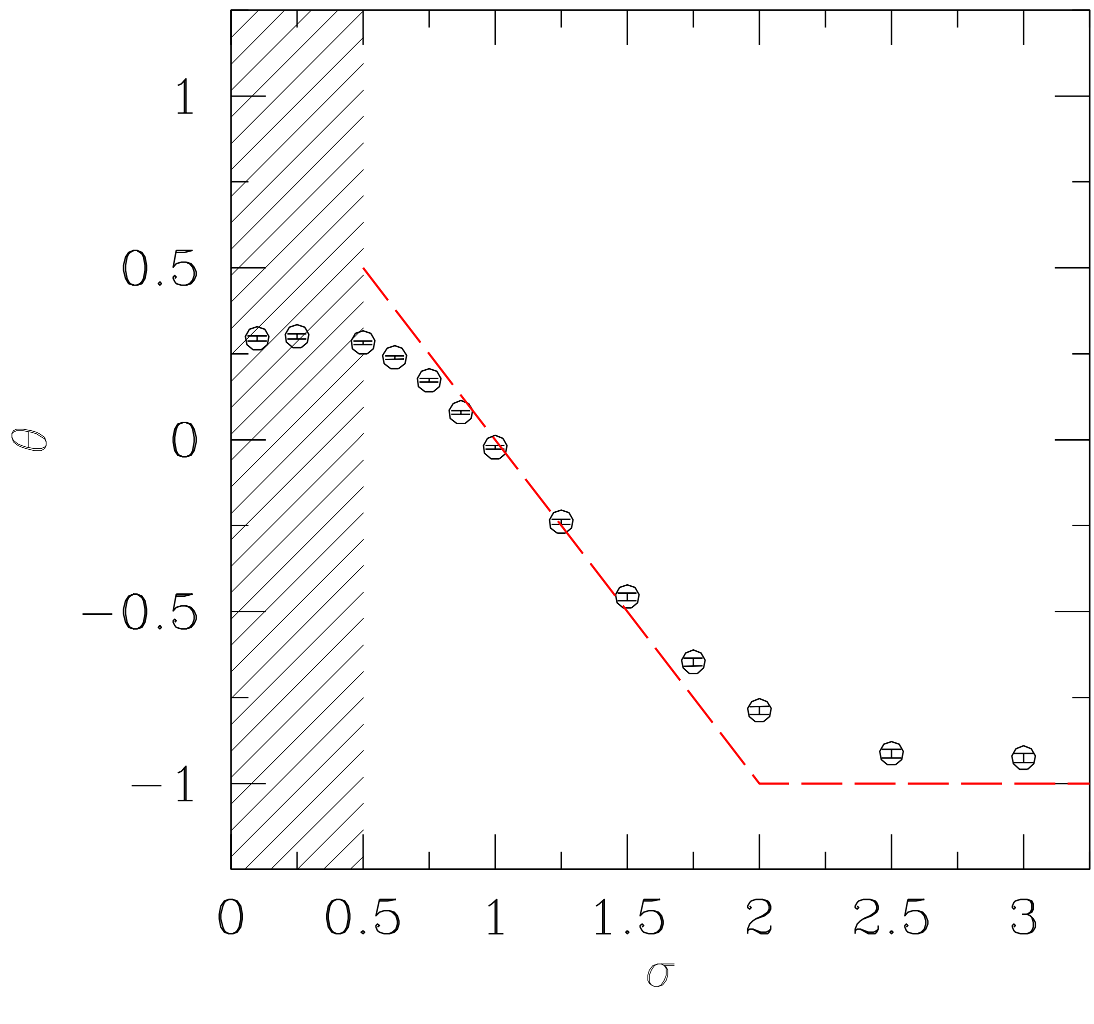
We expect $\Delta E \sim aL^{\theta}$. The solid lines connect the data for $\sigma = 0.75$. We find

$$\theta(\sigma = 0.75) = 0.173 \pm 0.005$$

which is incompatible with $\theta' = 0$ from thermally excited droplets, i.e. $\theta \neq \theta'$ for a large range of sizes.

$\rightarrow$ BC excitations and thermal droplets behave different.
$\rightarrow$ corrections to DP?

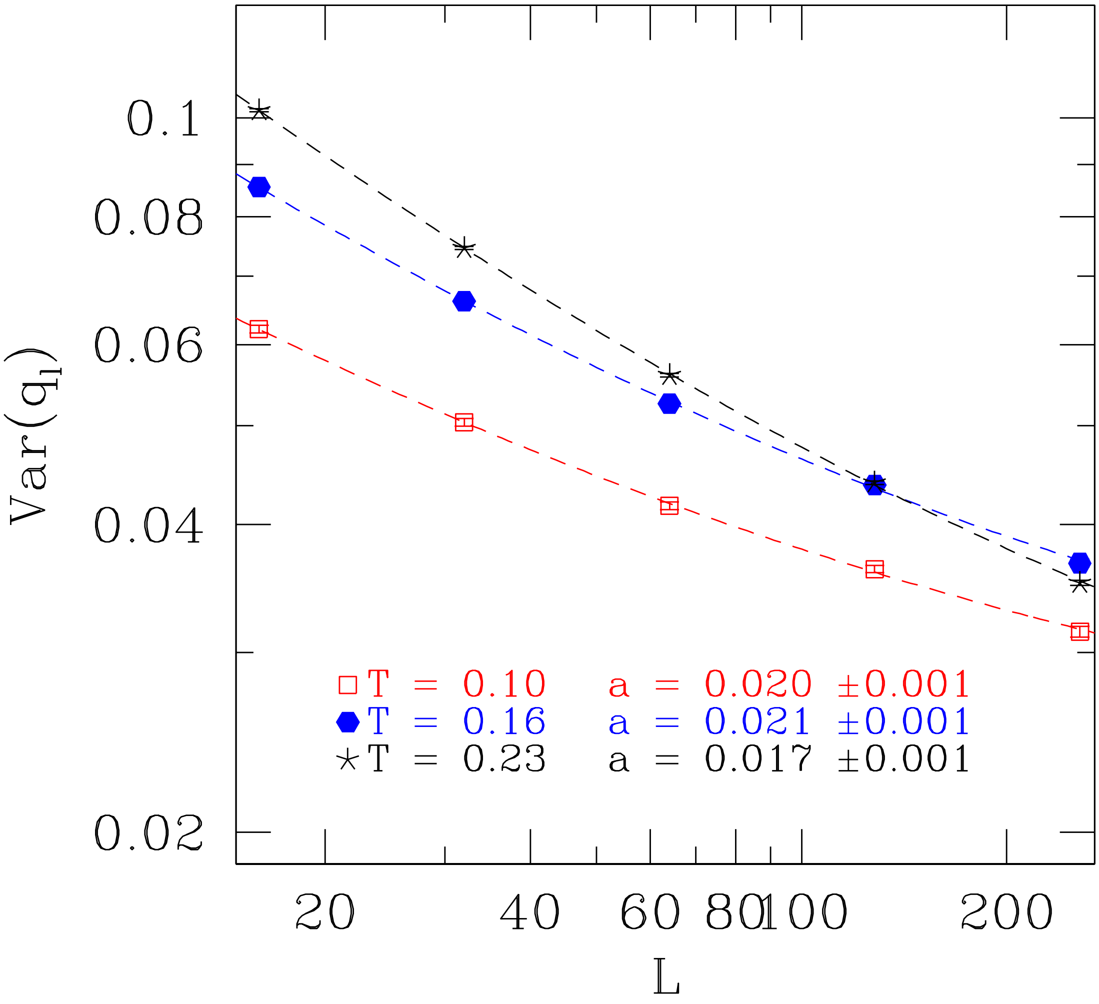
LR chain: $\theta(\sigma)$ at $T = 0$



The dashed line represents the theoretical prediction of the DP.

The data points are calculated by fitting $\Delta E \sim aL^{\theta}$.

Droplet Geometry LR Chain



The data do not fit well a power-law Var$(q_l) \sim cL^{-b}$ unless corrections to scaling are included (Palassini et al. 02).

A fit of the form Var$(q_l) \sim a + cL^{-b}$ gives $a > 0$, i.e. droplets are compact and $d = d_s$.

(Work in progress. . .)

Summary

•Our results for the short-range EA Ising spin glass in three and four dimensions agree qualitatively with the intermediate picture.

•Our results on the one-dimensional Ising spin chain show that

$$\theta \neq \theta'$$

i.e., the exponent for excitations of domain walls (θ) is not compatible with the stiffness exponent for the excitation of thermal droplets (θ') for a large range of sizes.

Results seem to indicate that the excitations are not fractal, i.e. $d = d_s$.

Future work

•Calculate $T = 0$ excitations by applying a coupling-dependent perturbation to the ground state.

•Study corrections to scaling.