New insights from one-dimensional spin glasses

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Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

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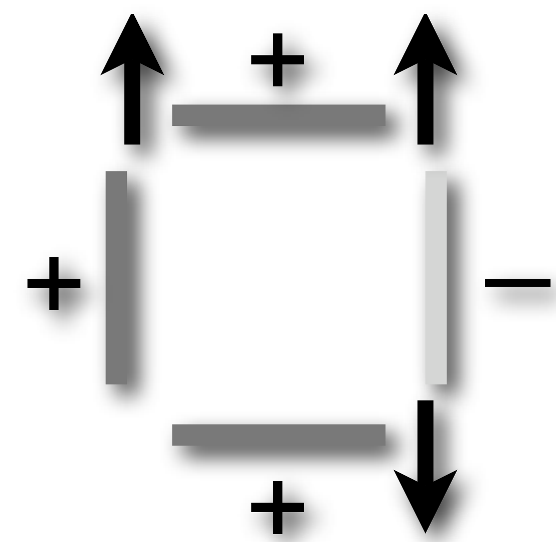
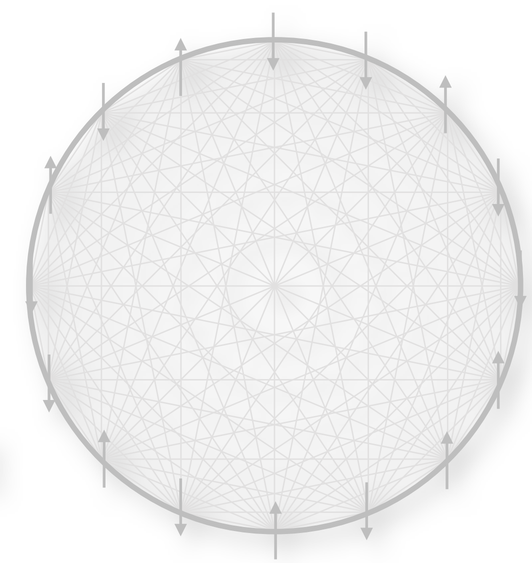
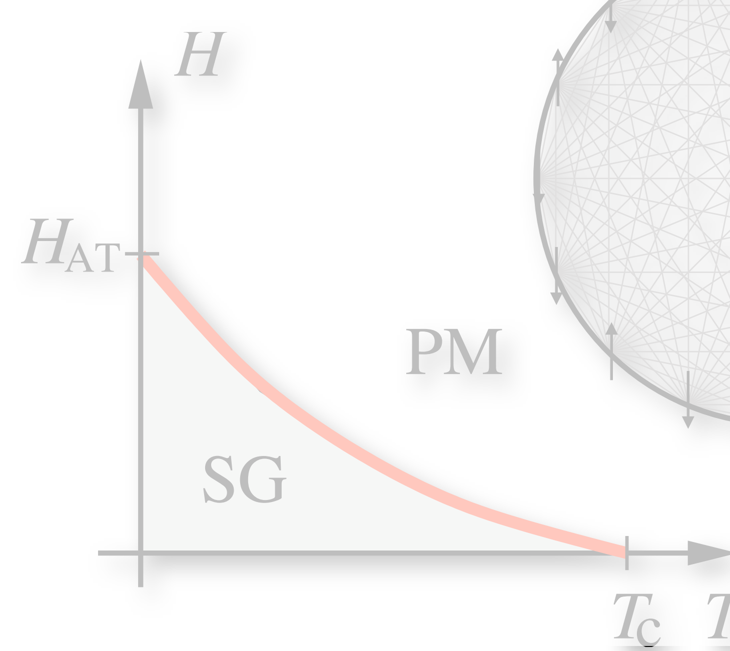
Outline and Motivation

- Introduction to spin glasses (disordered magnets)
  - What are spin glasses?
  - Why are they hard to study?



- How well does the mean-field solution work?
  - Model: 1D chain
  - Do spin glasses order in a field?
  - Ultrametricity in spin glasses?





  - Applications to other problems and algorithm benchmarking.

- Work done in collaboration with W. Barthel, S. Böttcher, B. Gonçalves, A. K. Hartmann, T. Jörg, F. Krzakala, and A. P. Young.

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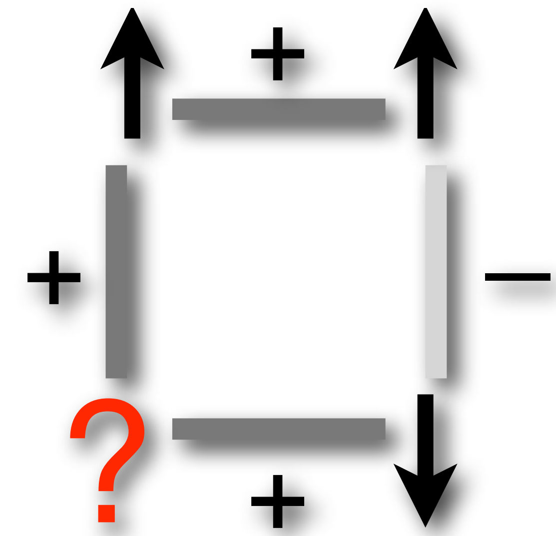

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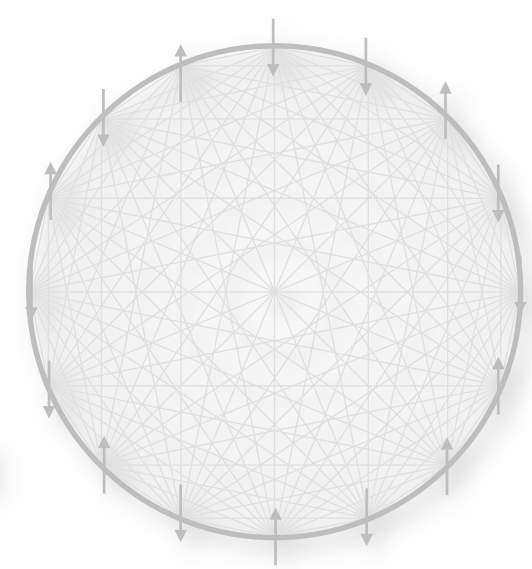

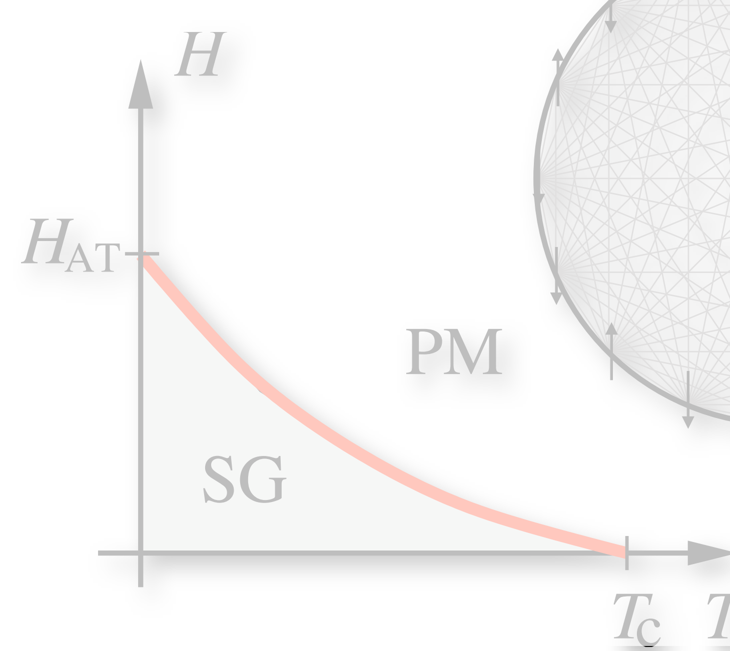

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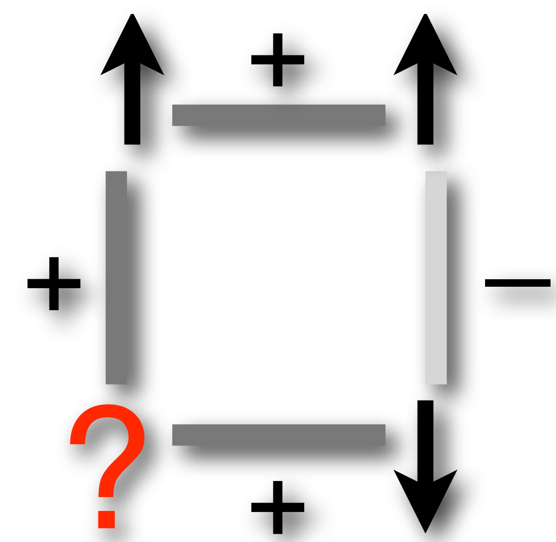

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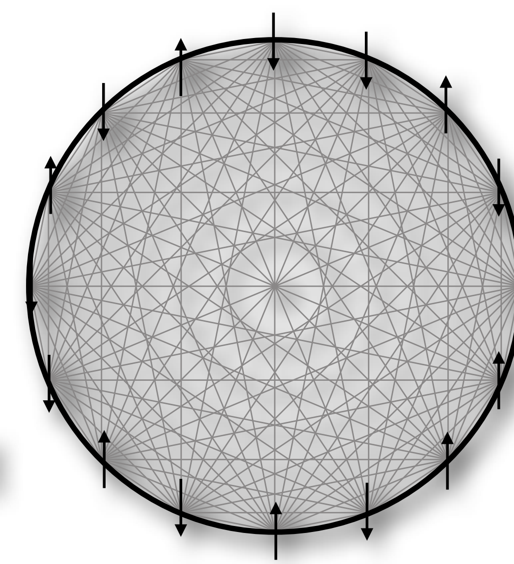

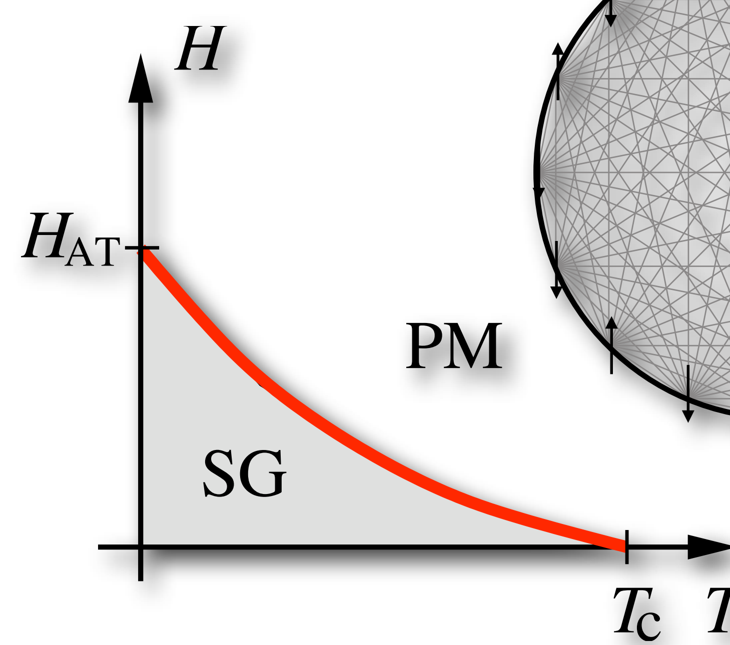

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Brief introduction to spin glasses

Building a spin glass from the Ising model

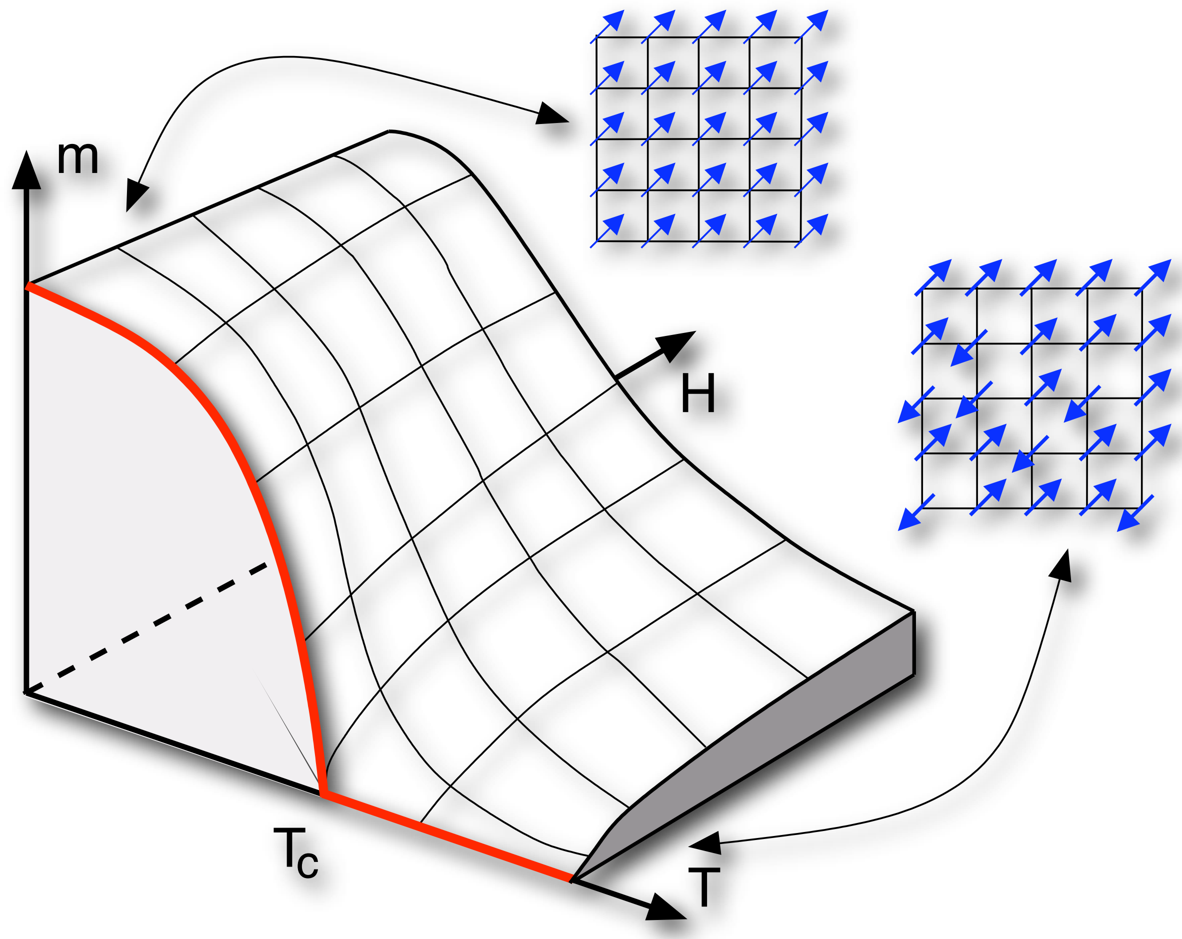
- **Hamiltonian:**

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - H \sum_i S_i$$

$$J_{ij} = 1 \ \ \forall i,j \quad i \neq j$$

- **Order parameter:**

$$m = \frac{1}{N} \sum_i S_i \quad \text{(magnetization)}$$

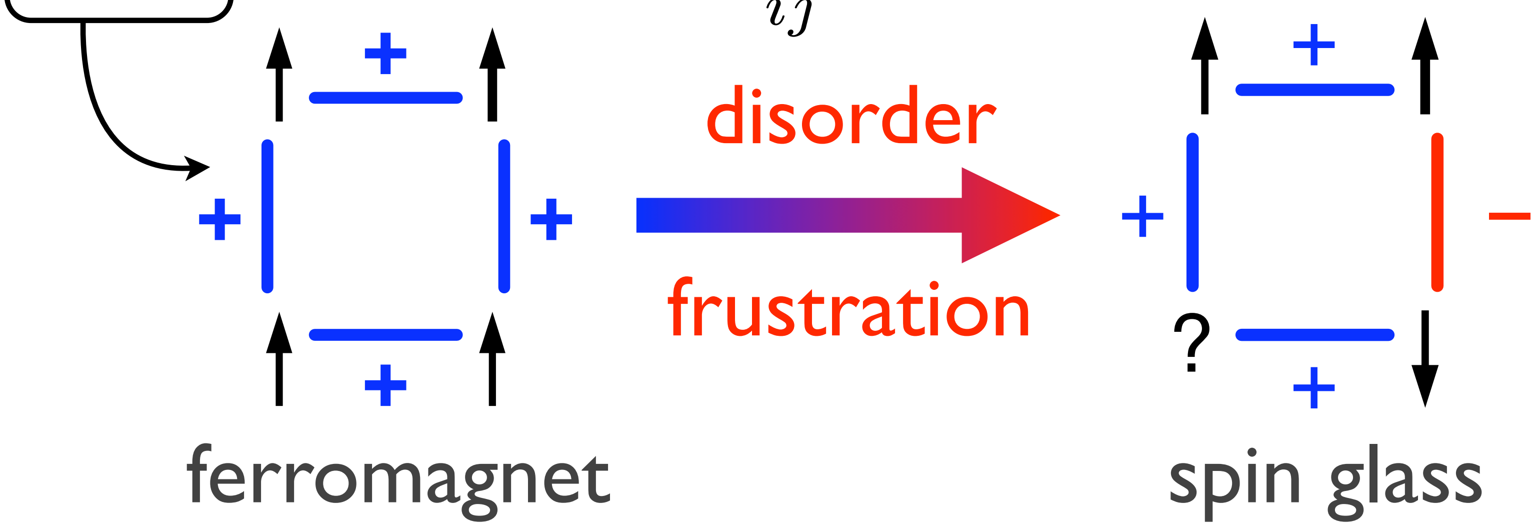


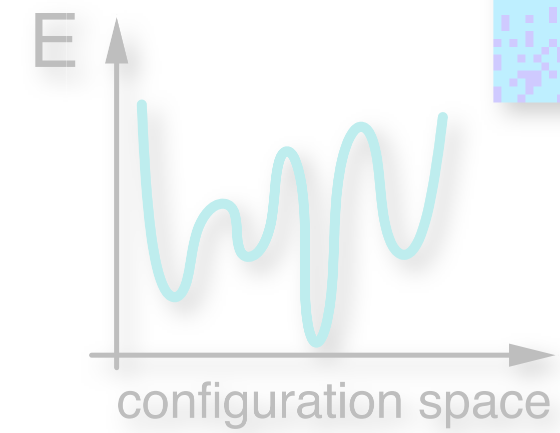
- **Some properties:**
  - Phase transition to an ordered state.
  - According to Harris criterion, if $d\nu > 2$ the system changes universality class when local disorder is added.
  - For the Ising model $d\nu \leq 2$ in 2D and 3D.

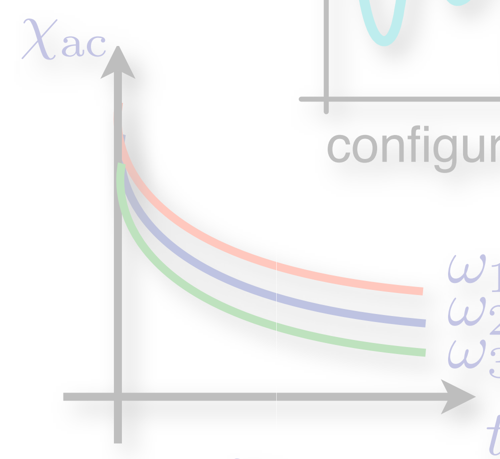
What is a spin glass?

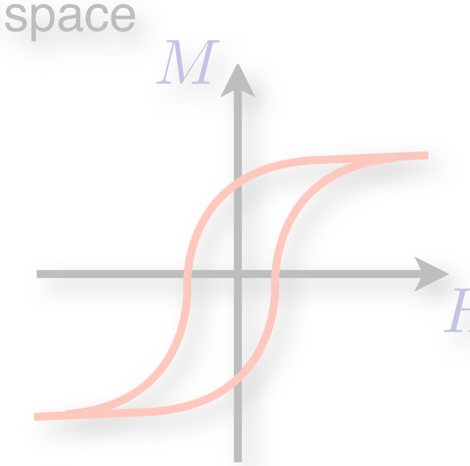
- Prototype model: Edwards-Anderson Ising spin glass

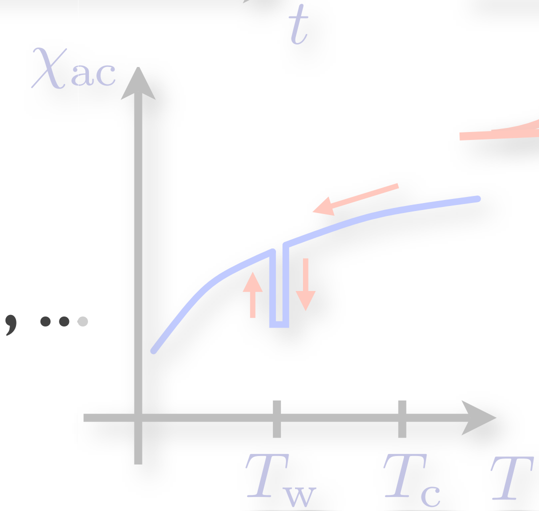
$$\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j - h \sum S_i \qquad J_{ij} \text{ random}$$











- Properties:
  - Phase transition into a glassy phase
  - Complex energy landscape
  - Some hallmarks: aging, memory, hysteresis, ...
  - Complex optimization problem
  - Very hard to treat analytically beyond mean-field.

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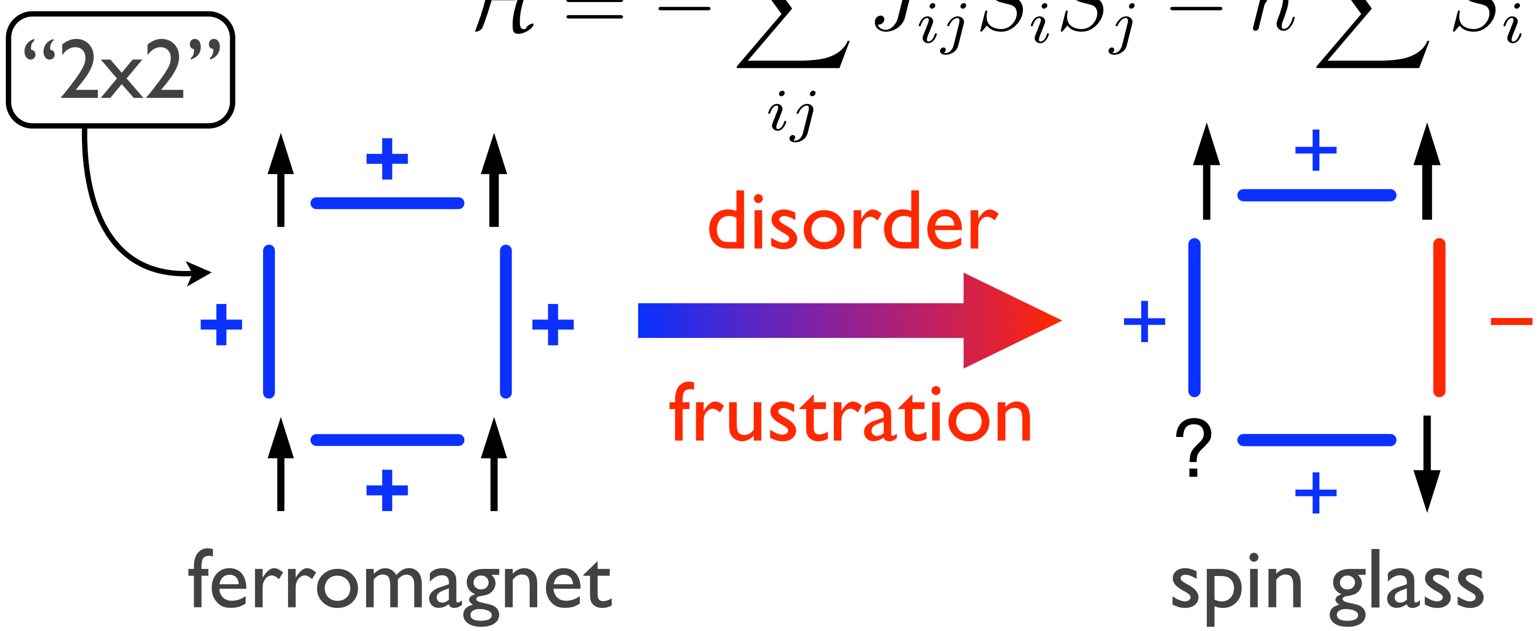

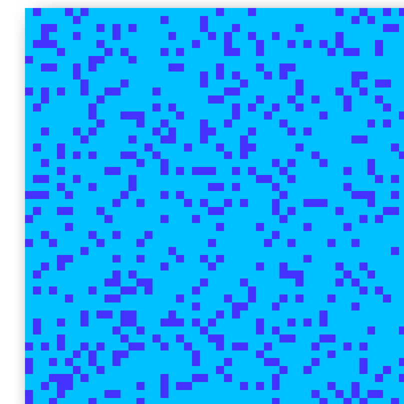

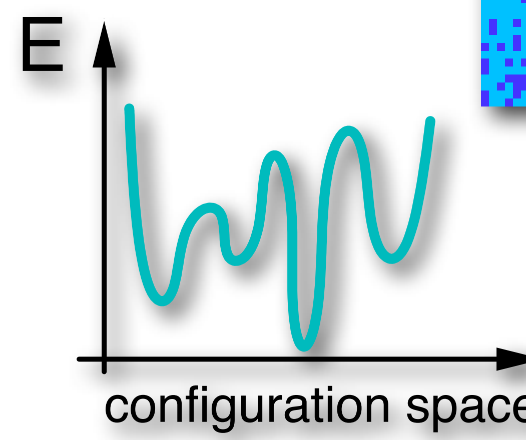

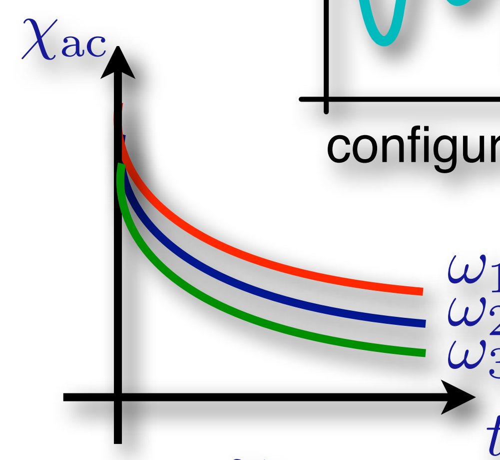

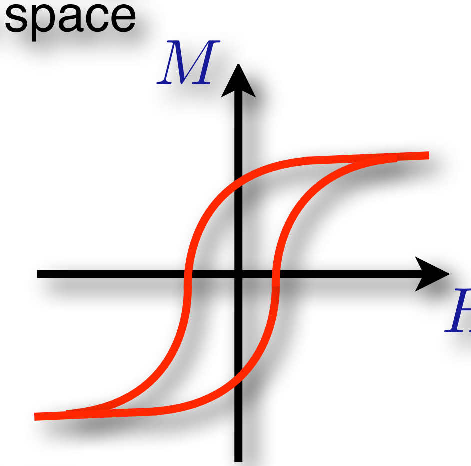

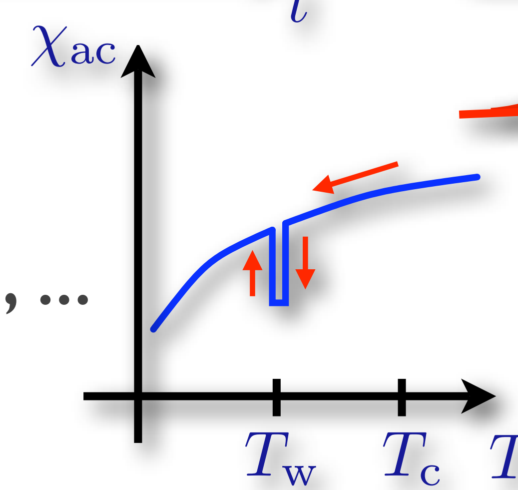

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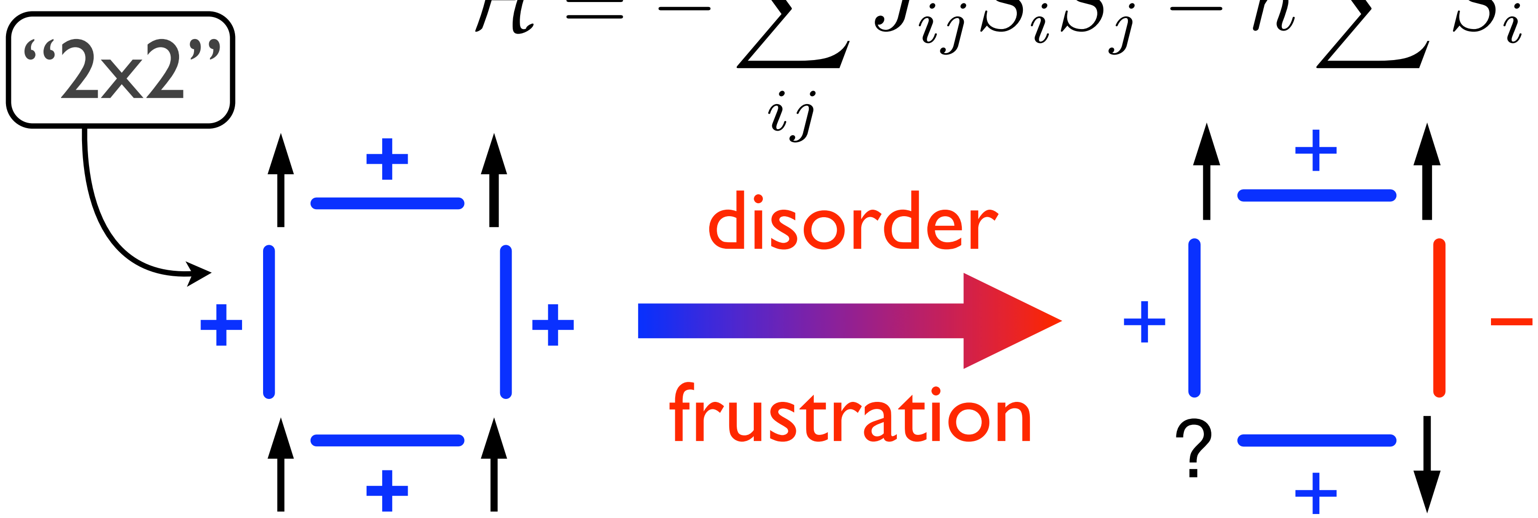
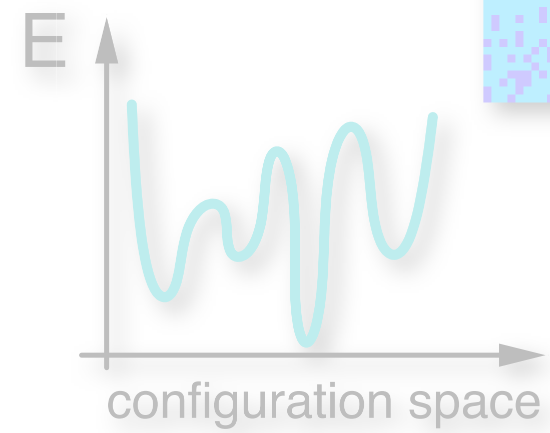
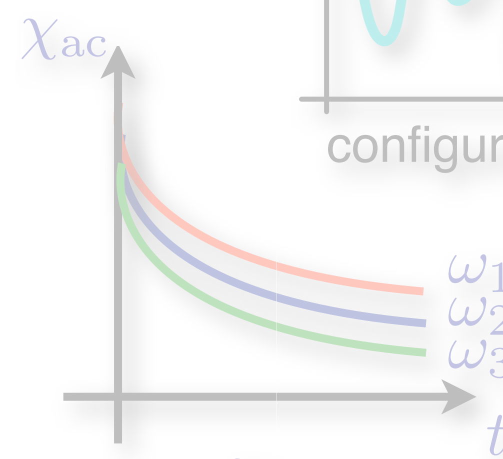
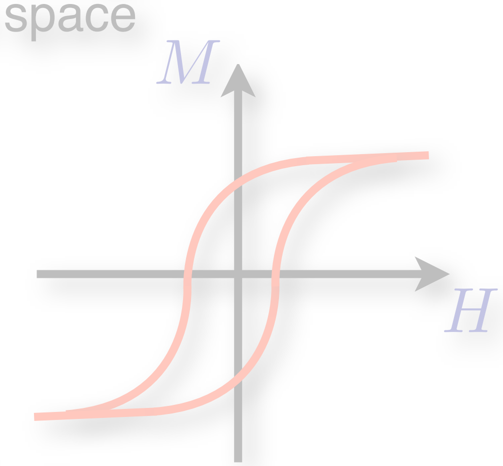
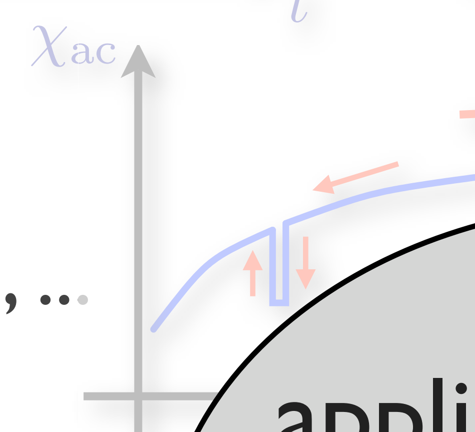


ferromagnet spin glass









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Many applications to other problems!

Applications beyond disordered magnets

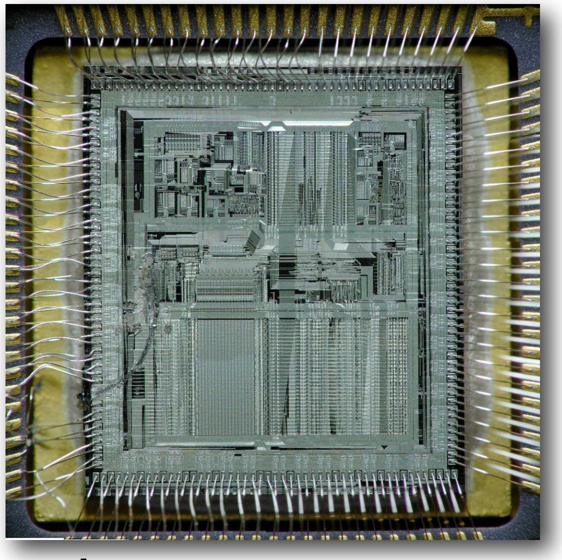
- The models can describe many systems with competing interactions on a graph:
  - Computer chips:

    S_i component

    J_{ij} wiring diagram
  - Economic markets:

    S_i agent inclination

    J_{ij} portfolio interactions
- Other applications:
  - Quantum error correction in topological quantum computing (current research).
  - Optimization problems (e.g., number partitioning problem).
  - Neural networks, …



chip optimization

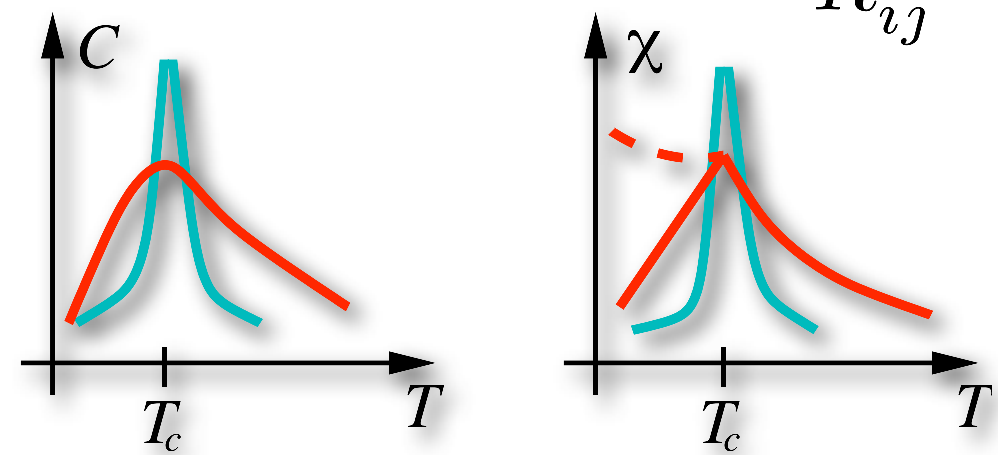
payload distribution

markets

Experimental discovery, theoretical pictures

- Early experimental observations:
  - 1970: Canella and Mydosh see a cusp in the susceptibility of Fe/Au alloys (disorder). Material with RKKY interactions (frustration):

$$J_{ij} \sim \frac{\cos(2k_{\mathrm{F}}R_{ij})}{R_{ij}^3}$$



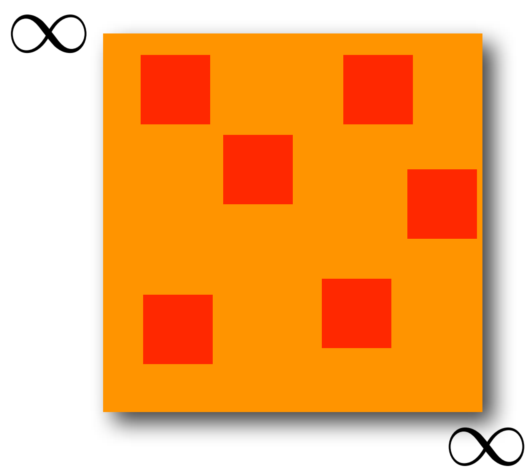
- Early theoretical descriptions:
  - 1975: Introduction of the Edwards-Anderson Ising spin-glass model (J_{ij} random):

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j \quad \xrightarrow{\text{mean-field approx.}} \quad \sum_{\langle ij \rangle} \to \sum_{i,j}$$

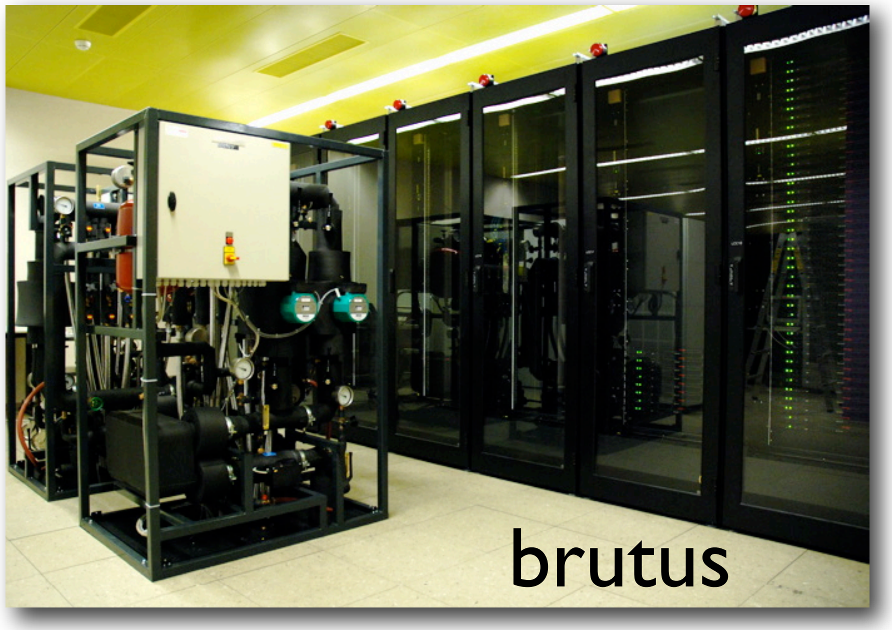
  - 1975: Mean-field Sherrington-Kirkpatrick model.
  - 1979: Parisi solution of the mean-field model (RSB).
  - 1986: Fisher, Huse, Bray, Moore introduce the phenomenological droplet picture (DP) for short-range systems.

How can we study these systems?

- Analytically: only the mean-field solution (RSB) or qualitative descriptions (DP).



- Numerically: Optimal problem for large computers
  - Challenges:
    - Exponential number of competing states (usually NP hard).
    - Relaxation times diverge exponentially with the system size.
    - Extra overhead due to disorder averaging.
    - Usually small systems only.
  - Solution:
    - Use large computer clusters.
    - Use better algorithms.
    - Use better models.
  - Average project requires 300’000 CPUh (4 months on 10^2 CPUs).



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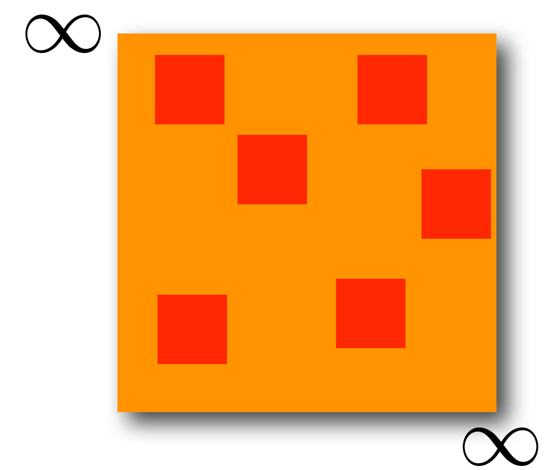

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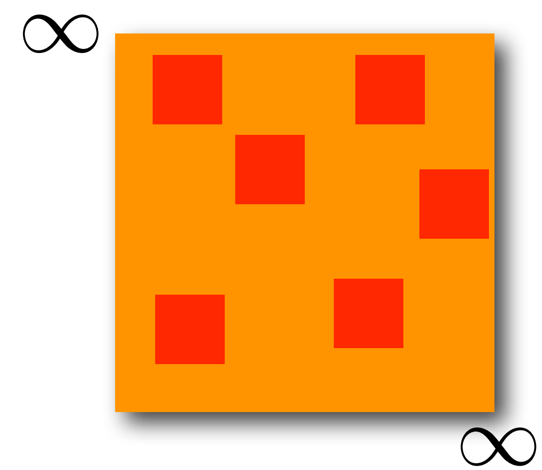

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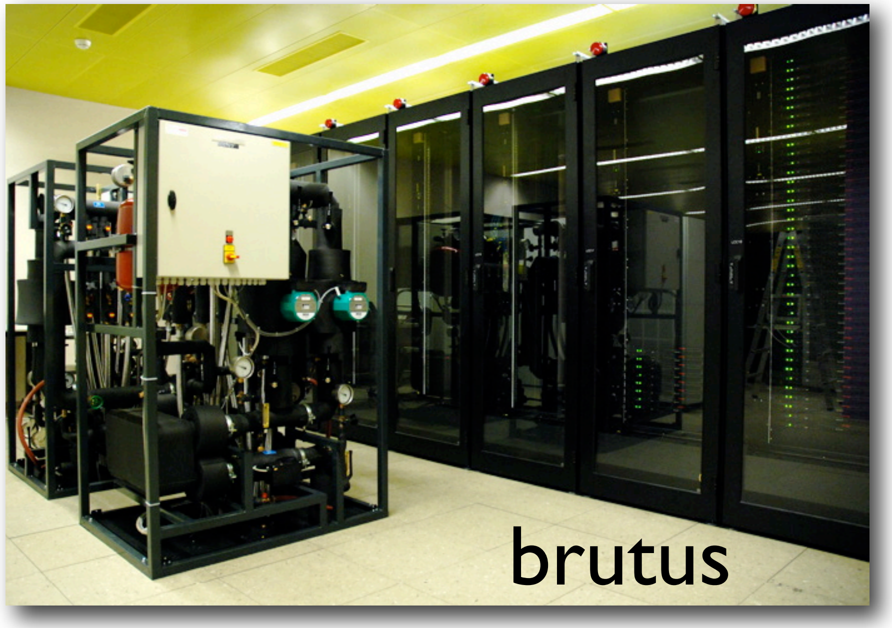

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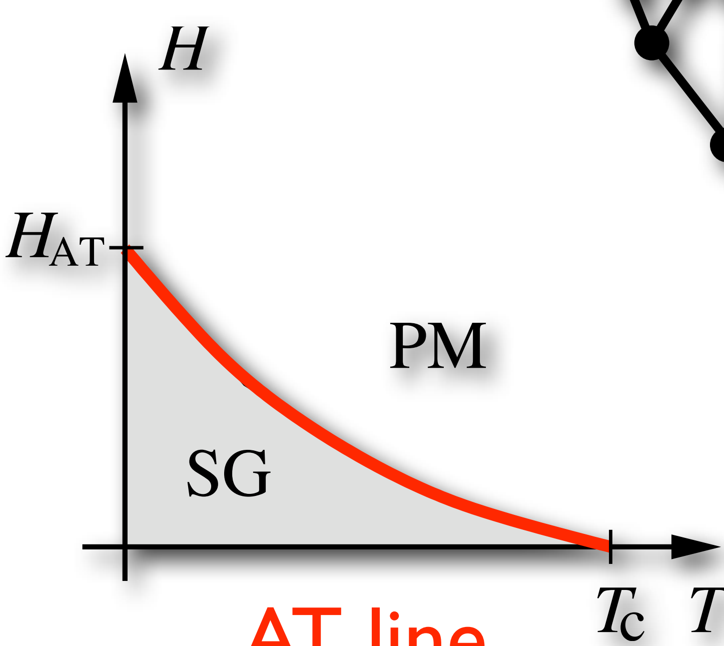
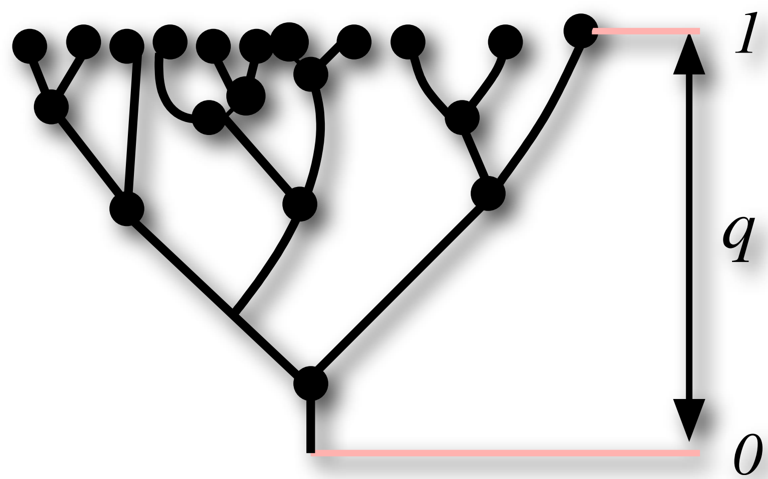
Some open problems... many challenges

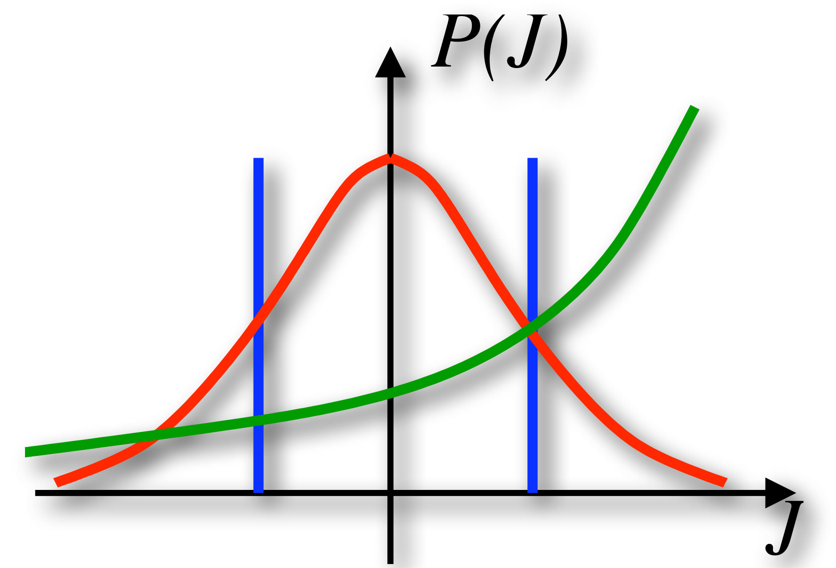
- Some open issues:



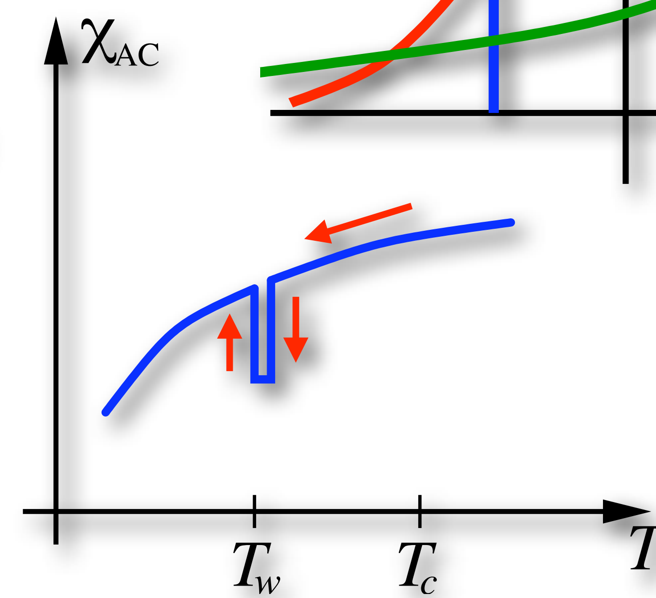
AT line



ultrametricity



universality



memory effect

- And many more:
  - Chaos in spin glasses
  - Nature of the low-temperature spin-glass phase
  - Properties of vector spin glasses, …

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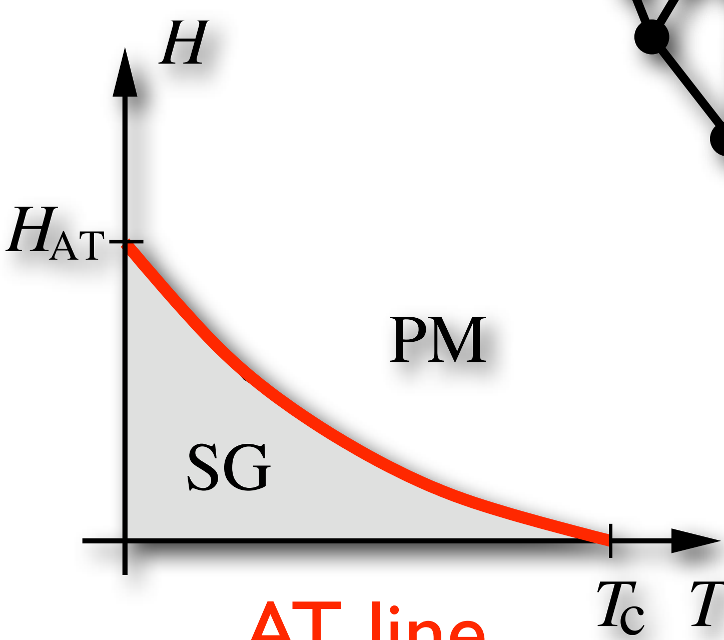

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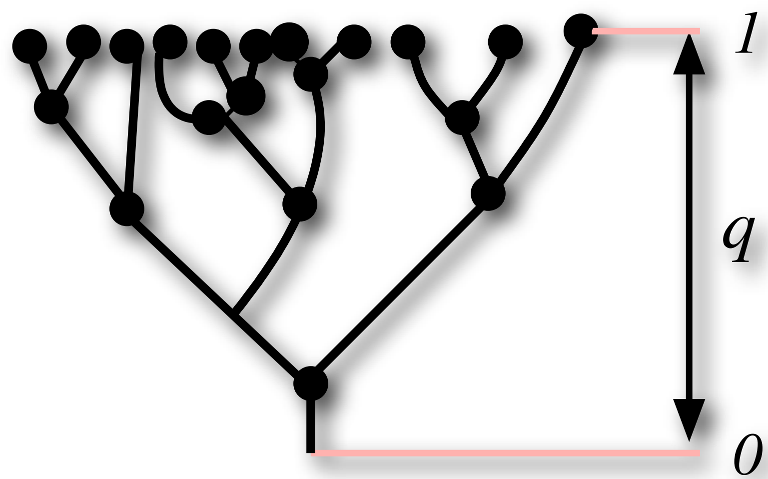

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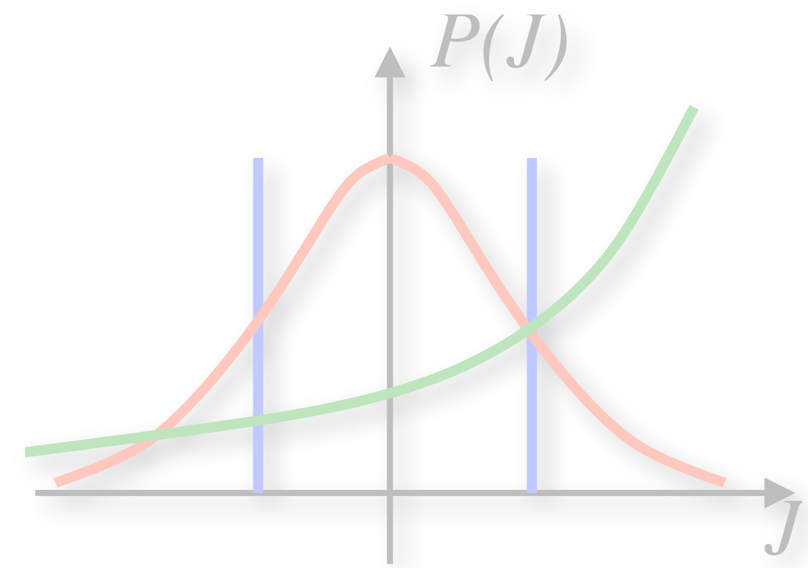

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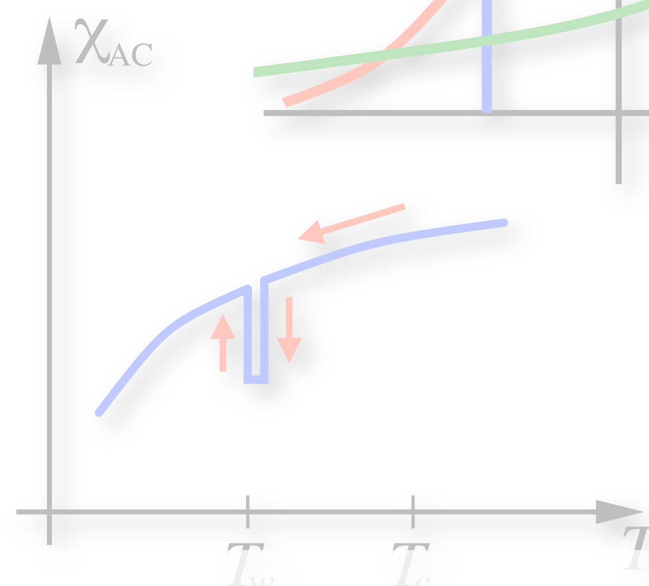

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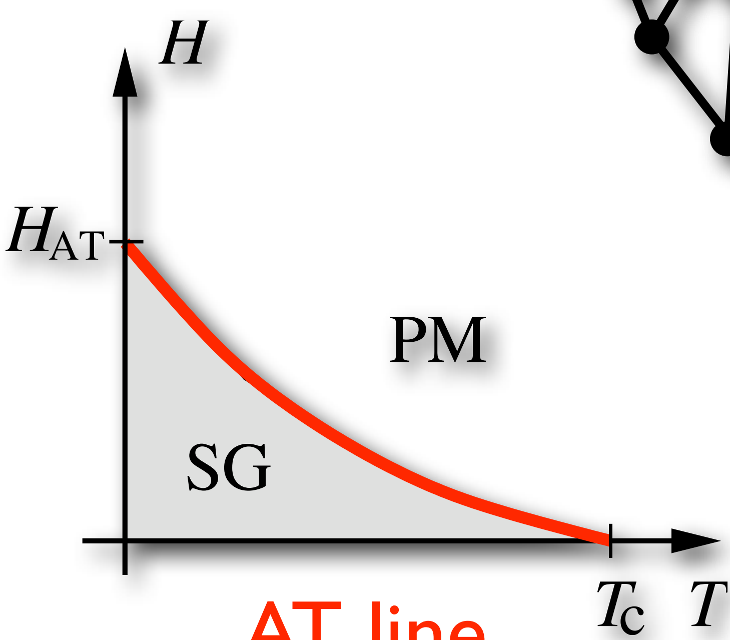

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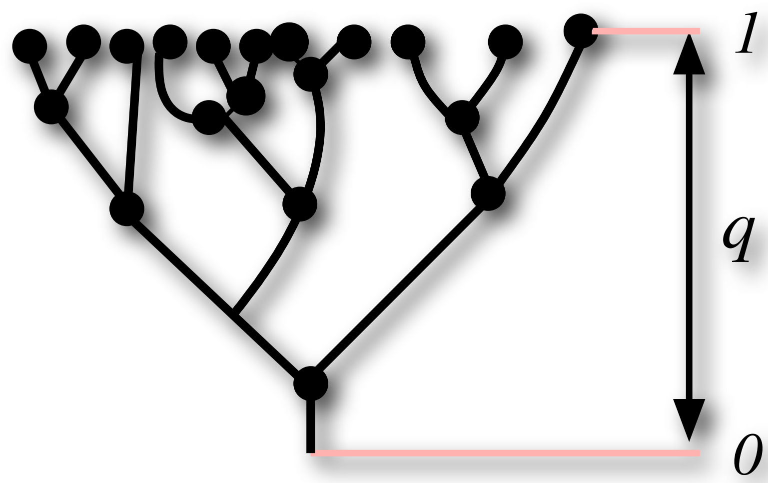

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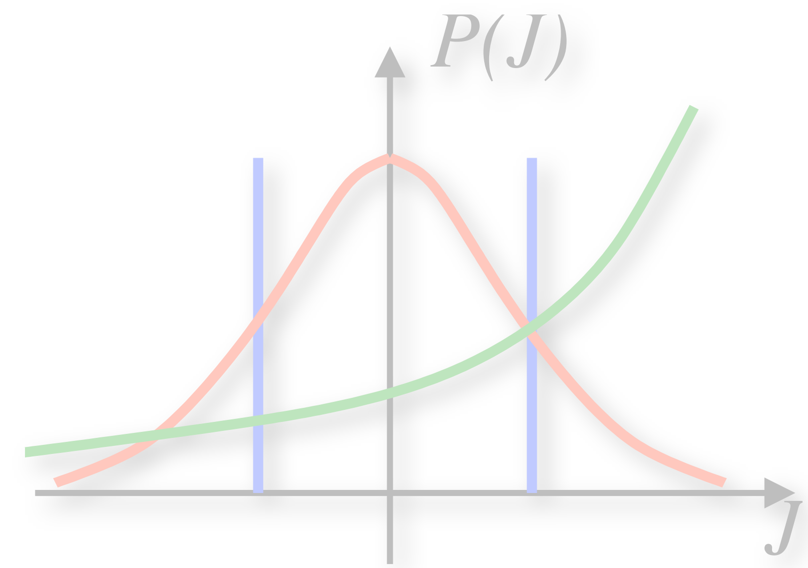

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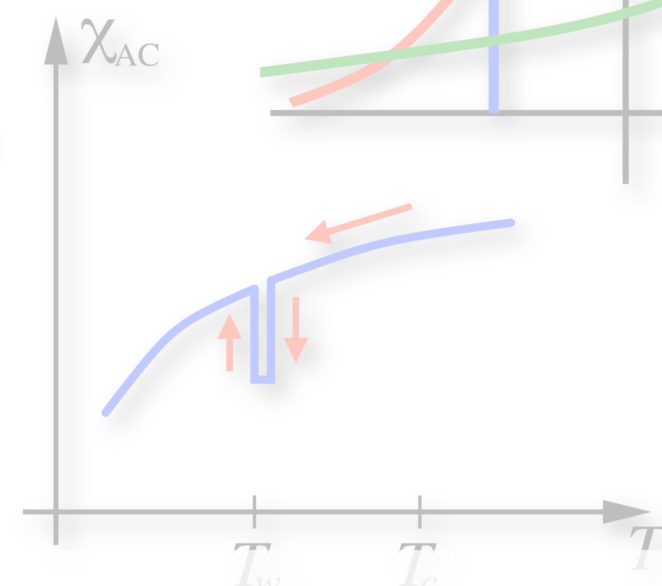

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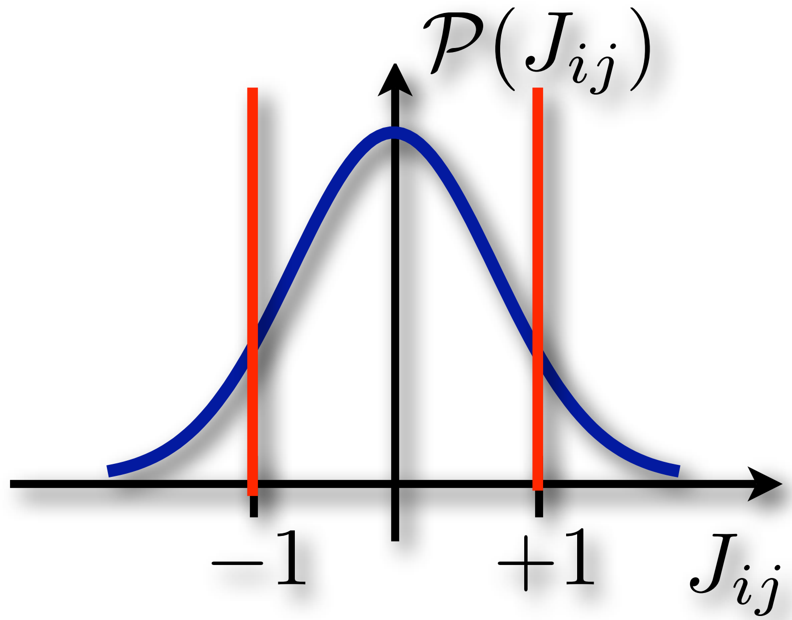
Which properties of the mean-field solution carry over to short-range systems?

Models: The 1D Ising chain

Traditional model: Edwards-Anderson

- Hamiltonian:

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



- Details about the model:
  - Nearest-neighbor interactions.
  - Simulations usually done with periodic boundary conditions.
  - Transition temperatures: $T_c = 0$ (2D), $T_c \sim 1$ (3D), $T_c \sim 2$ (4D).
  - Most studied spin-glass model to date.

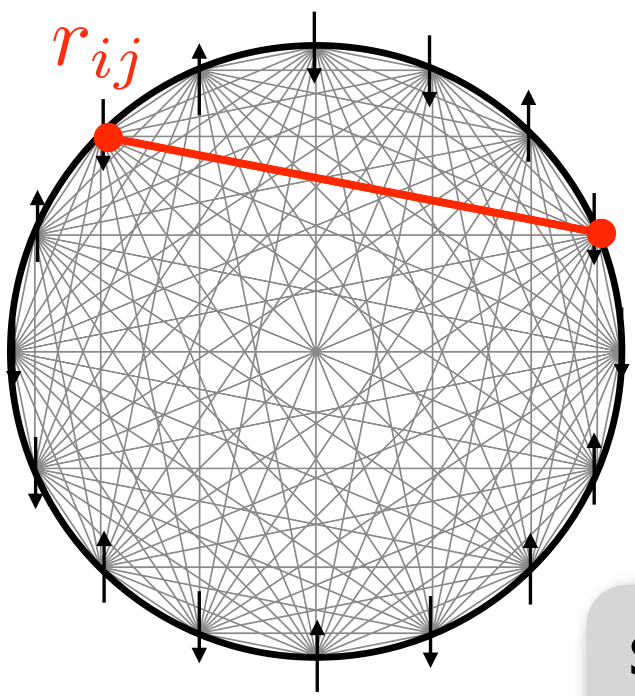
- Disadvantages of the model:
  - Cannot be solved analytically.
  - In high space dimensions only small systems can be simulated ($D \geq 5$ almost impossible).

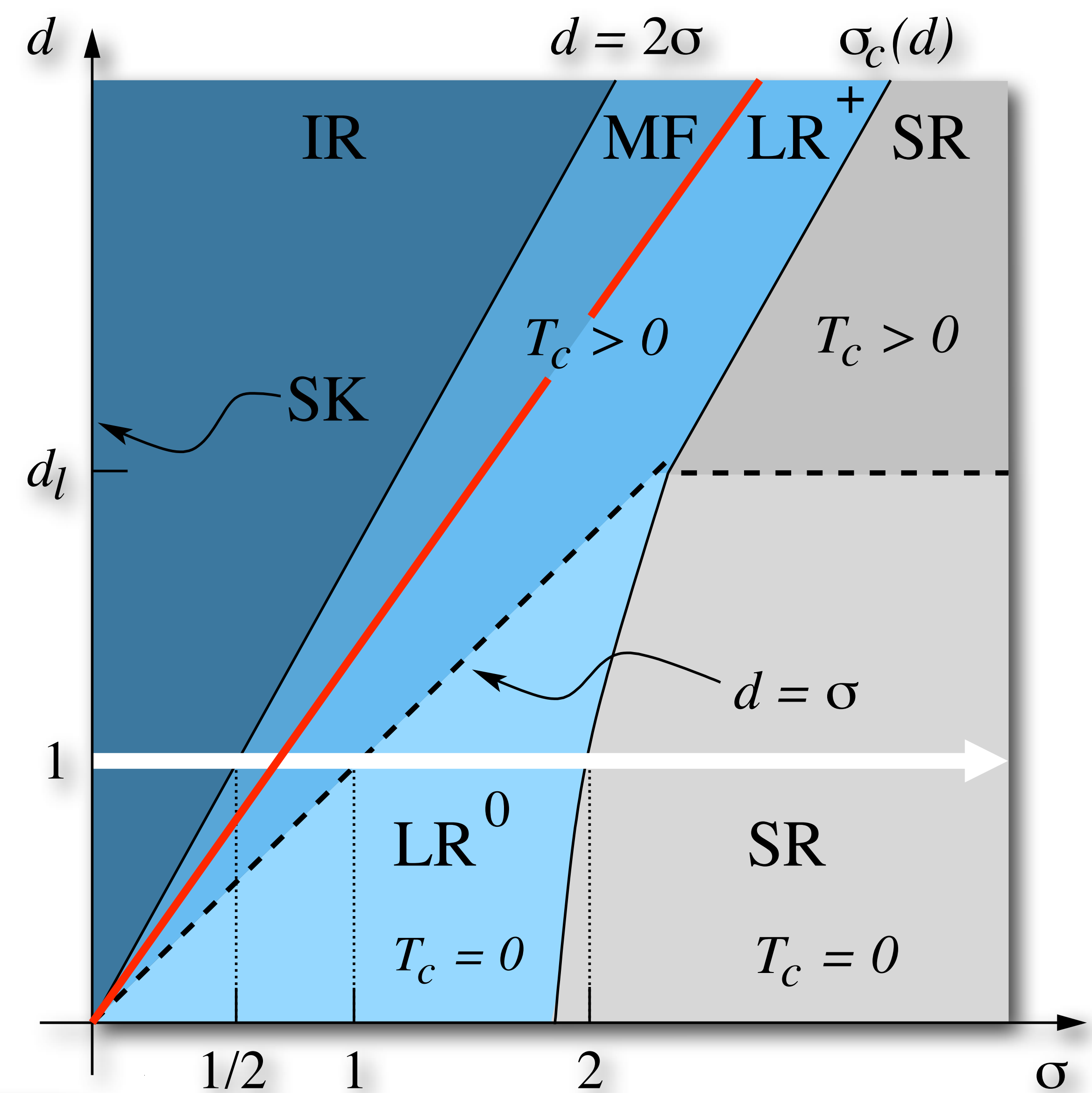
Better: The one-dimensional Ising chain

$$\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j - \sum_i h_i S_i$$

- Properties:
  - The sum ranges over all spins
  - Power-law random interactions

$$J_{ij} \sim \frac{\varepsilon_{ij}}{r_{ij}^{\sigma}}$$





- Advantages:
  - Large range of sizes.
  - Tuning the power-law exponent changes the universality class.

small σ
large d_{eff}

Fisher & Huse, PRB (88)
Kotliar et al., PRB (83)

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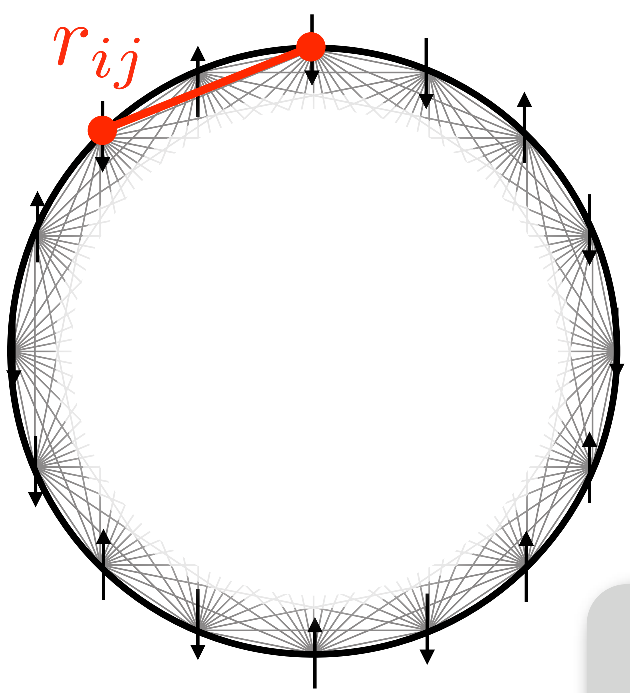

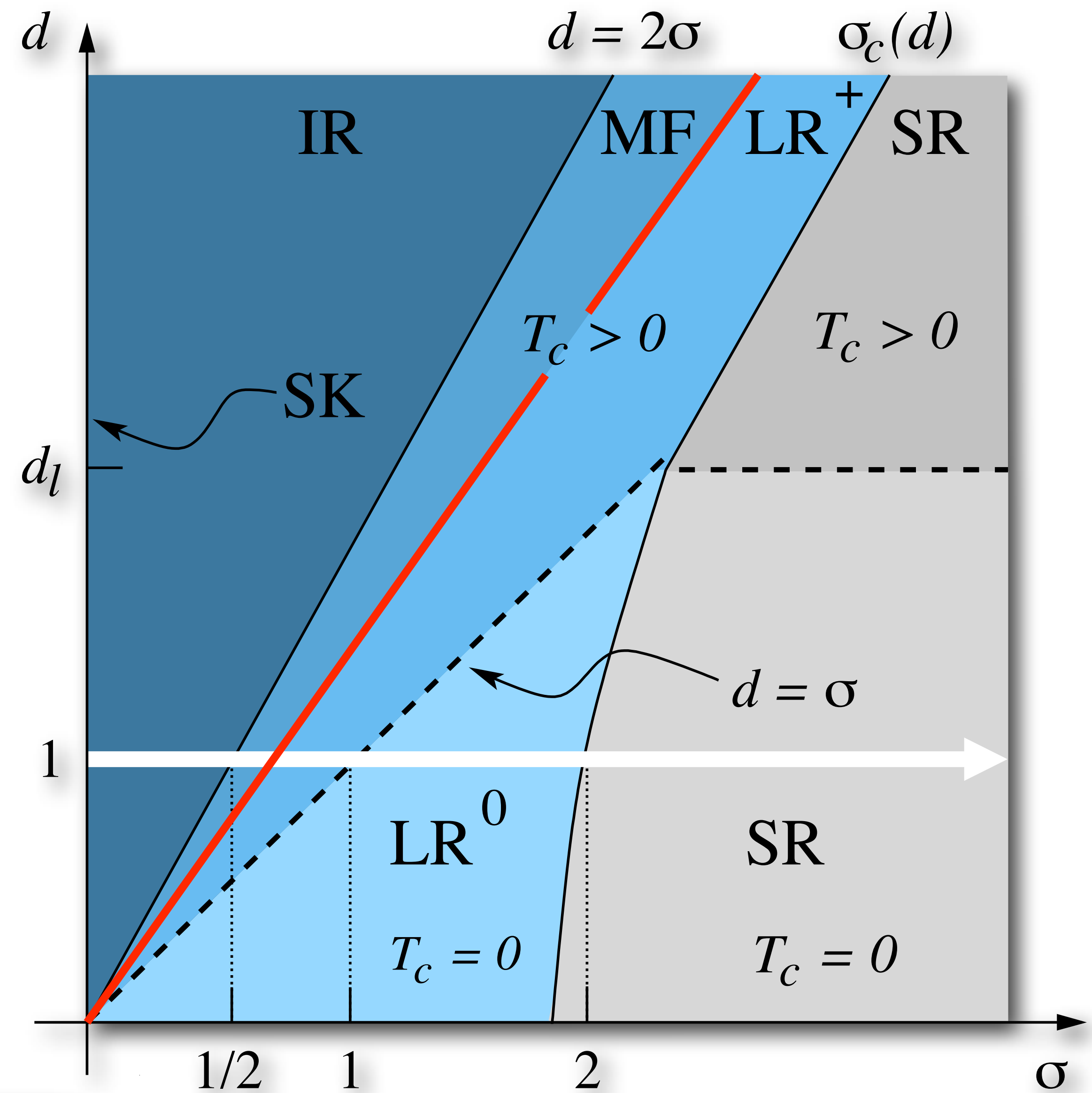

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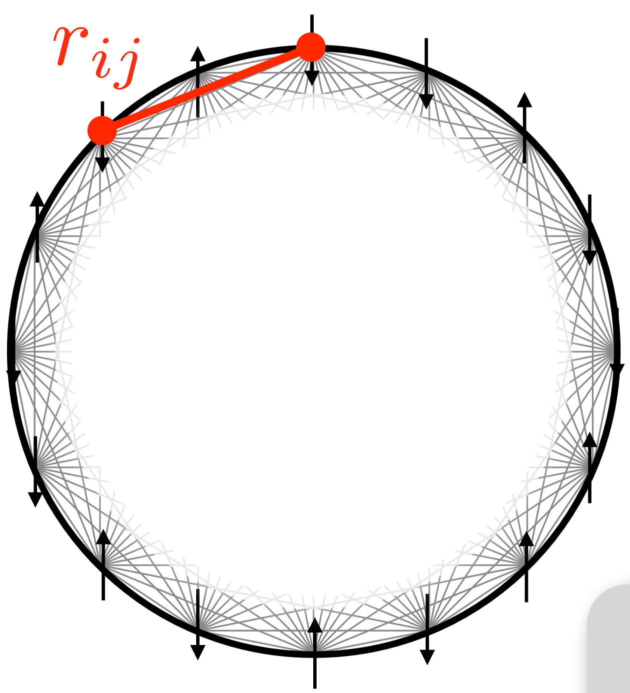

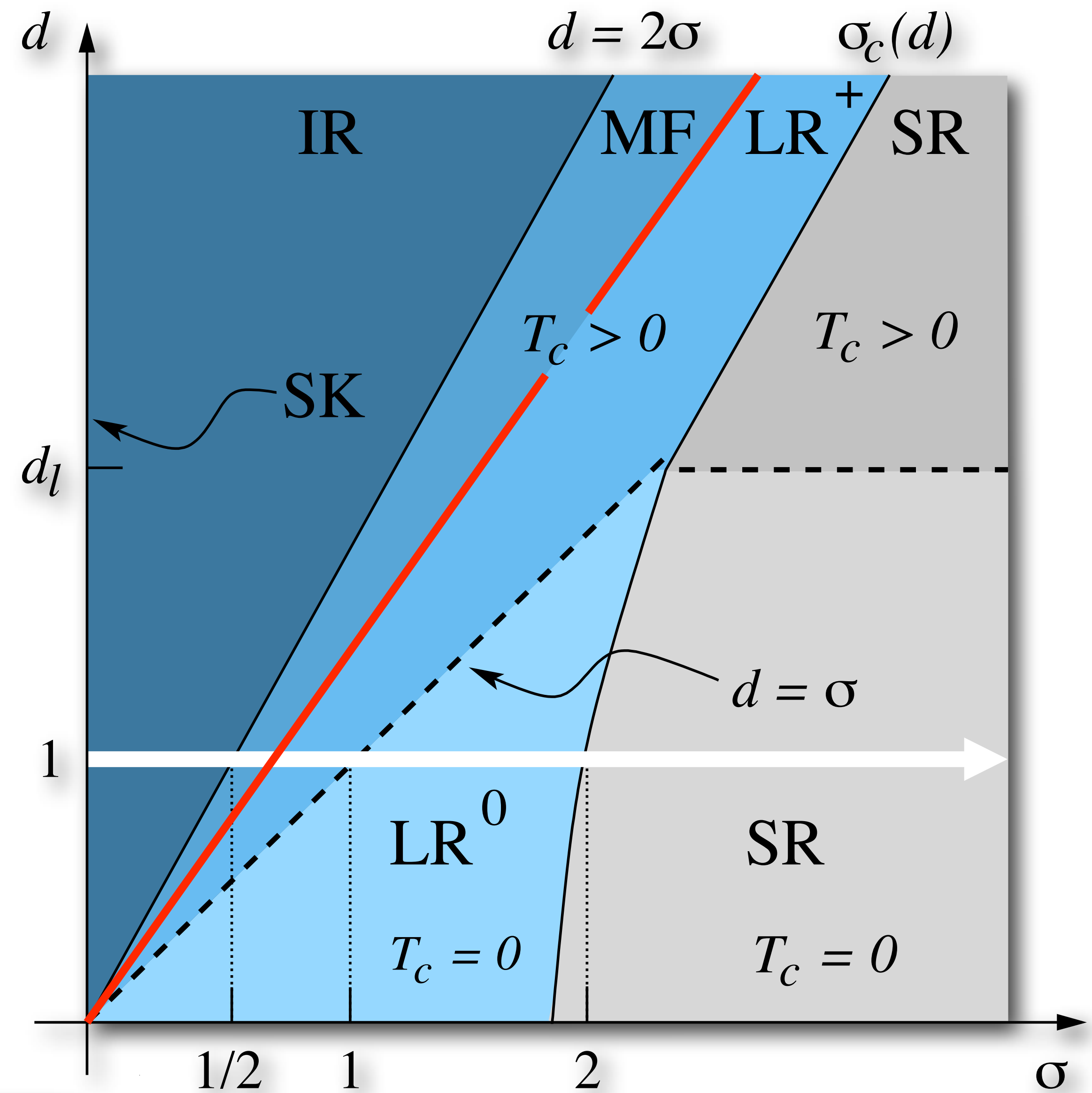

- Advantages:
  - Large range of sizes.
  - Tuning the power-law exponent changes the universality class.

large σ
small $d_{\rm eff}$

Fisher & Huse, PRB (88)
Kotliar et al., PRB (83)

Tuning the universality class

- Short-range spin glasses:
  - Upper critical dimension $d_u = 6$ (for $d \geq d_u$ MF behavior)
  - Lower critical dimension $d_l = 2$ (for $d \leq d_l$ $T_c = 0$)

$$d_{\mathrm{eff}} \approx \frac{2}{2\sigma - 1}$$

- Phase diagram of the 1D chain:

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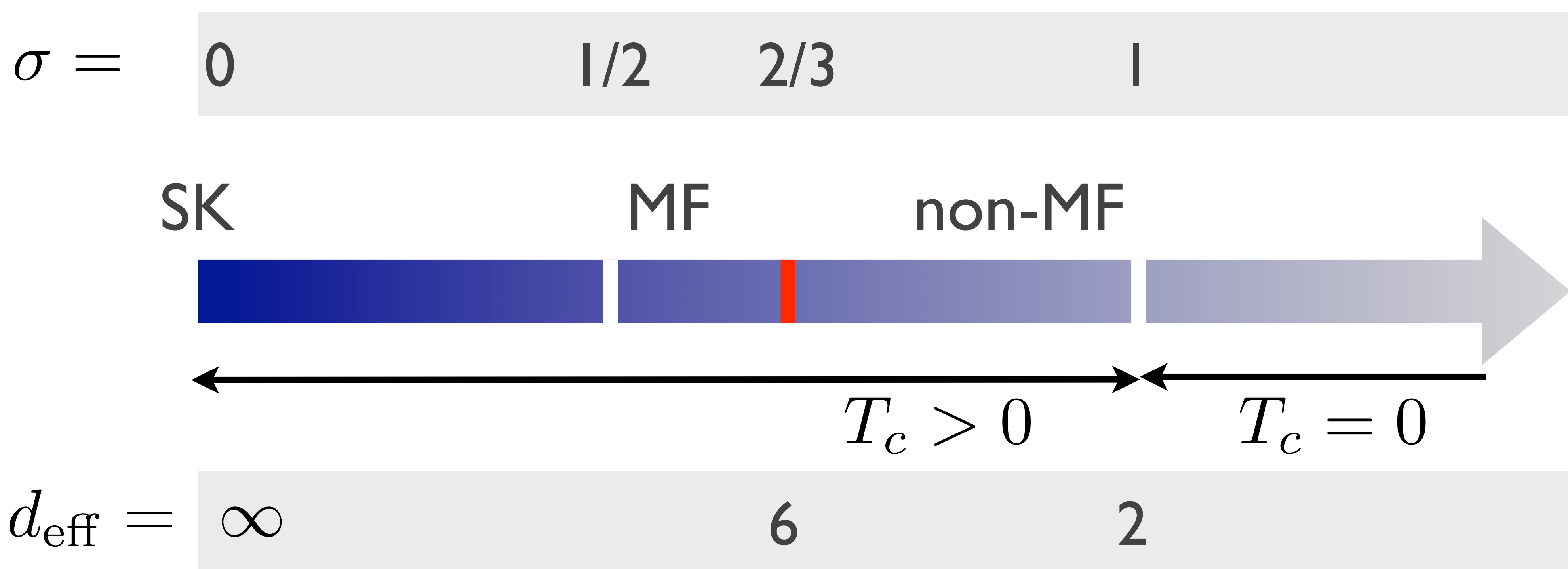

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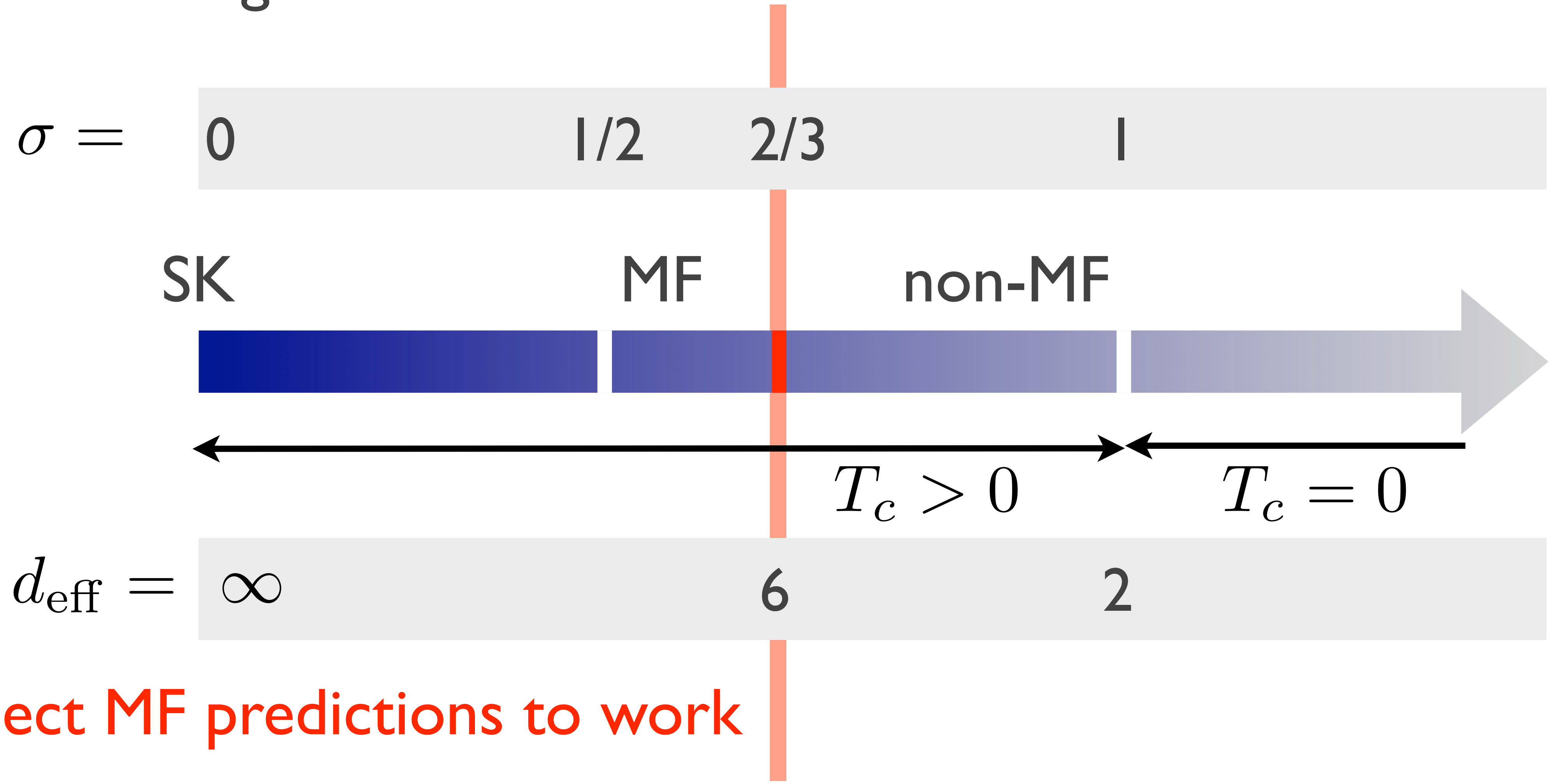


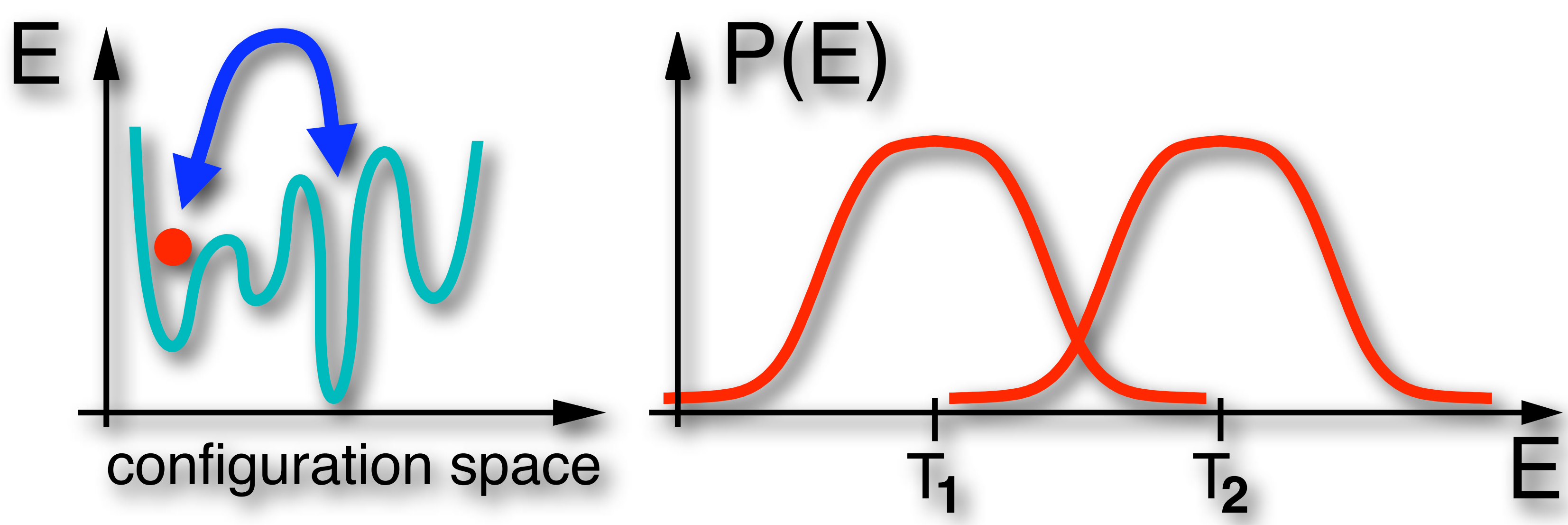
expect MF predictions to work

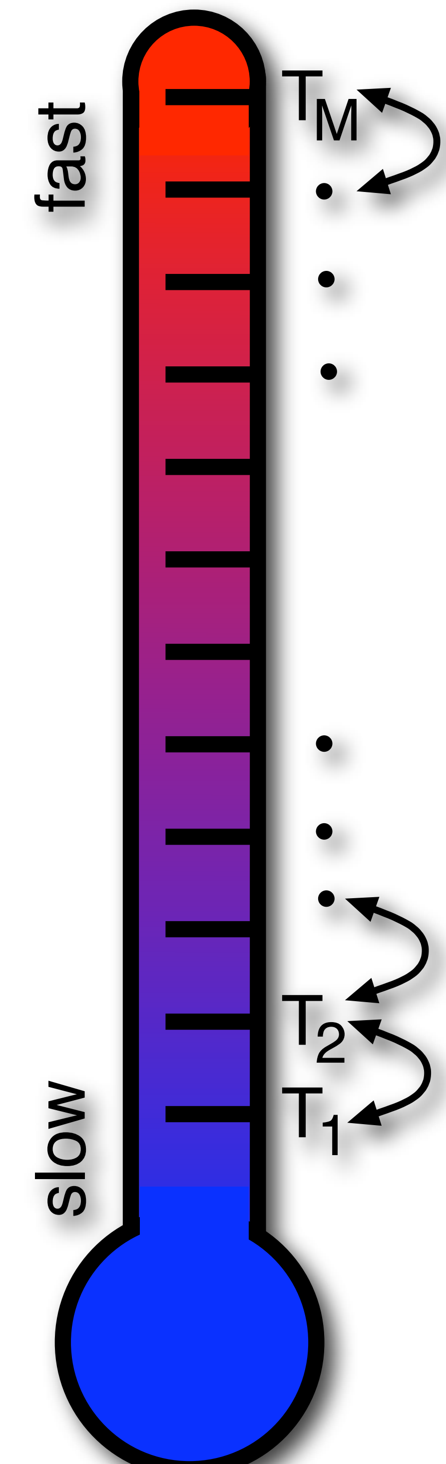
Algorithms

Reminder: Exchange Monte Carlo

Hukushima & Nemoto (96)

- Efficient algorithm to treat spin glasses at finite *T*.
- Idea:
  - Simulate *M* copies of the system at different temperatures with $T_{max} > T_c$ (typically $T_{max} \sim 2T_c^{MF}$).
  - Allow swapping of neighboring temperatures: easy crossing of barriers.



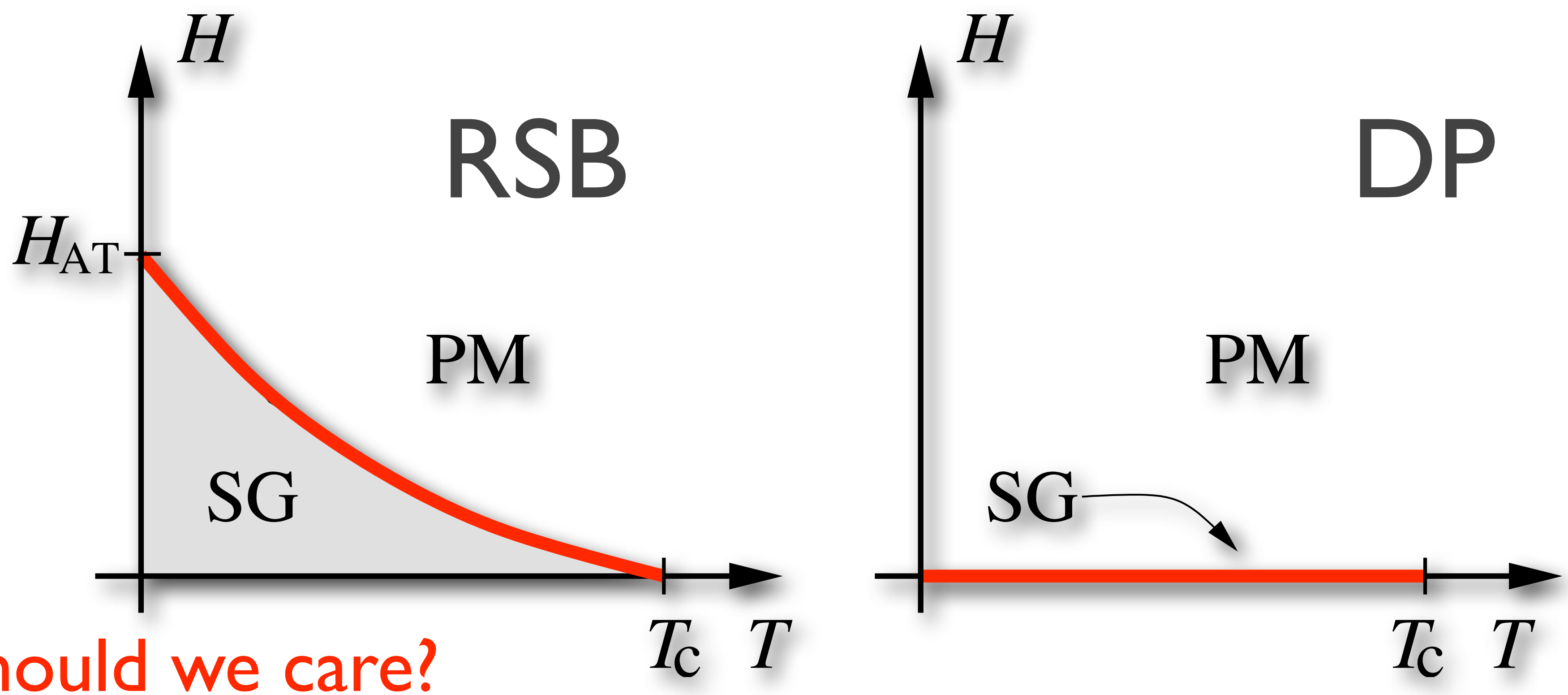


- Extremely fast equilibration at low temperatures.
- For the following applications we use this algorithm...

Do spin glasses order in a field?

Spin-glass state in a field?

- Two possible scenarios:
  - Replica Symmetry Breaking (RSB): existence of an instability line [Almeida & Thouless (78)] for the mean-field SK model.
  - Droplet picture (DP): there is no spin-glass state in a field.



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  - The question lies at the core of theoretical descriptions.
  - Field terms are ubiquitous in applications/experiments.
  - Experimentally, numerically, and theoretically controversial.

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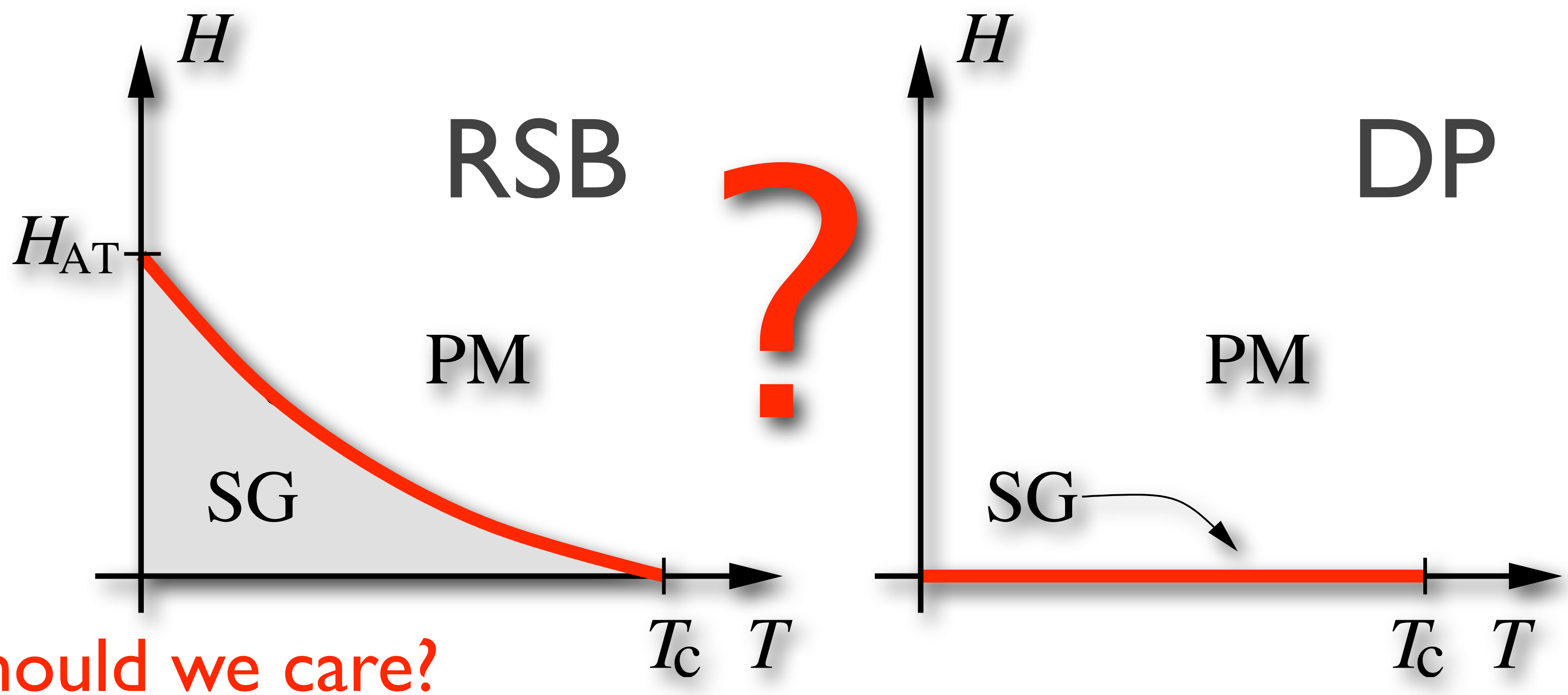

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Spin-glass state in a field?

Outline:
1. Tool to probe transition
2. Review of old 3D results
3. Improved results in 1D

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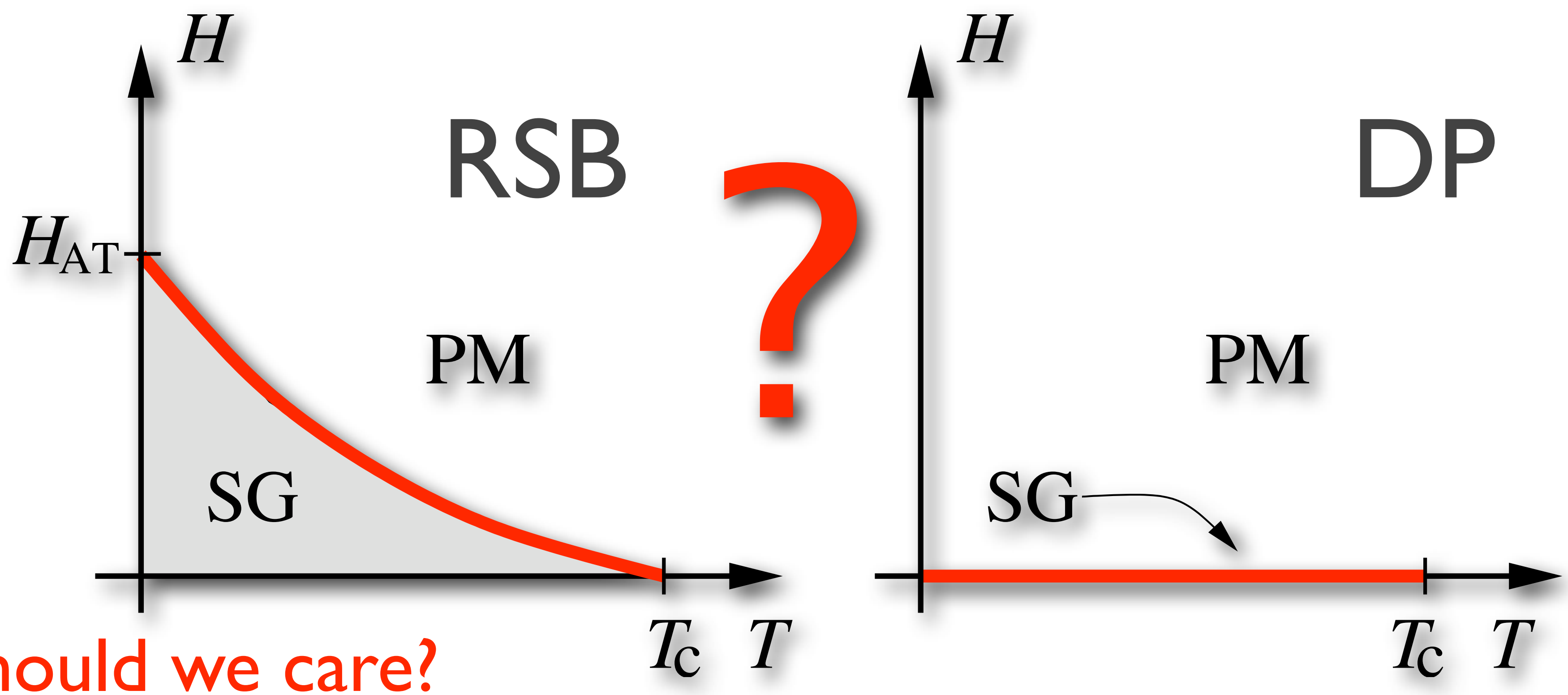

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Probing criticality: correlation length

Ballesteros *et al.* PRB (00)

- Use the finite-size correlation length to probe criticality in spin-glass systems:
  - Wave-vector-dependent connected spin-glass susceptibility:

$$\chi_{\rm SG}(\mathbf{k}) = \frac{1}{N}\sum_{ij}\left[\left(\langle S_i S_j\rangle_T - \langle S_i\rangle_T\langle S_j\rangle_T\right)^2\right]_{\rm dis} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}$$

  - Perform an Ornstein-Zernicke approximation:

$$[\chi_{\rm SG}(k)/\chi_{\rm SG}(0)]^{-1} = 1 + \xi_L^2 k^2 + \mathcal{O}[(\xi_L k)^4]$$

  - Compensate for finite-size effects and periodic boundaries:

$$\xi_L = \frac{1}{2\sin(k_{\rm min}/2)}\left[\frac{\chi_{\rm SG}(0)}{\chi_{\rm SG}(k_{\rm min})} - 1\right]^{1/2}$$

  - Finite-size scaling: $\frac{\xi_L}{L} = \tilde{X}\left(L^{1/\nu}[T - T_c]\right)$
  - Better than Binder ratio.

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How well does this work for zero field?

Katzgraber et al., PRB (06)

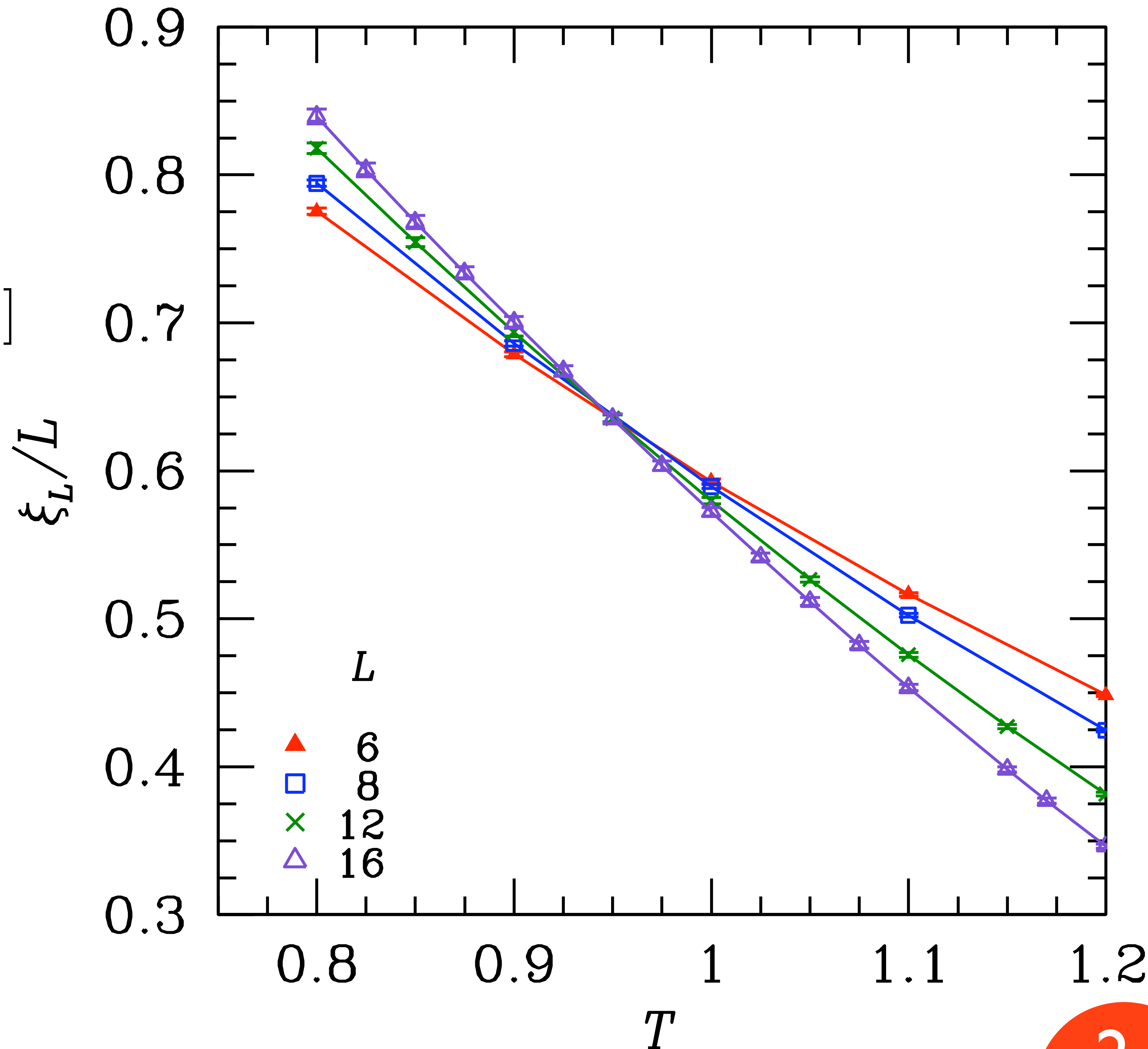
- Study the 3D model:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j$$

- Remember:

$$\frac{\xi_L}{L} = \tilde{X}[L^{1/\nu}(T - T_c)]$$

- The data cross at $T_c \approx 0.96$.
- Spin-glass state at zero field.
- Next: apply a field…



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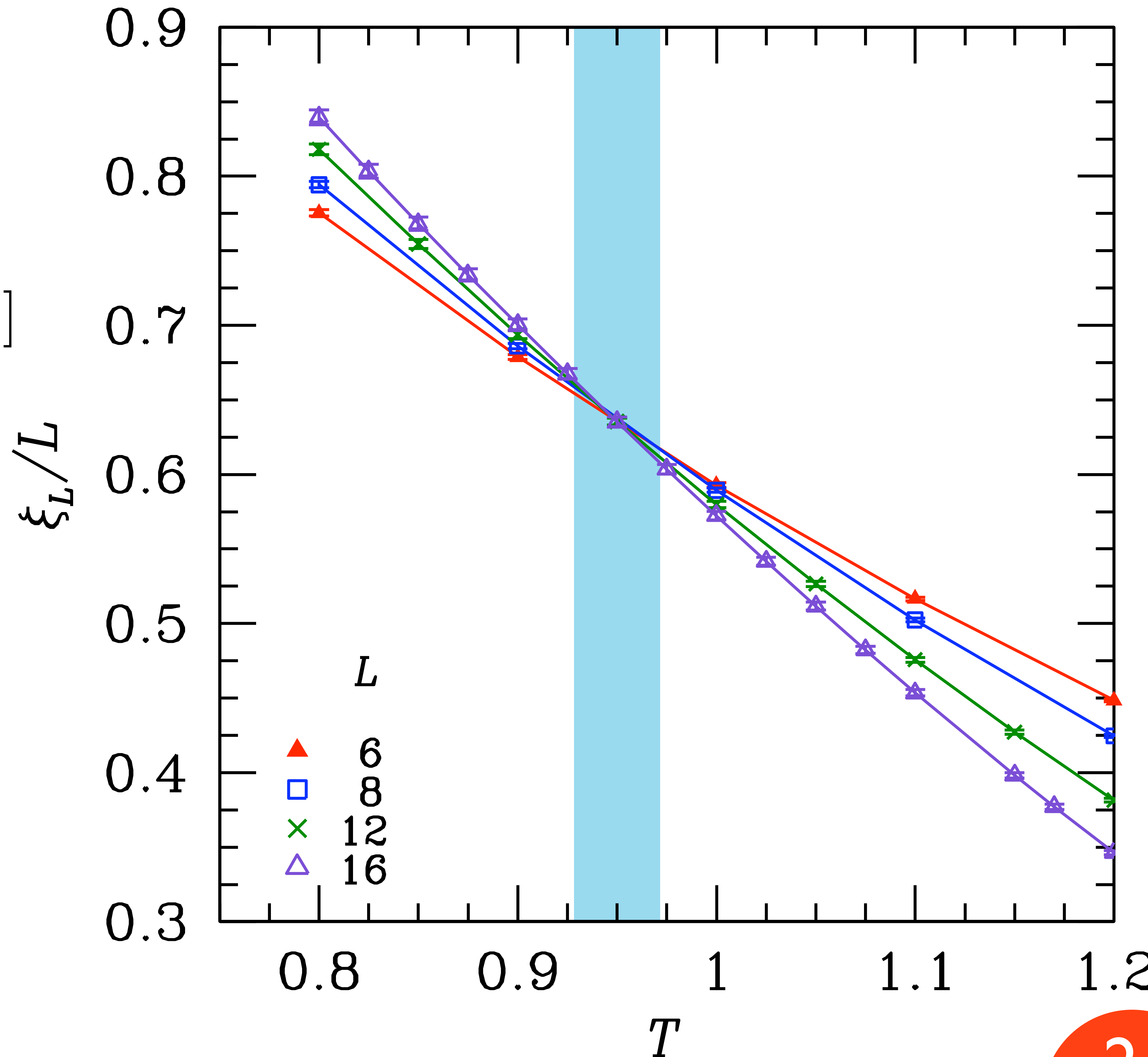

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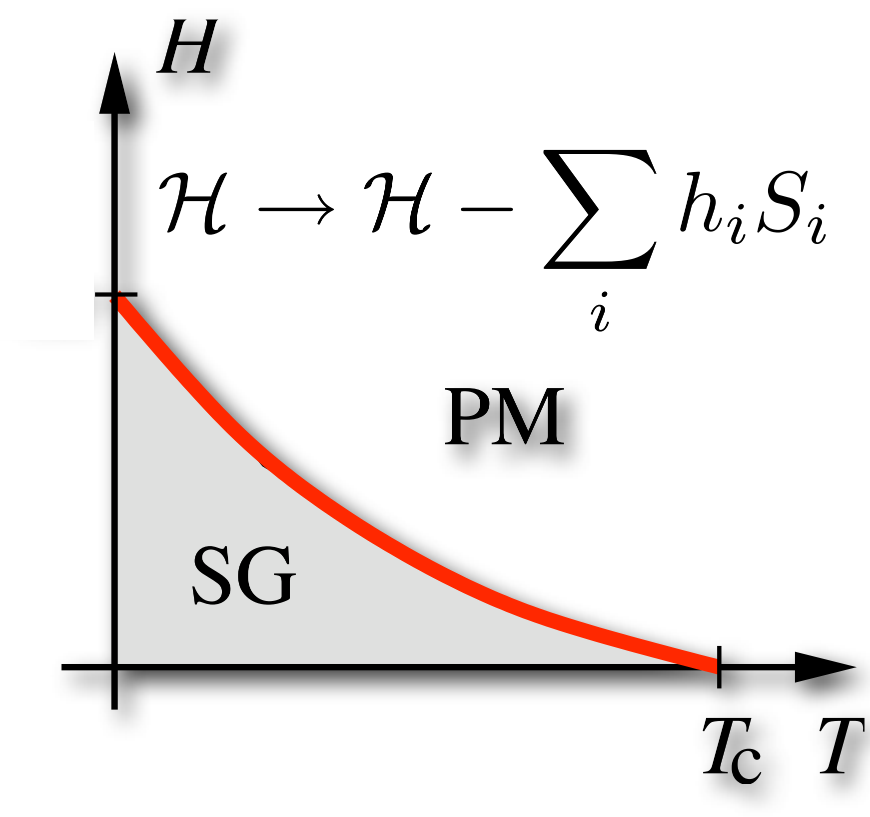
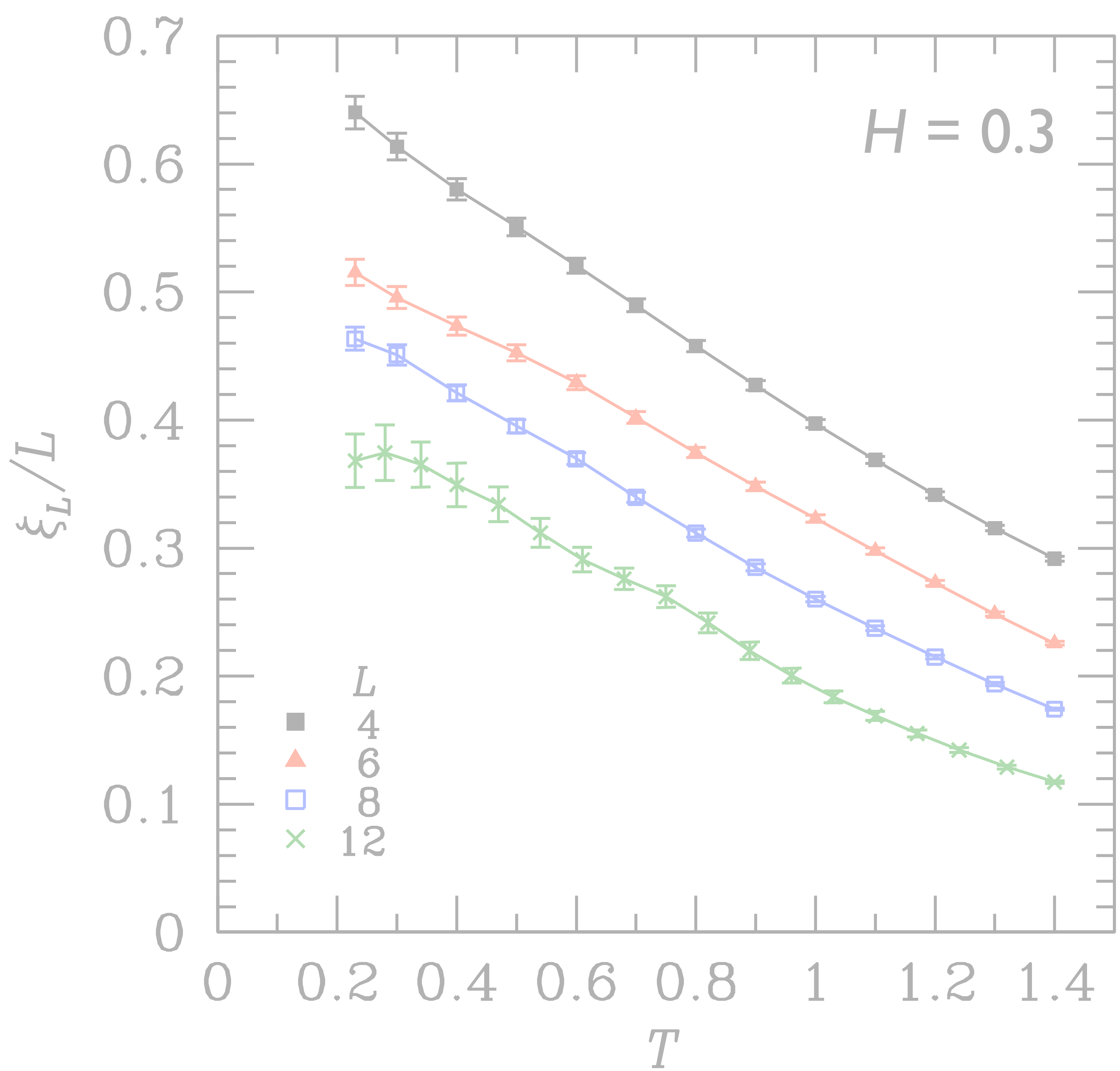
2.

"Old" 3D results in a field

Katzgraber & Young, PRL (04)

- Perform "slices" at different horizontal fields.





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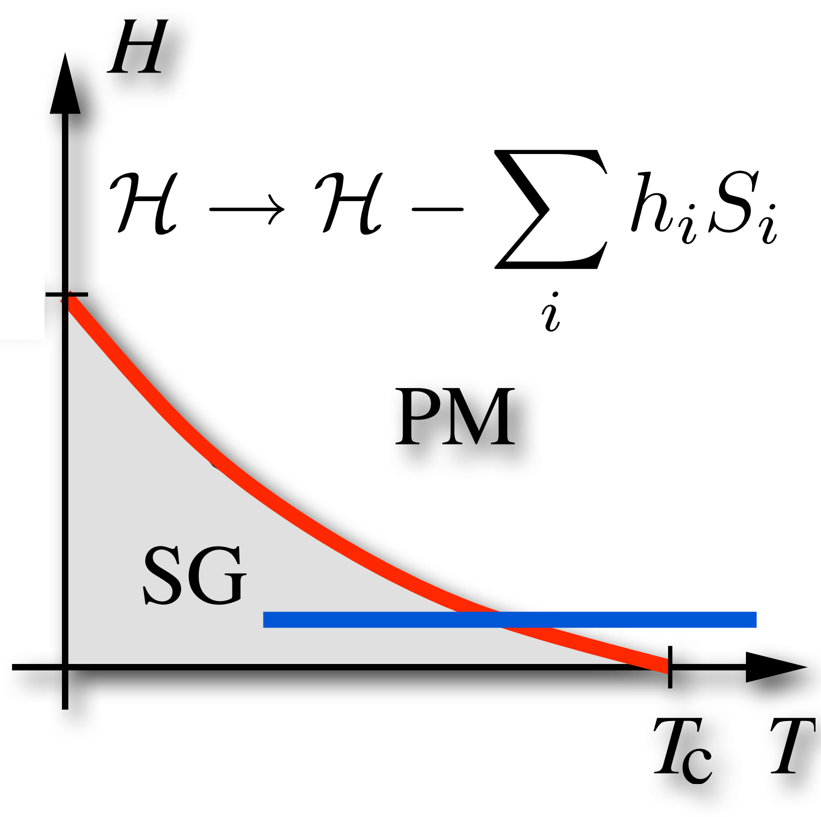

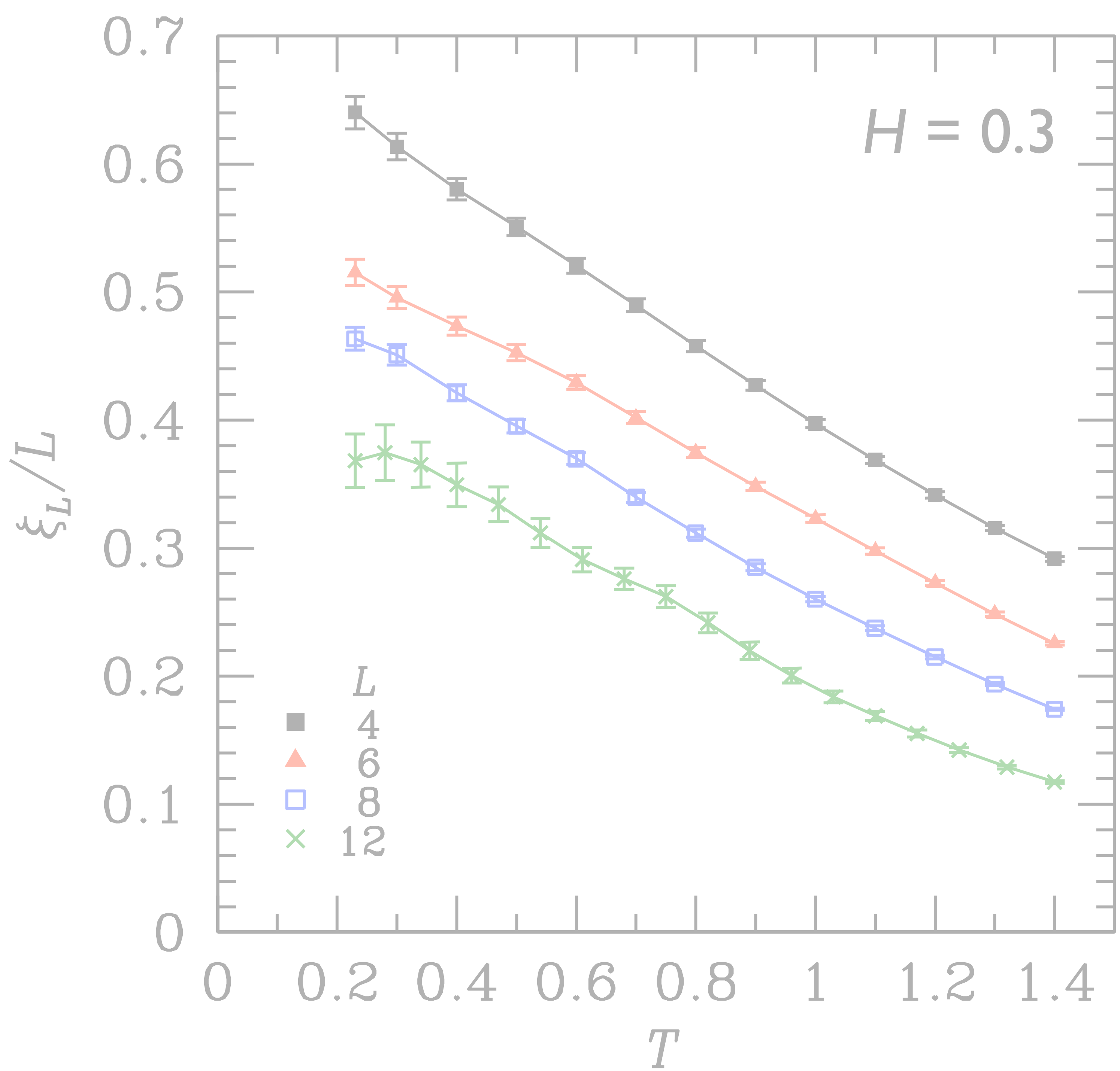

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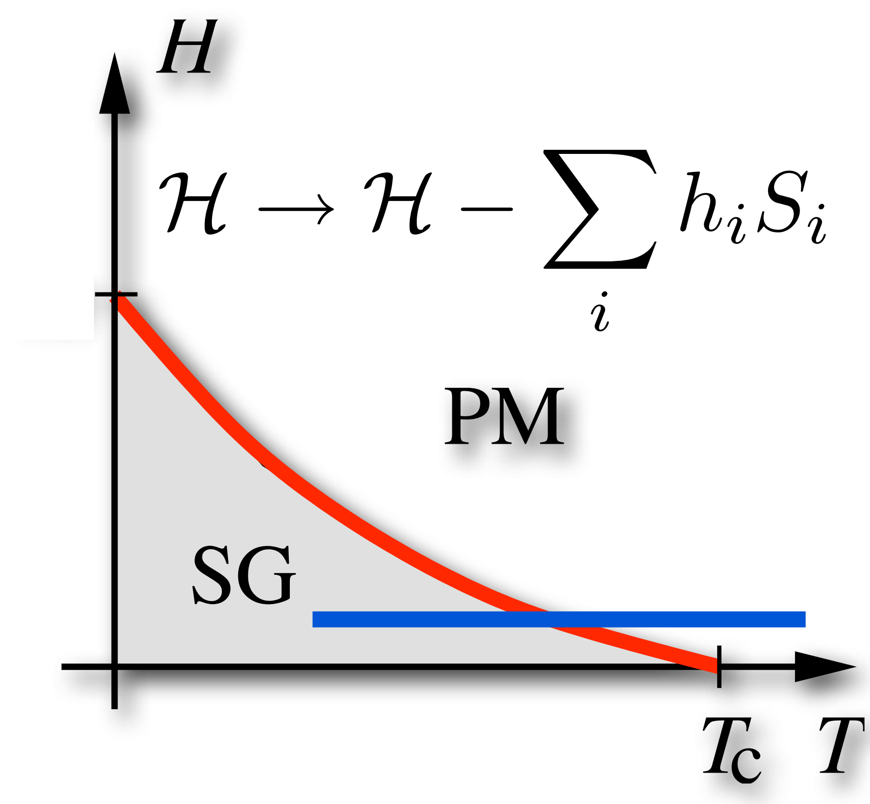

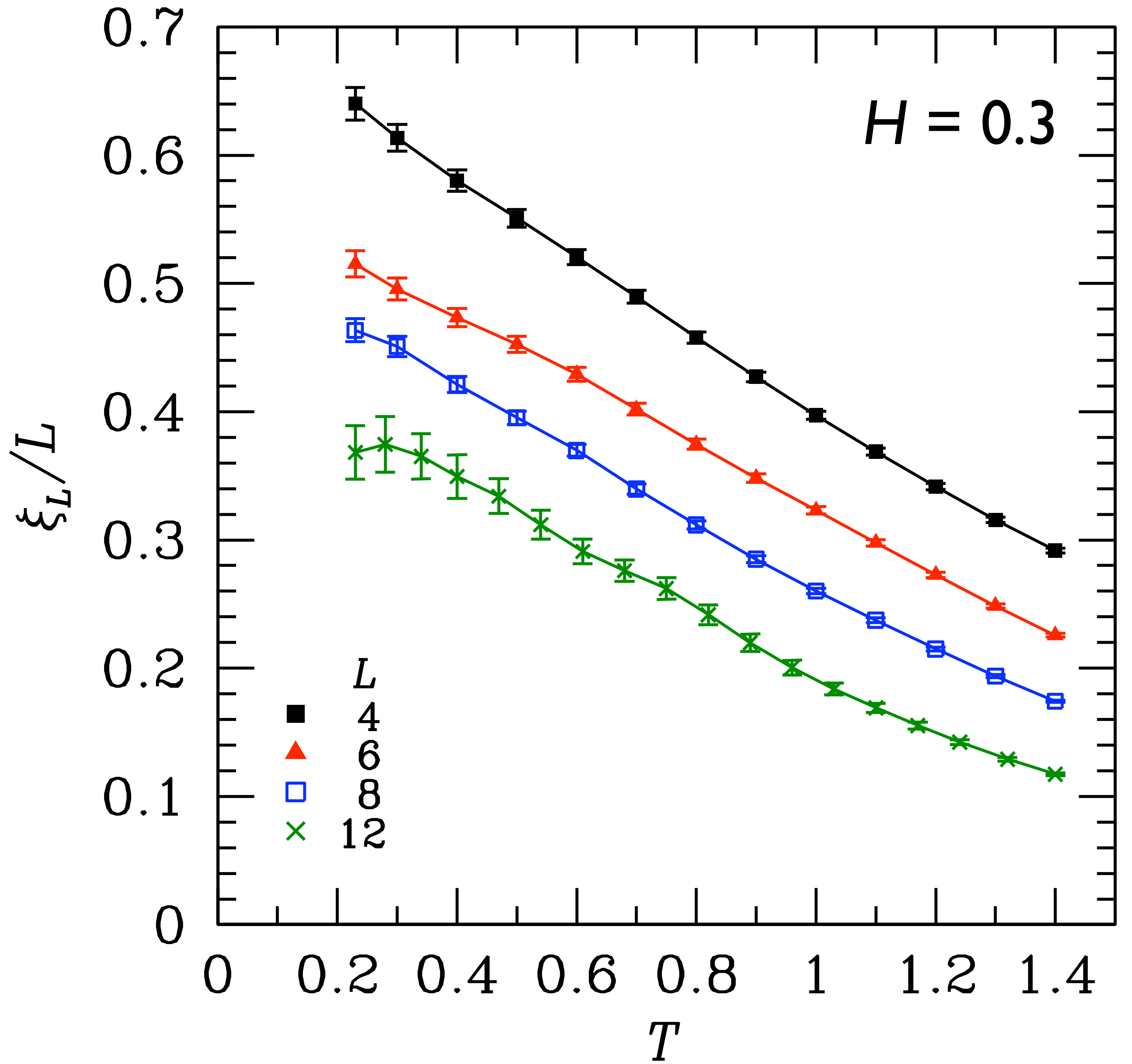

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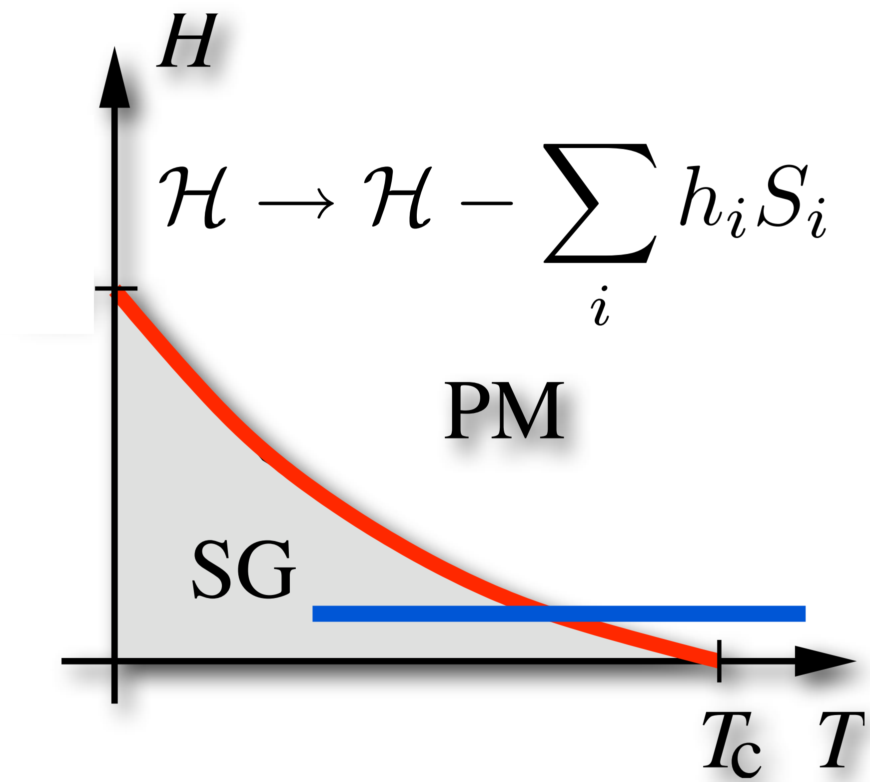

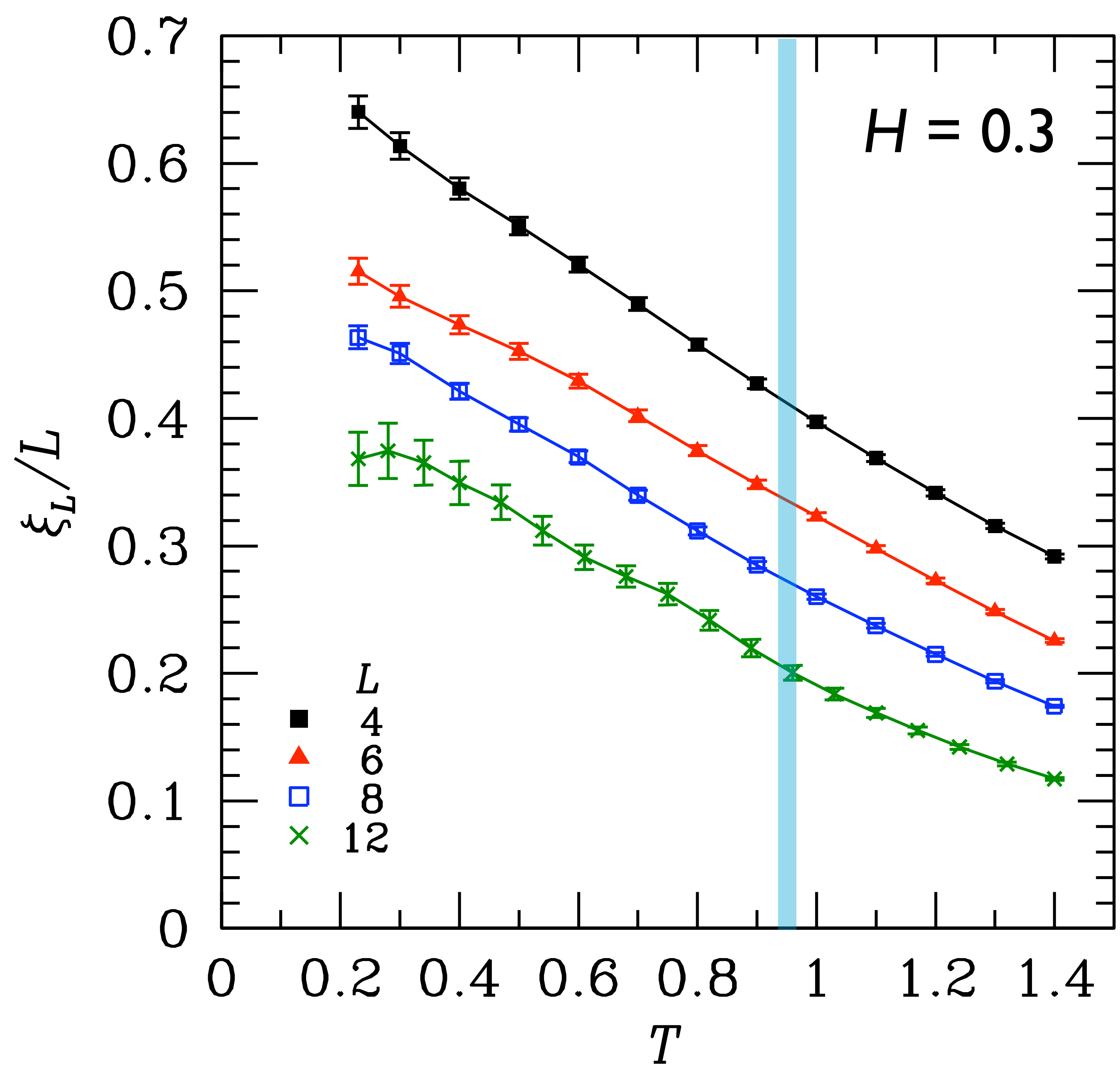

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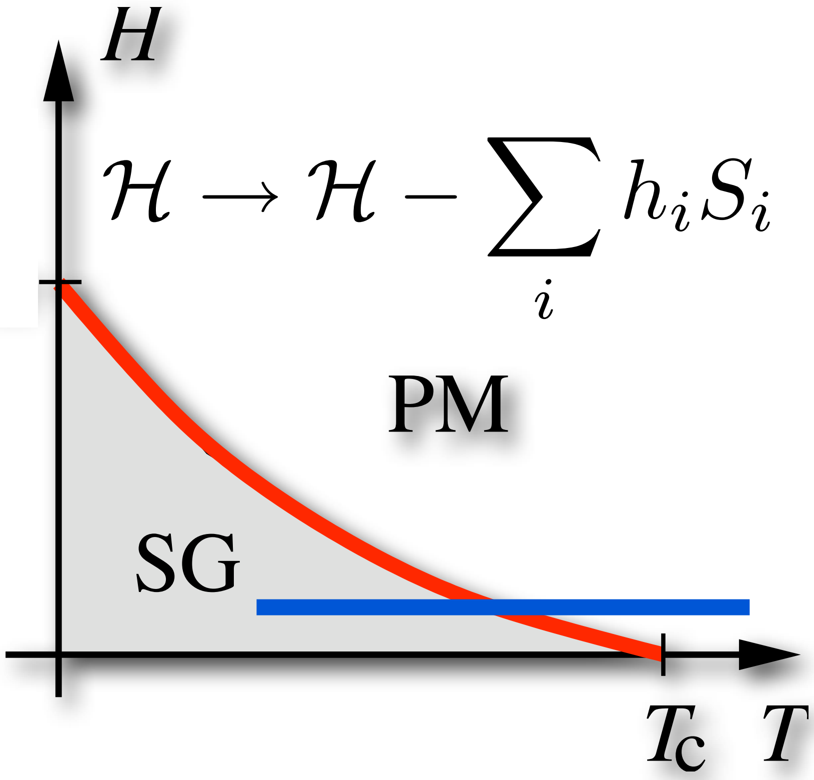

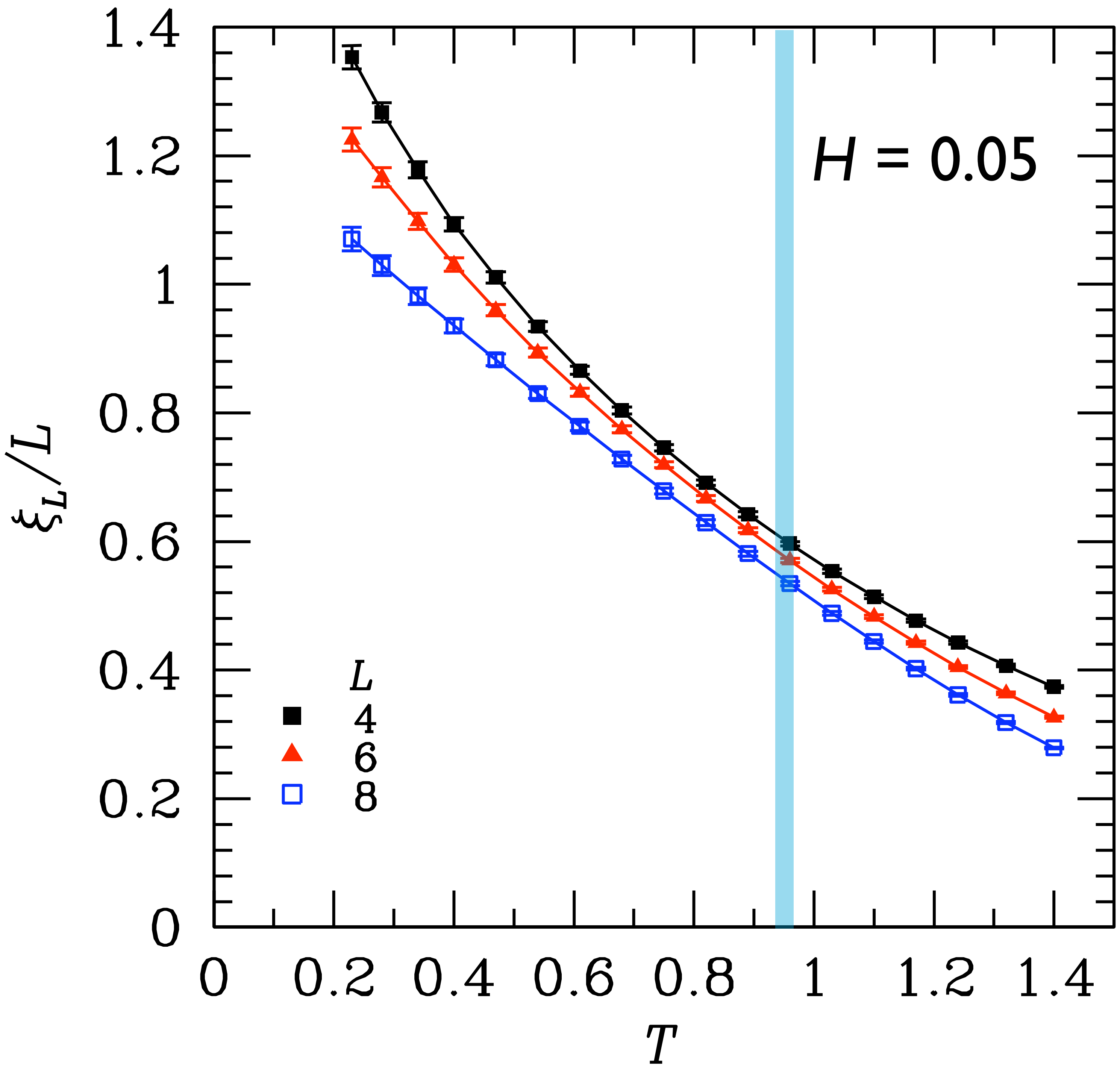

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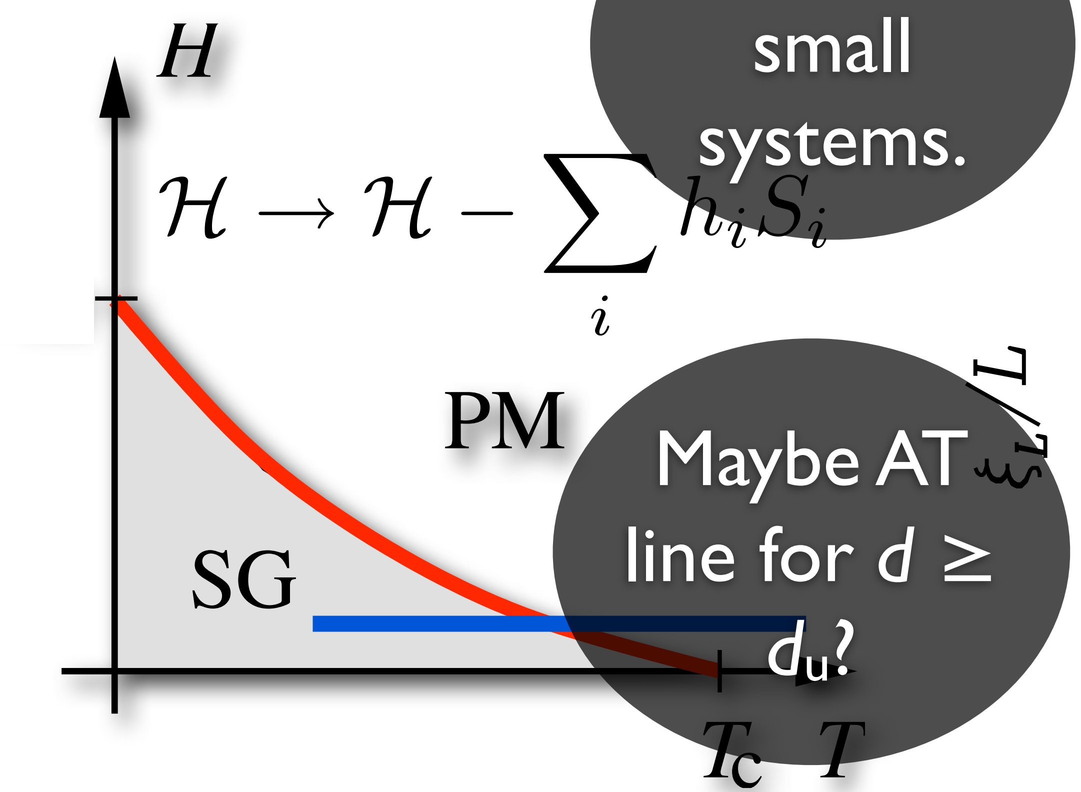

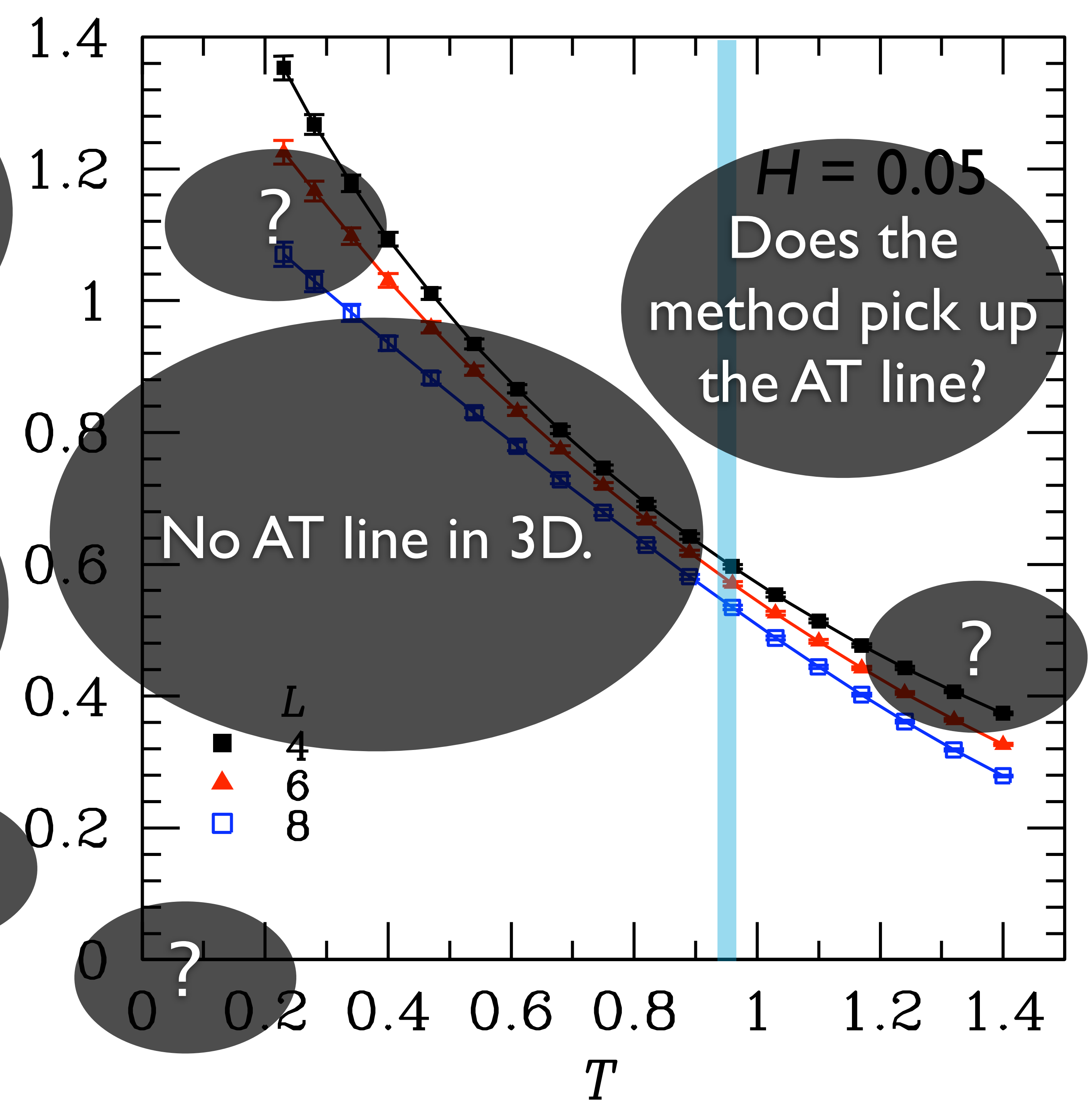

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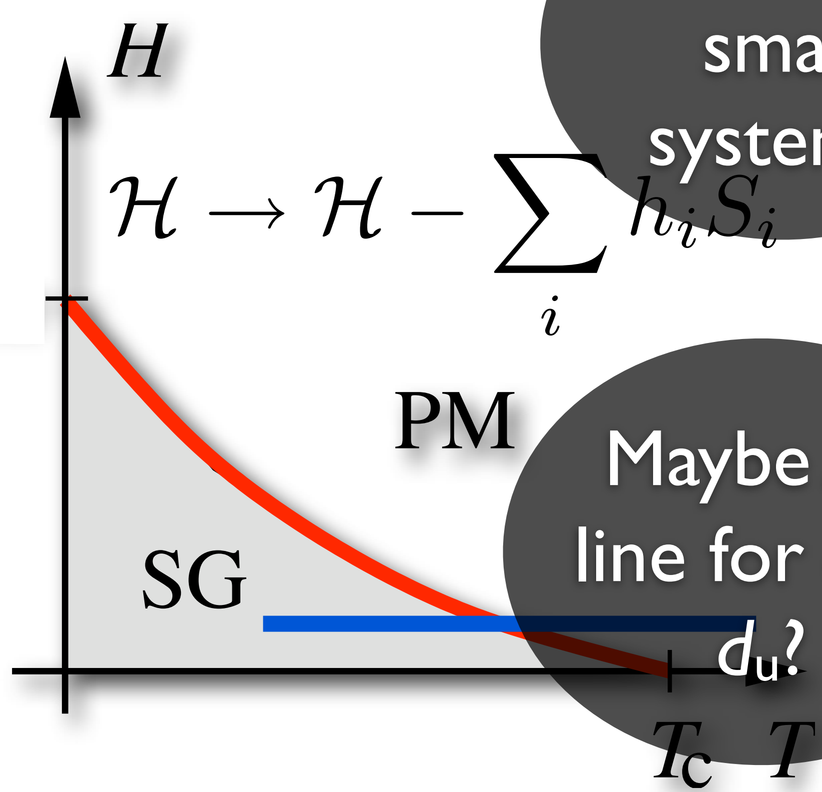
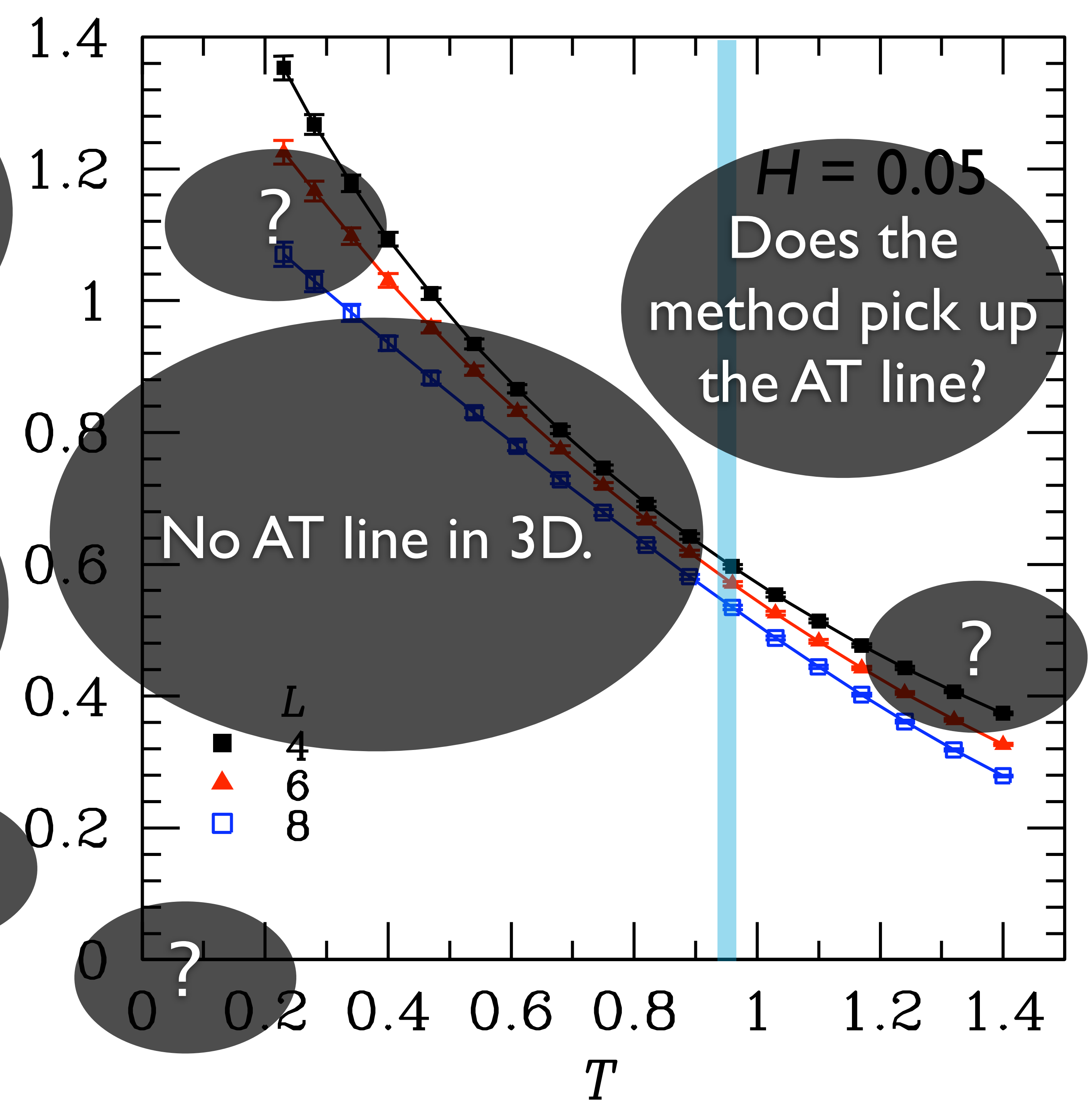


Problem: small systems.

Maybe AT line for $d \geq d_u$?

?



Does the method pick up the AT line?

No AT line in 3D.

?

?

?

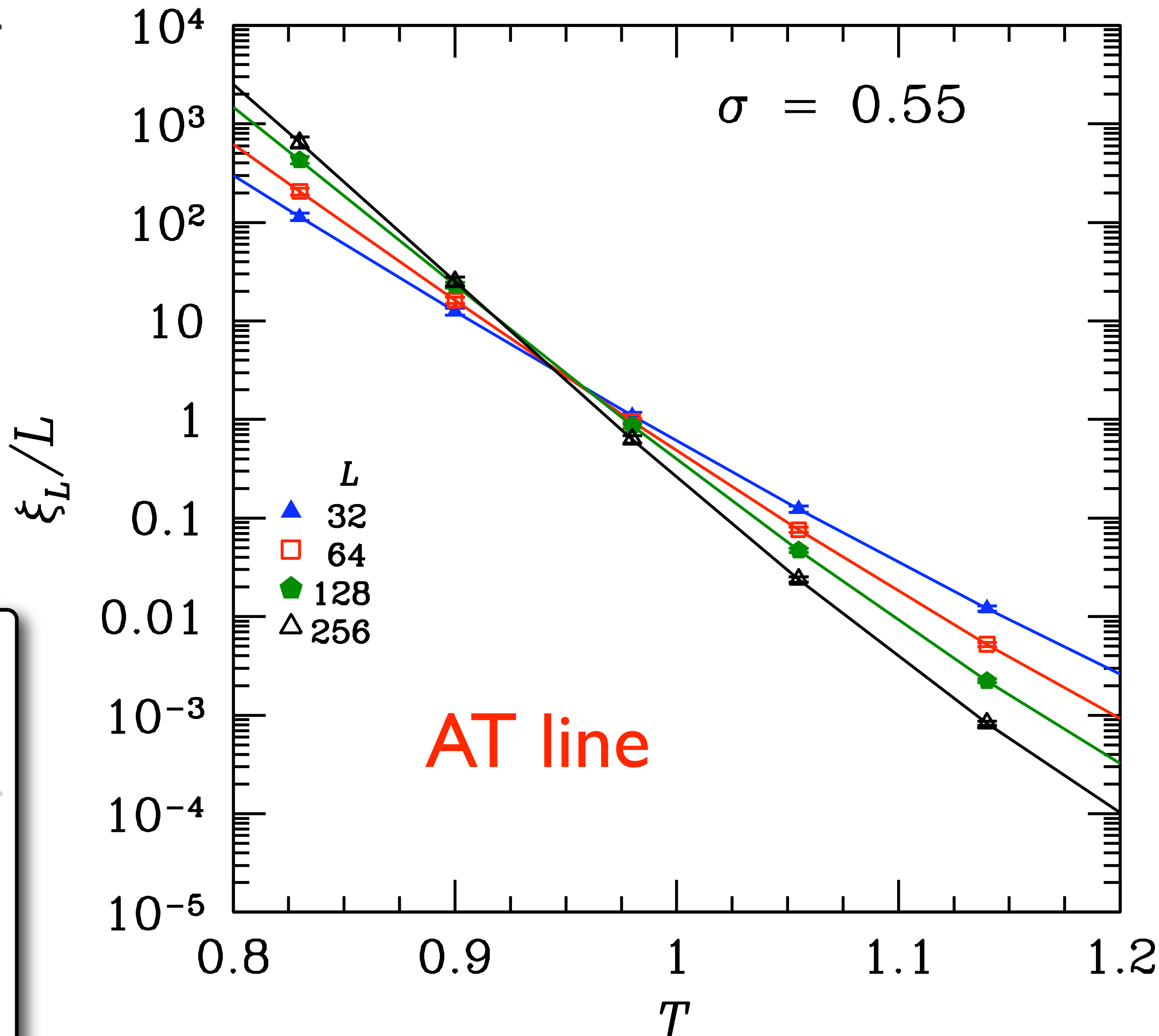
- Solution: Use 1D chain
  - Can probe large systems.
  - Can probe MF region to check if the method works.

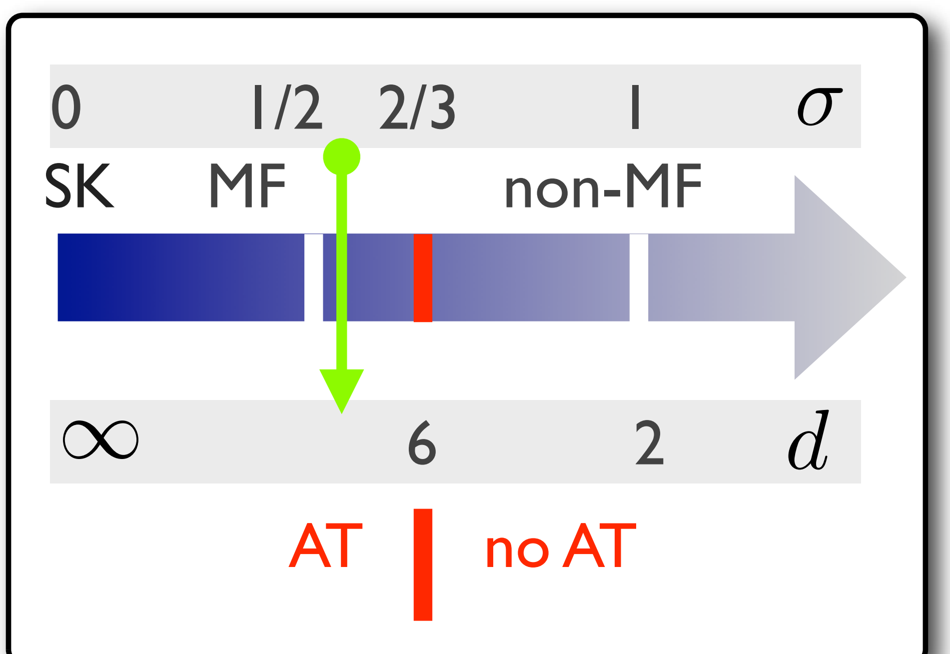
2.

Tuning the universality class (1D chain)

Katzgraber & Young, PRB (2005)

- External field $H = 0.10$.
- The data span a large range of system sizes.
- The AT line vanishes outside the MF regime ($\sigma \geq 2/3$).





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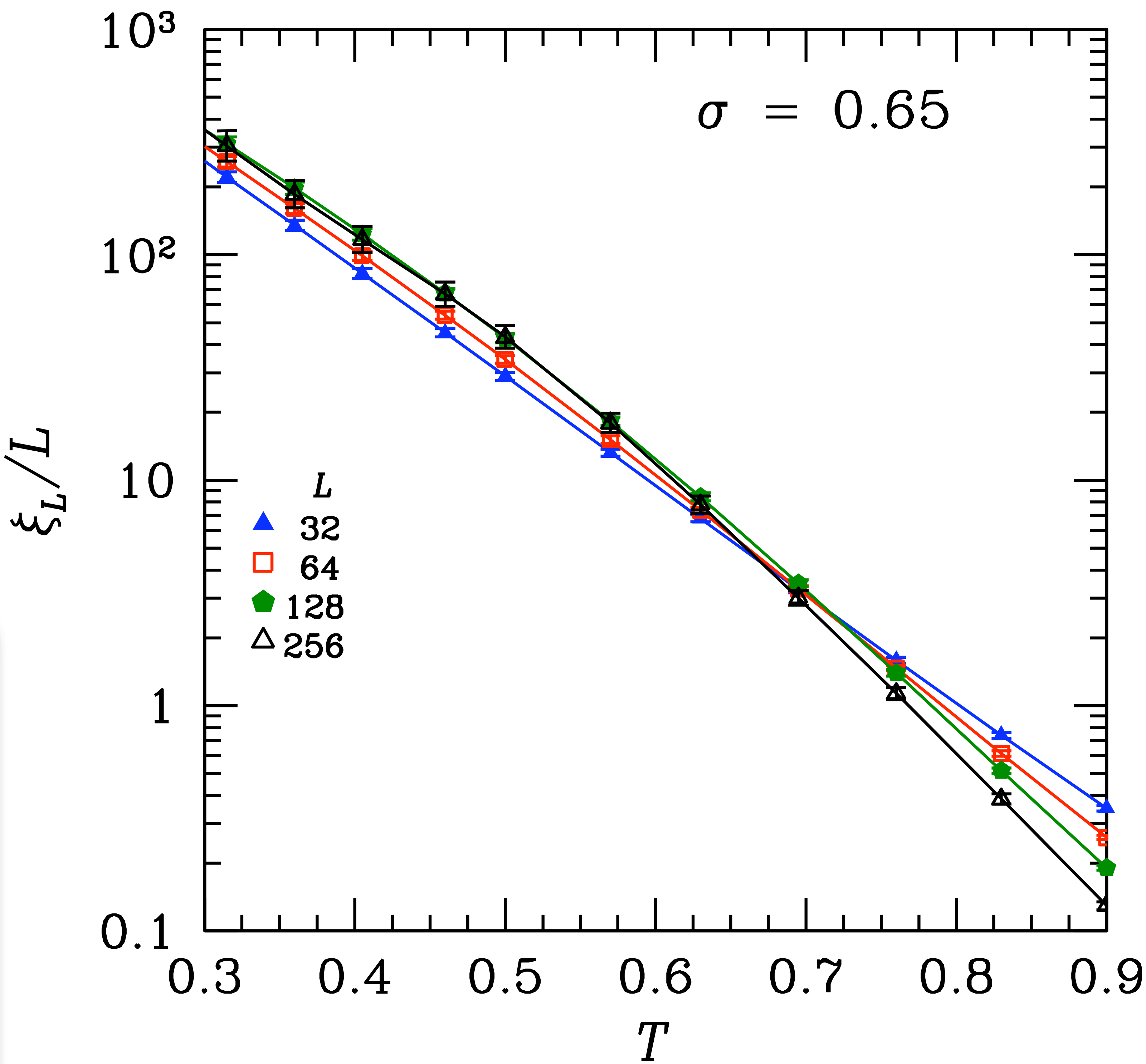

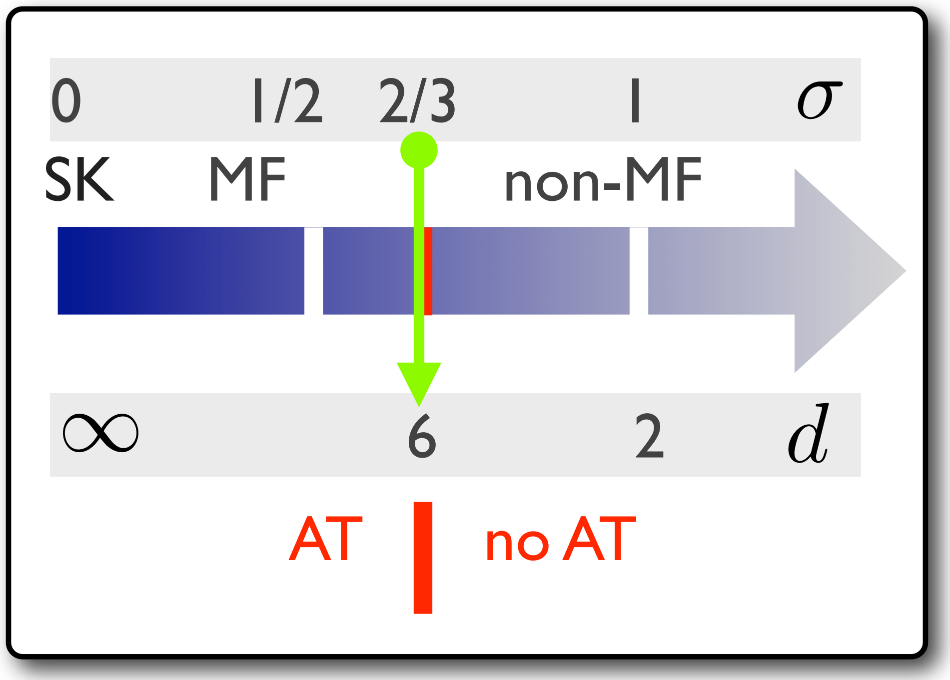

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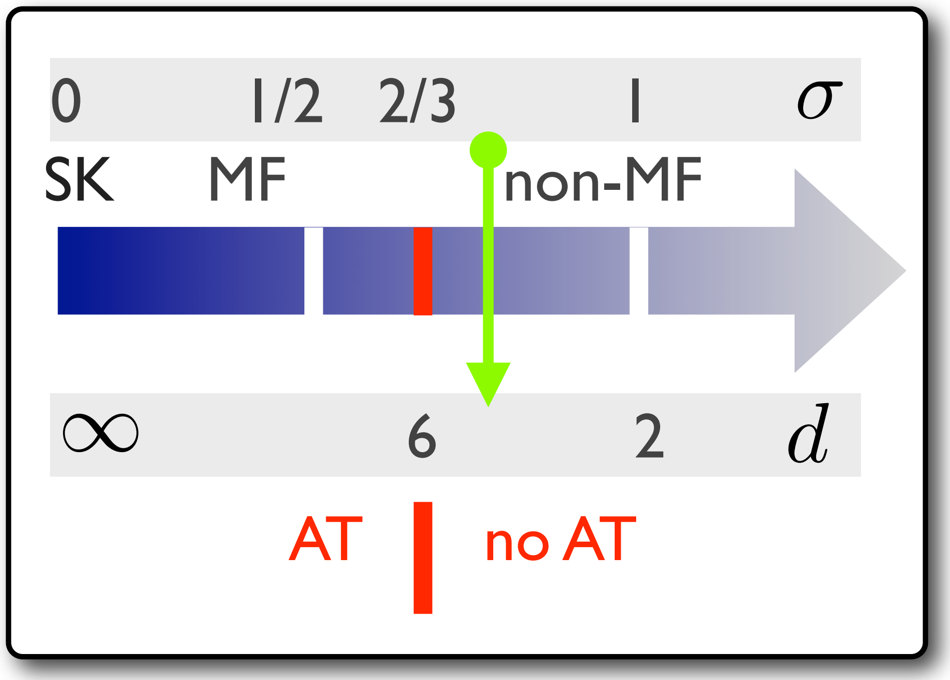

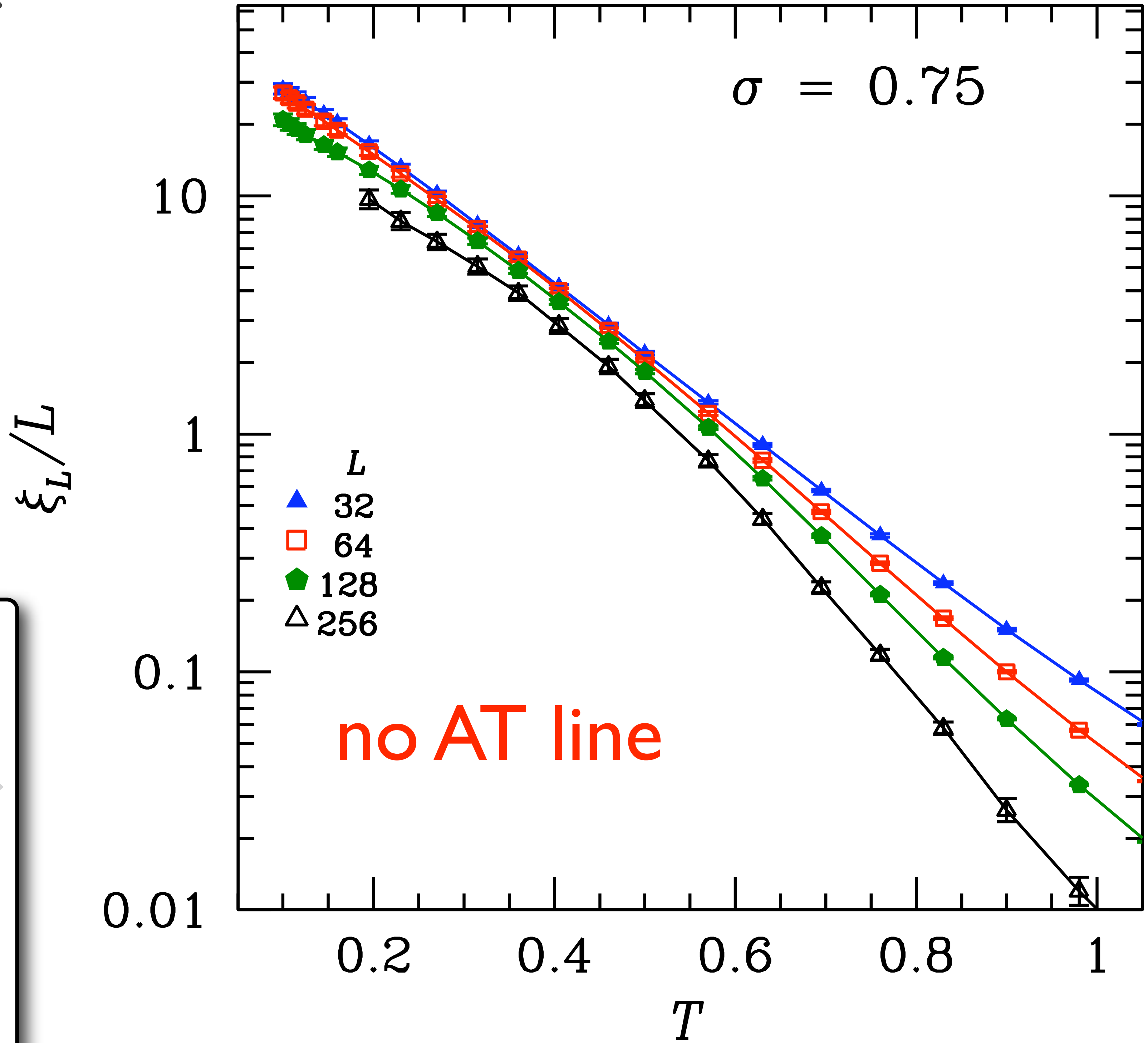

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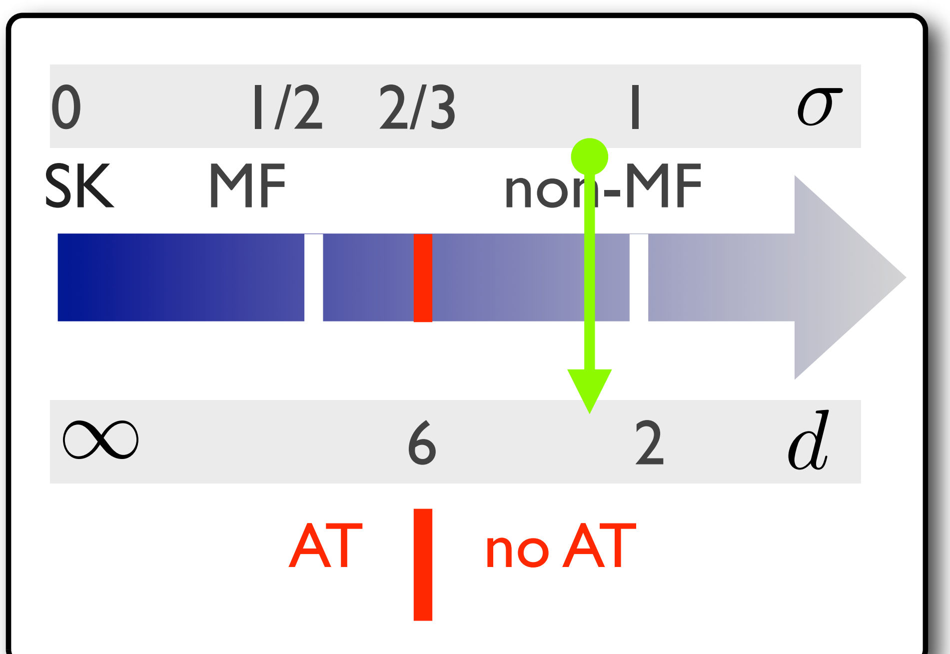

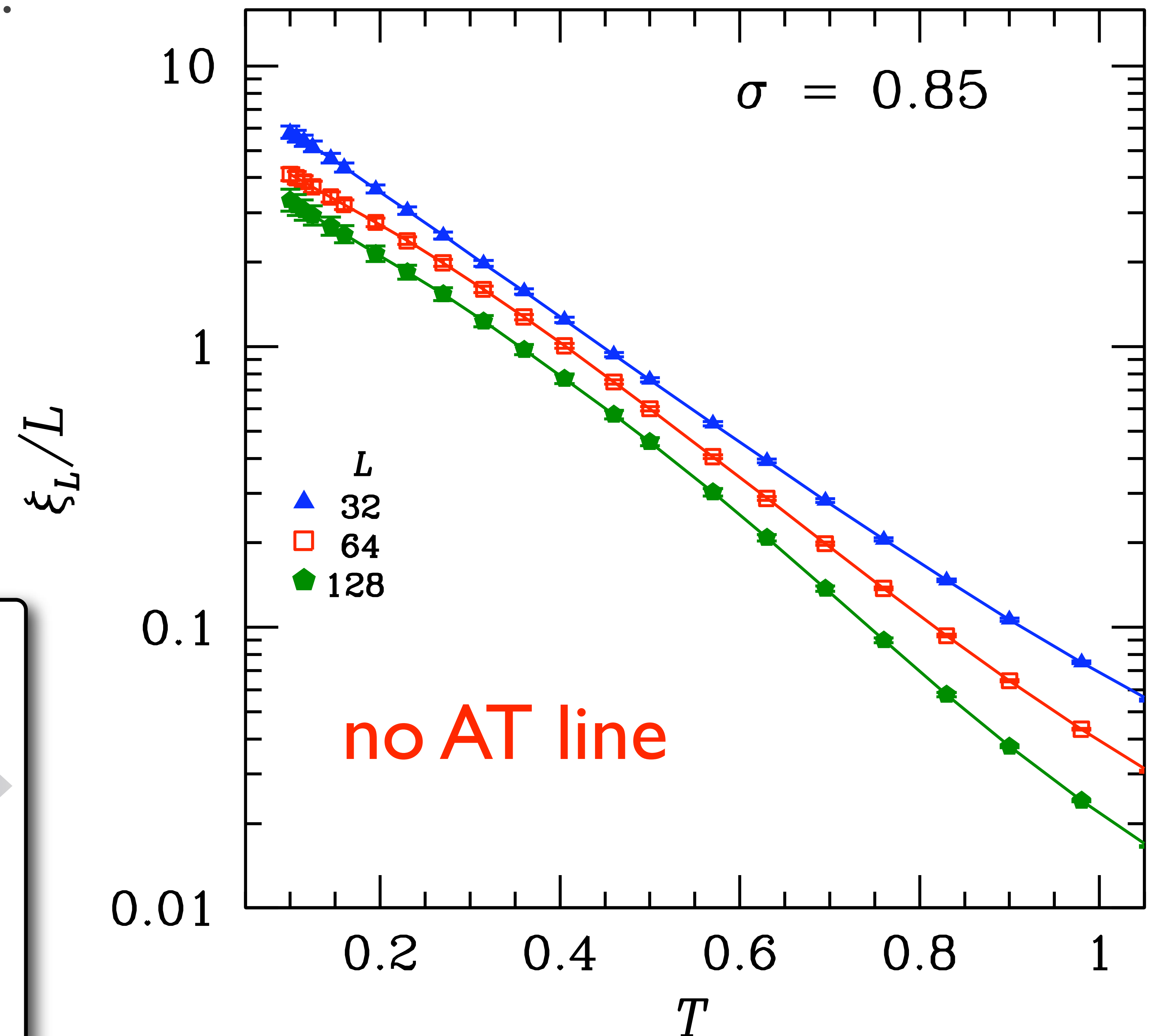

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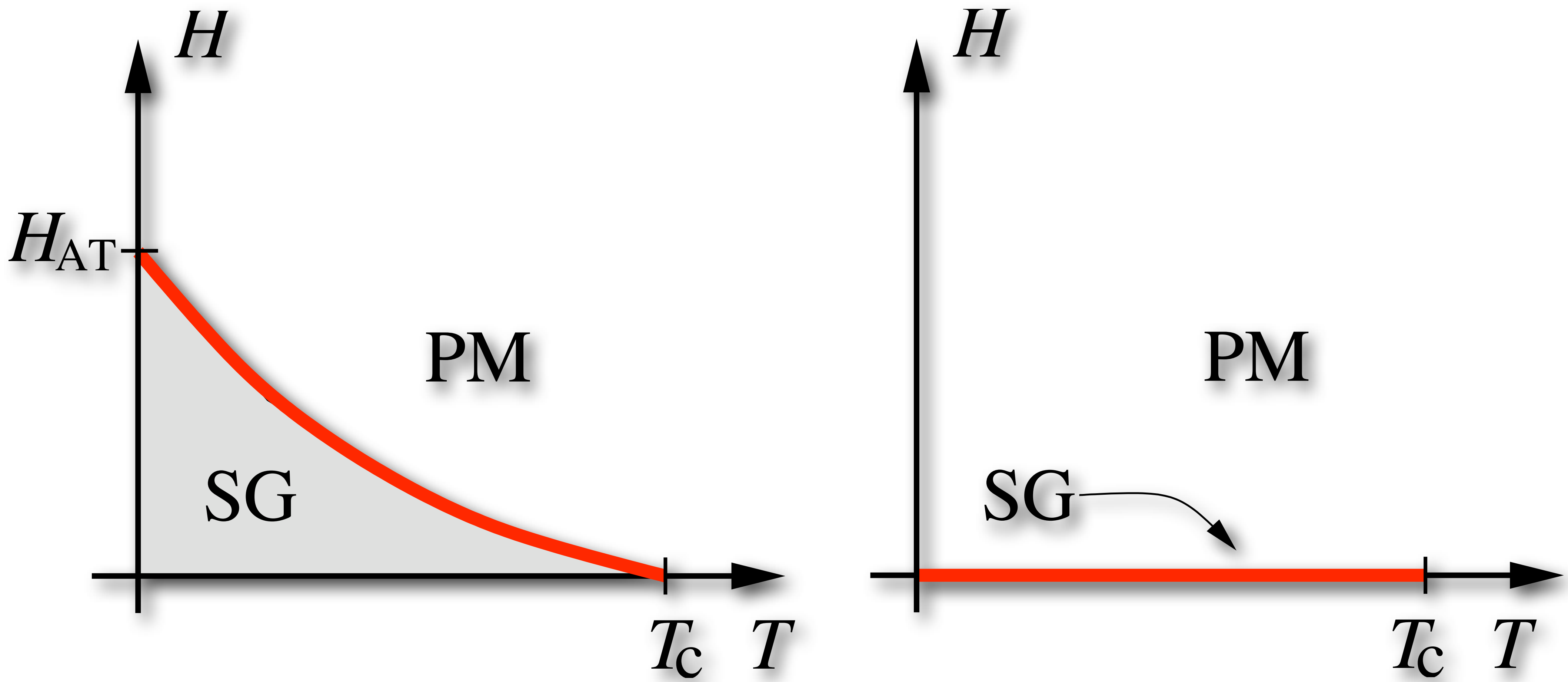
Spin-glass state in a field?

- The AT line vanishes when not in the mean-field regime.
- For short-range spin glasses below the upper critical dimension:



- Does the behavior change for even larger system sizes?
- What happens for "narrow" AT lines? (see cond-mat/0712.2009)

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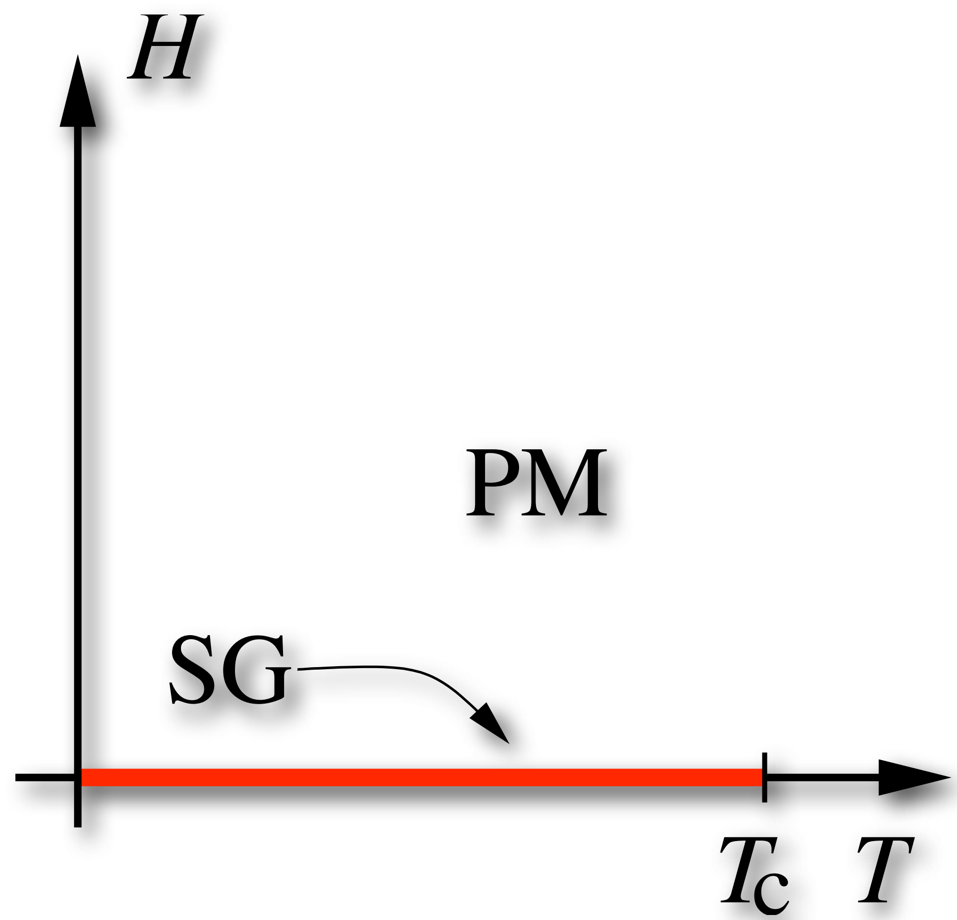

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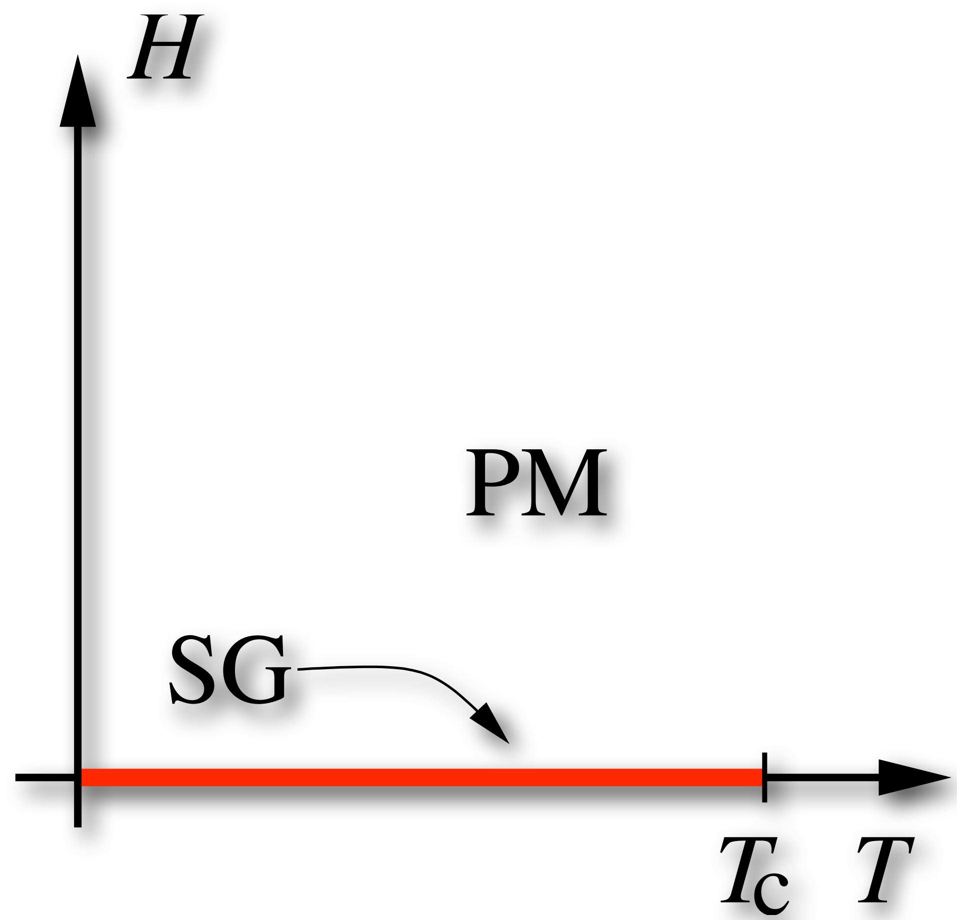

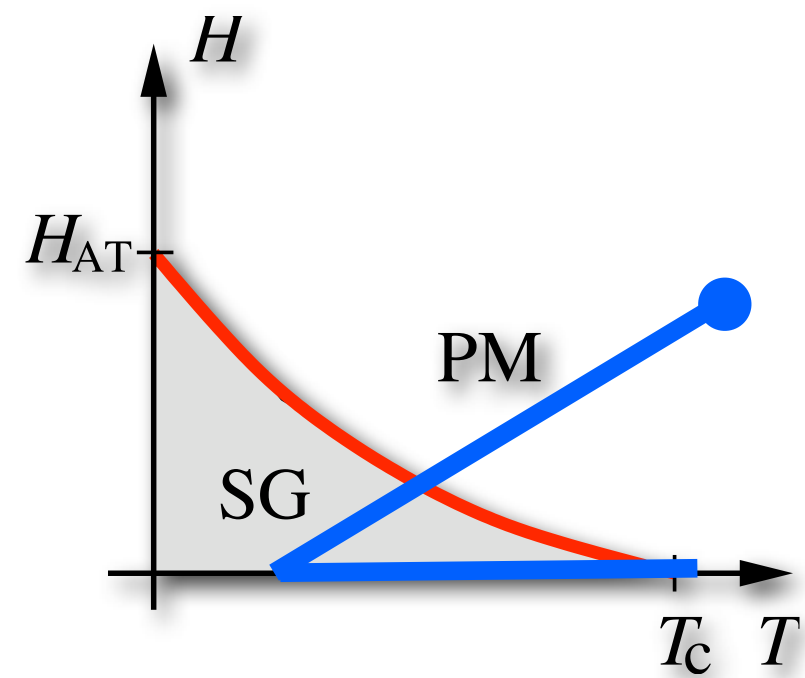

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Ultrametricity in spin glasses

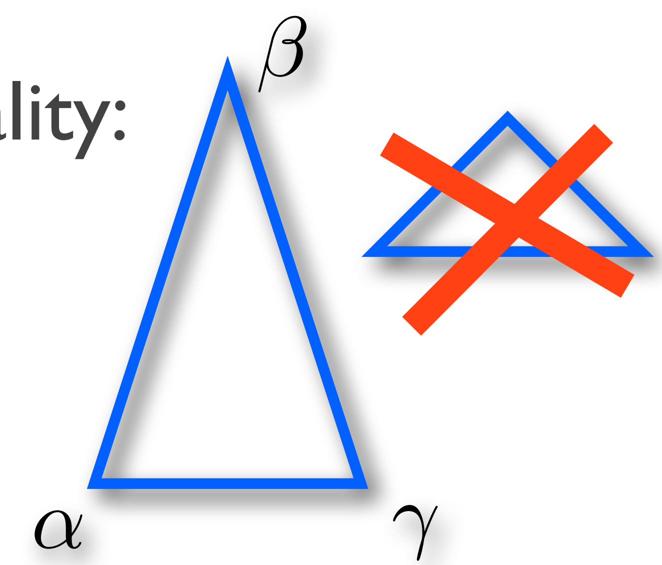
What is ultrametricity?

- Formal definition:
  - Given a metric space with a distance function.
  - In general, the distance function obeys the triangle inequality:

$$d(\alpha,\gamma) \leq d(\alpha,\beta) + d(\beta,\gamma)$$

  - In an ultrametric space we have a stronger inequality:

$$d(\alpha,\gamma) \leq \max\{d(\alpha,\beta), d(\beta,\gamma)\}$$



- Note:
  - Every triangle is isosceles in an ultrametric space.
- Examples:
  - Linguistics (space where words differ)
  - Taxonomy (classification of species).
  - Number theory (p-adic numbers), ...

What is ultrametricity?

Outline:
1. Definitions
2. Tools
3. Results

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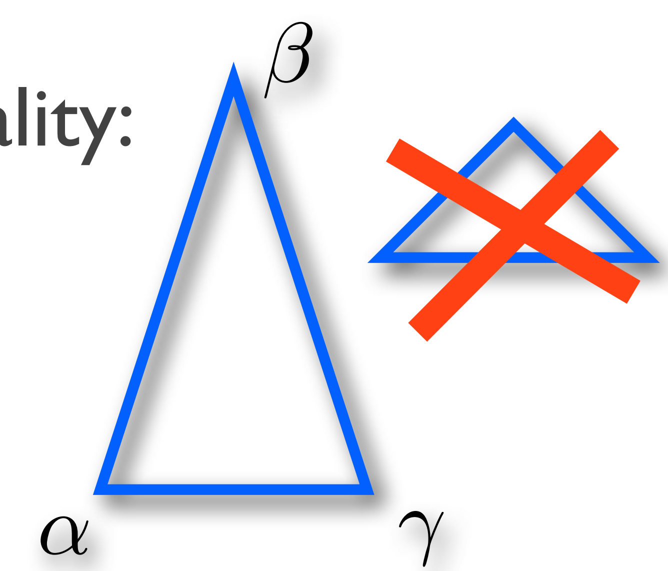

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Relevance to spin glasses (hand-waving...)

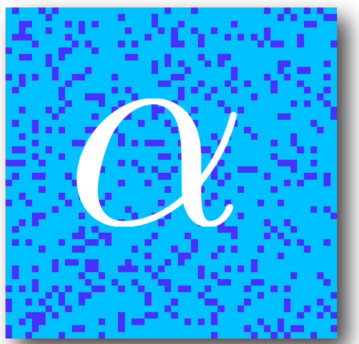
- Replica symmetry breaking solution of the mean-field model:

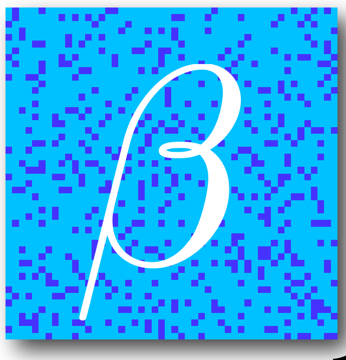
Parisi (79)
Talagrand (06)

$$F = -kT[\log Z]_{\mathrm{av}} \qquad \log Z = \lim_{n\to 0}\left(\frac{Z^n - 1}{n}\right)$$

- Order parameter: overlap function

$$q = \frac{1}{N}\sum_{i=1}^{N} S_i^{\alpha} S_i^{\beta}$$

$q = \frac{1}{N}\Big($ 

$\times$ 

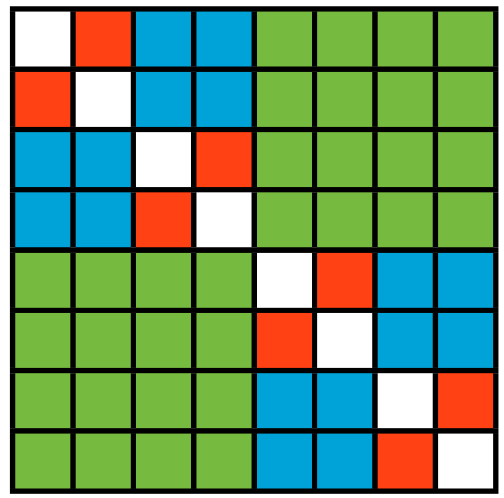
$\Big)$

- After replication one obtains:

$$[\log Z]_{\mathrm{av}} \sim \int \Pi_{\alpha,\beta} dQ_{\alpha\beta} e^{NG(Q_{\alpha\beta})}$$

- Typical structure:

$$Q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^{(\alpha)} S_i^{(\beta)} =$$



$$1 \le \alpha, \beta \le n$$

- One can show that for three states in $Q_{\alpha\beta}$ with $q_{\alpha\gamma} \ge q_{\gamma\beta} \ge q_{\alpha\beta}$ one has $q_{\gamma\beta} = q_{\alpha\beta}$ in the thermodynamic limit.

I.

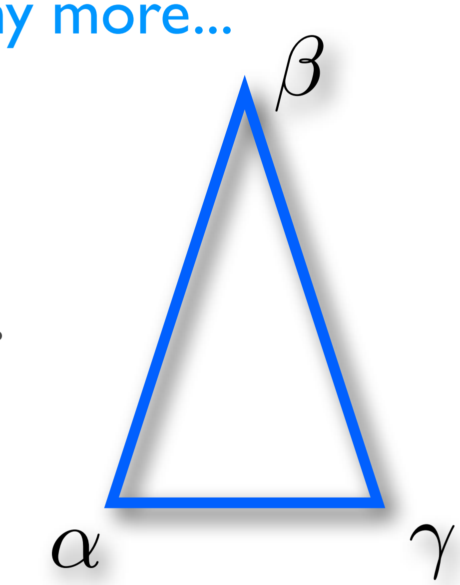
What does it mean to be ultrametric?

- Simple test to see if the mean-field solution is applicable to a model:
  - Ultrametricity is a cornerstone of the mean-field solution.
  - If a model has no ultrametricity, the RSB solution is not valid for it.

- Current state of affairs:
  - Are short-range models ultrametric? Very controversial!
  - Many contradicting predictions.

Hed et al., PRL (04)
Contucci et al., PRL (06)
Jörg & Krzakala, PRL (07)
and many more...

- Problems:
  - Only small short-range systems can be studied.
  - The states for the test have to be selected very carefully.



- Solution:
  - Analysis of the 1D chain [similar to Hed *et al.* (04)].

I.

Achtung! Problems when picking 3 states…

Hed *et al.*, PRL (04)

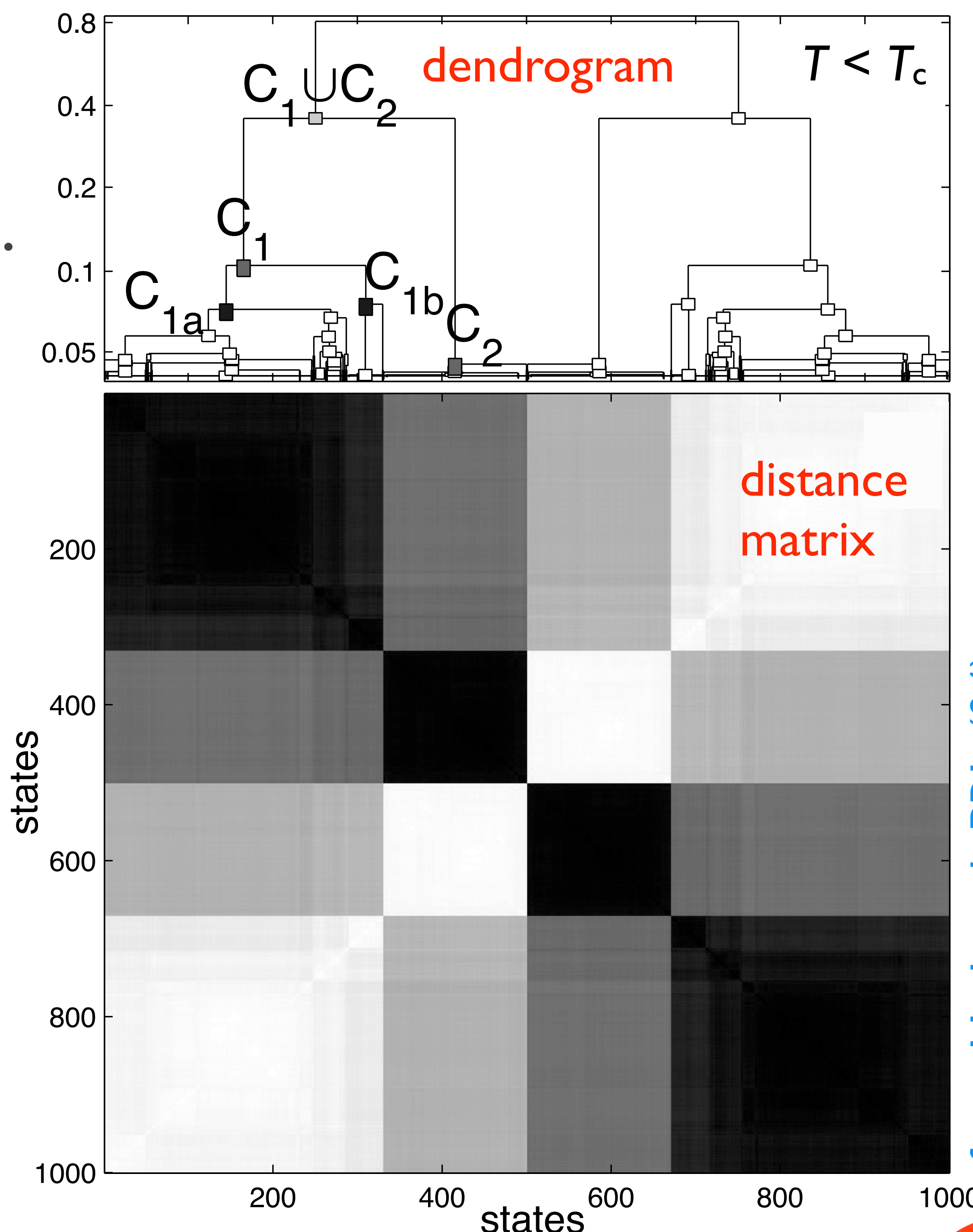
- Possible pitfalls:
  1. If time-reversal symmetry is unbroken, one has to ensure that all three states used belong to the same "side" of phase space.
  2. The temperature must be much smaller than T_c.
  3. If the temperature is too small, for large systems most triangles are equilateral (carry no information). Do not study too low T's.

- Solutions:
  1. Can be avoided with a clustering analysis: Pick 3 states only from the left tree.
  2. Simulations done at $T < T_c$, but not below $T = 0.2T_c$. Data shown for $T = 0.4T_c$.
  3. To avoid equilateral triangles pick the 3 states from different branches in the left subtree (C_{1a}, C_{1b}, C_2). Next…

2.

Selection of states (similar to Hed *et al.*)

- Generation of states:
  - Equilibrate system.
  - Store 10^3 states per realization.
- Selection of states:
  - Sorted *dendrograms* using Wards clustering method.
  - Pick left tree ("spin down").
  - Split left tree into $|C_1| \geq |C_2|$.
  - Split C_1 into C_{1a} and C_{1b}.
  - Pick three random states: $\alpha \in C_{1a}\,,\, \beta \in C_{1b}\,,\, \gamma \in C_2\,.$
- Distance matrix:
  - Darker colors mean closer distances $d_{\alpha\beta} = (1 - q_{\alpha\beta})/2\,.$

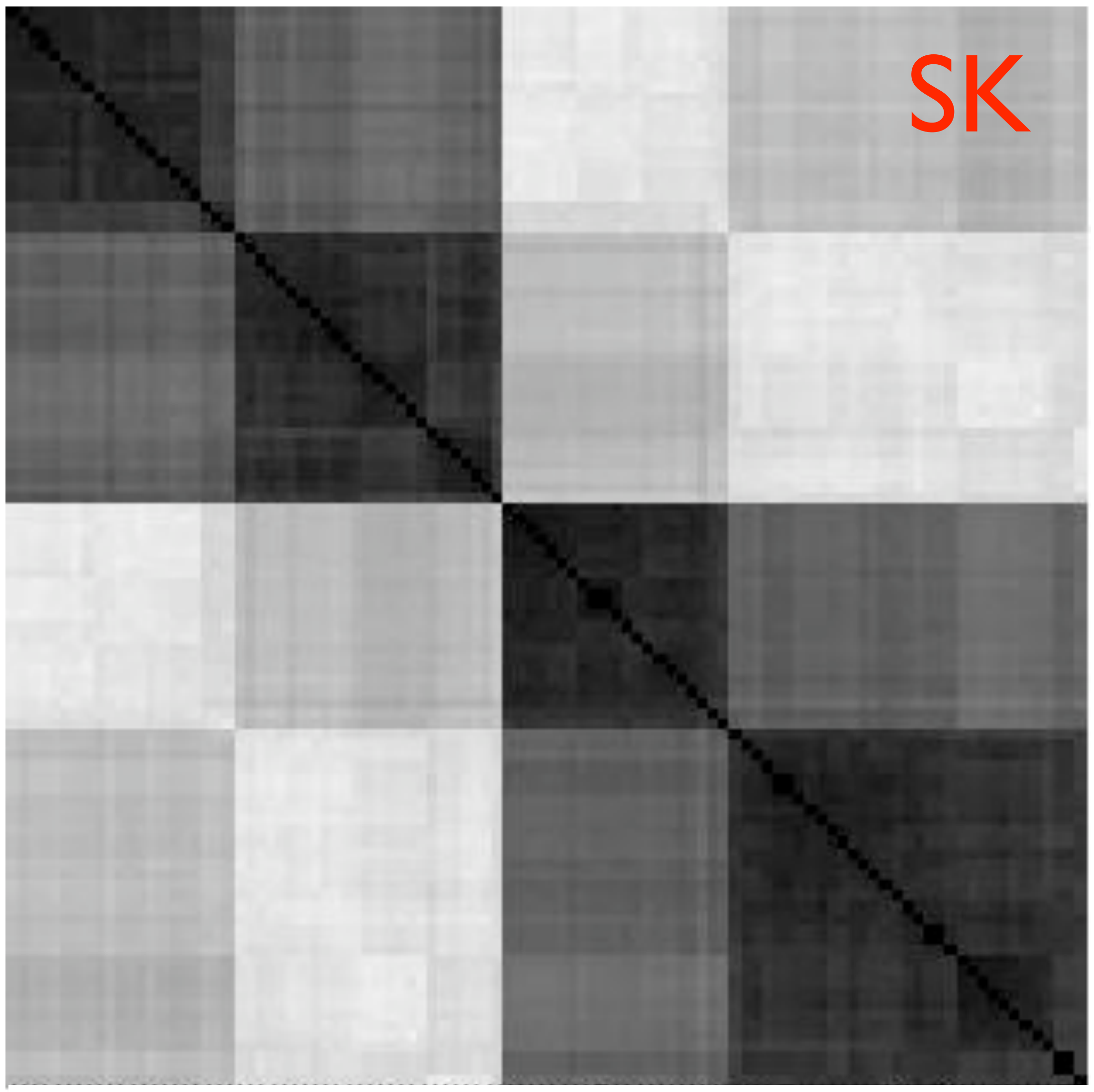


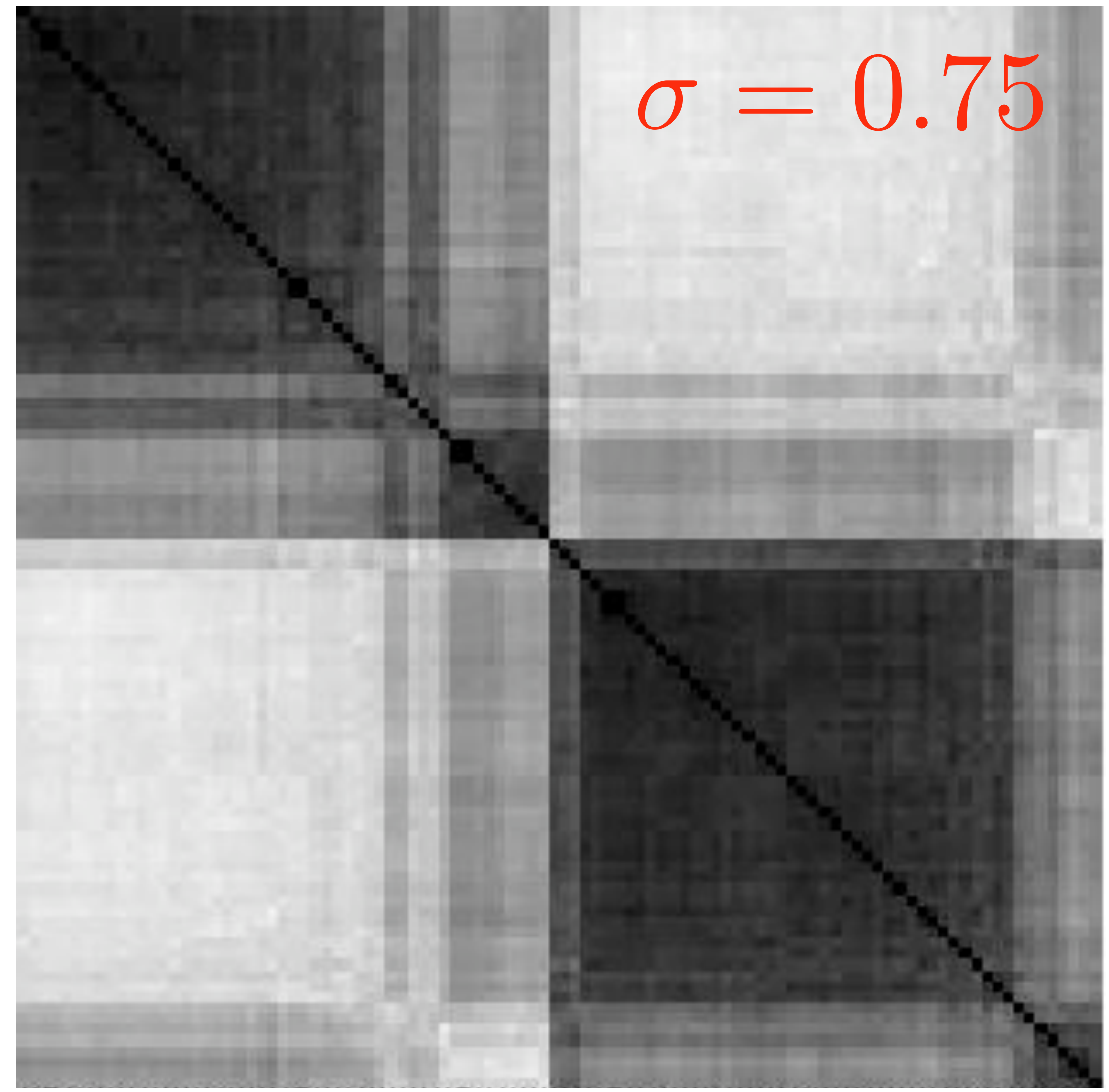
from Hed *et al.*, PRL (04)

2.

Typical distance matrices at $T < T_c$

- Data for the 1D chain, $L = 512$, $T = 0.4T_c$.





- Darker colors correspond to closer hamming distances.
- Both systems show structure at low temperatures.

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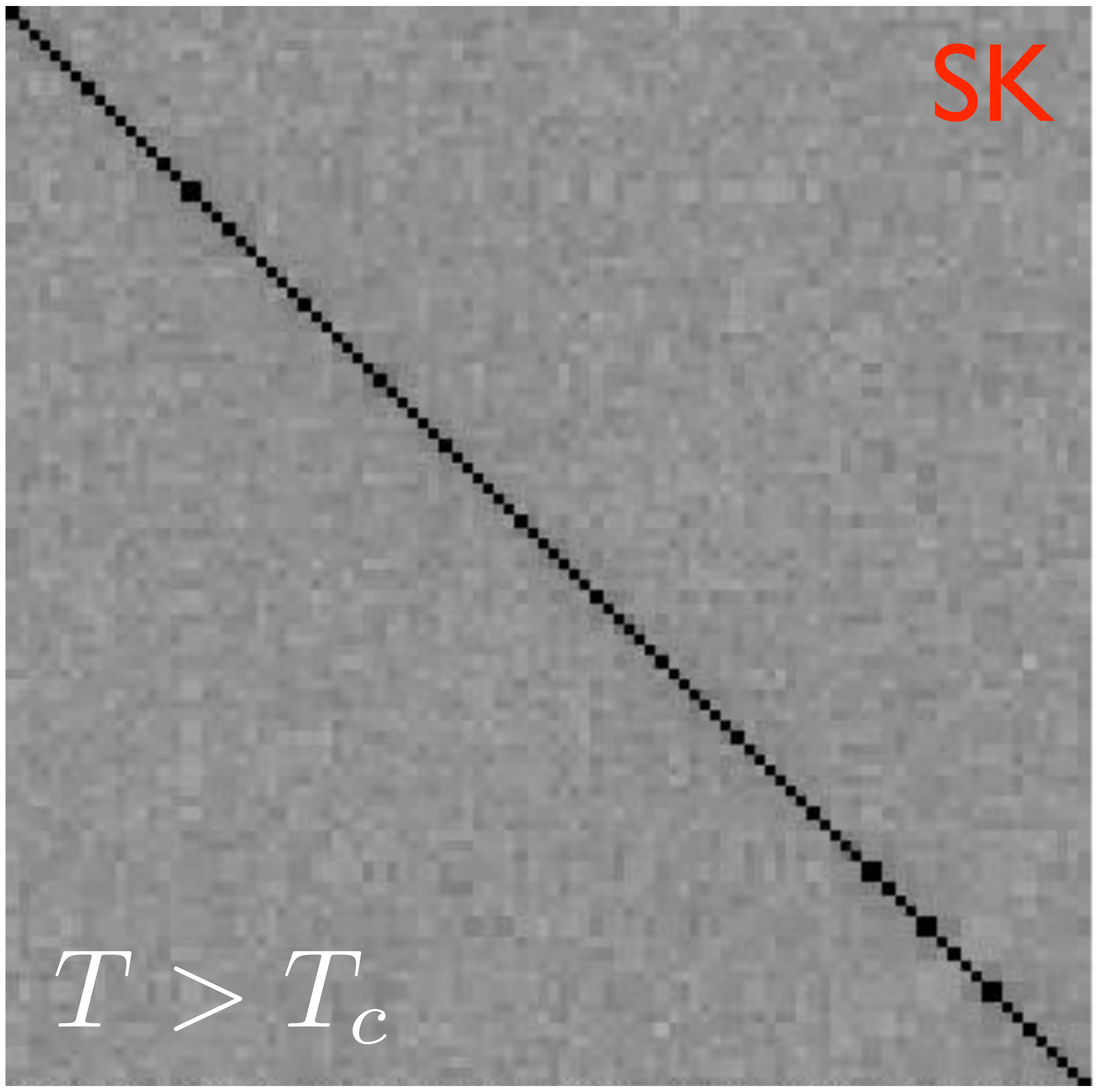

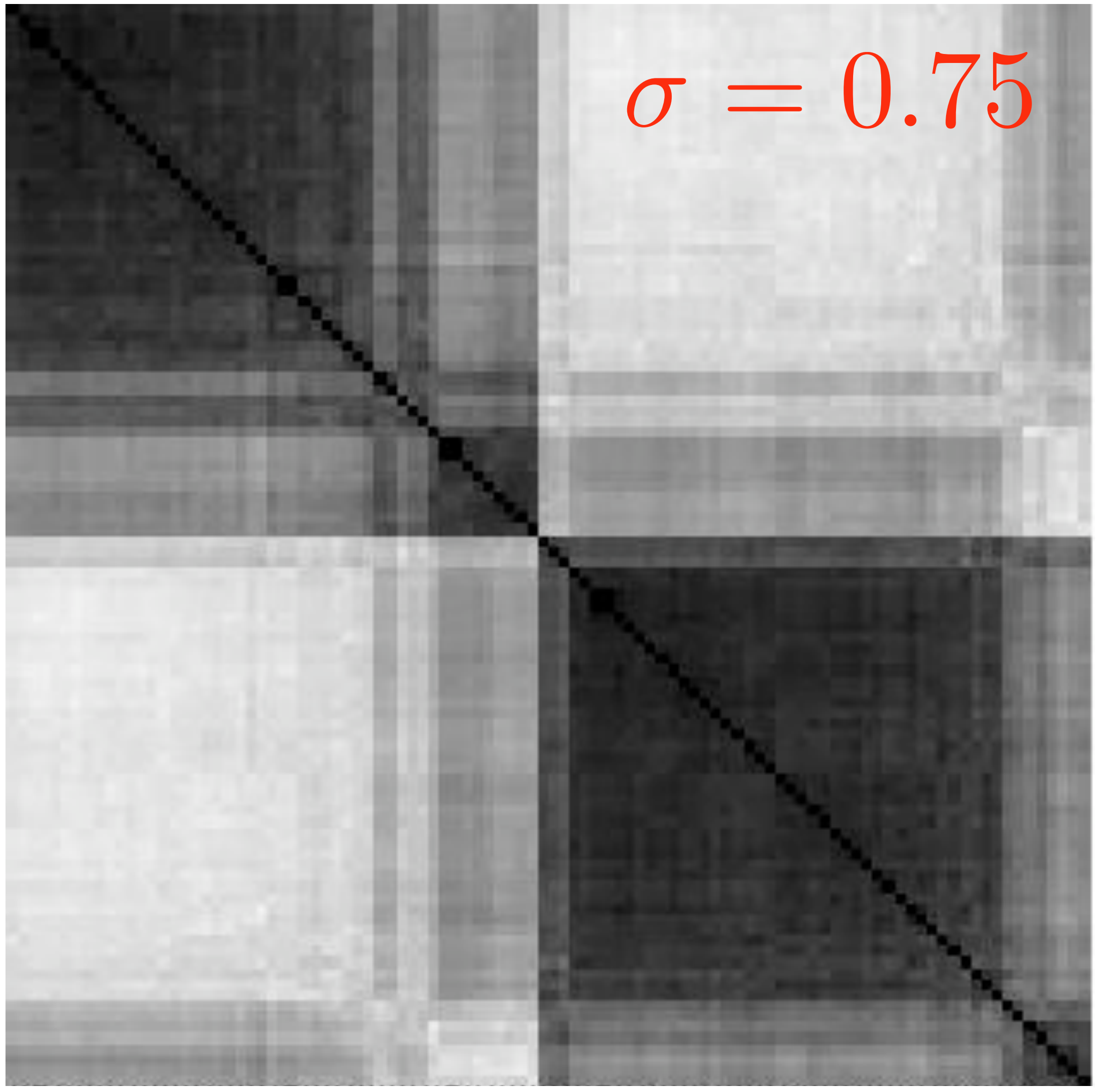

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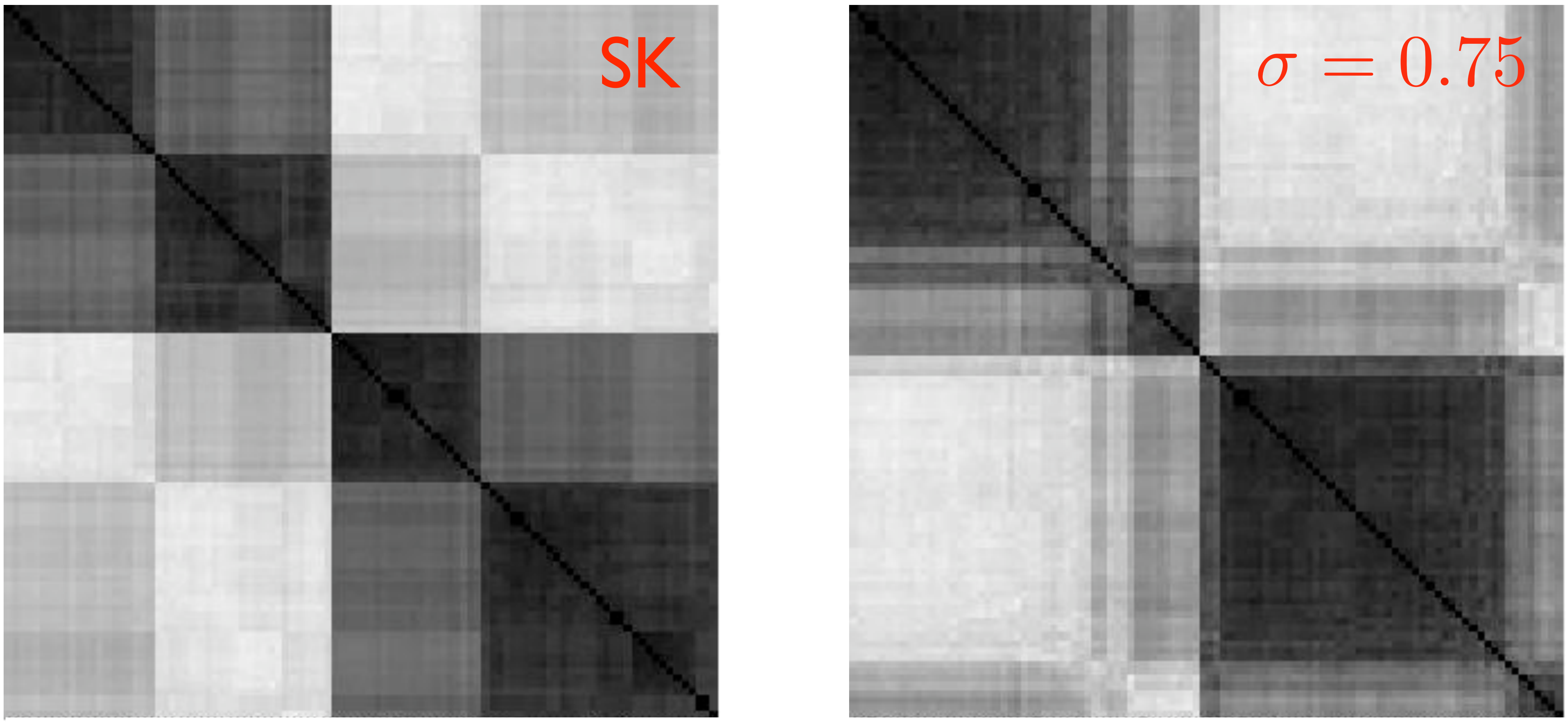

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How to measure ultrametricity

- Observable:
  - Select three states with the aforementioned recipe.
  - Compute the hamming distance between them: $d_{\alpha\beta} = (1 - q_{\alpha\beta})/2$.
  - Sort the distances: $d_{\max} \geq d_{\mathrm{med}} \geq d_{\min}$.
  - Compute:

$$K = \frac{d_{\max} - d_{\mathrm{med}}}{\rho(d)}$$

Here $\rho(d)$ is the width of the distance distribution.

- Signs of ultrametricity:
  - If the space is ultrametric, we expect $d_{\max} = d_{\mathrm{med}}$ for $N \to \infty$.
  - Study the distribution $P(K)$. We expect:

$$P(K) \sim \delta(K = 0) \qquad N \to \infty$$

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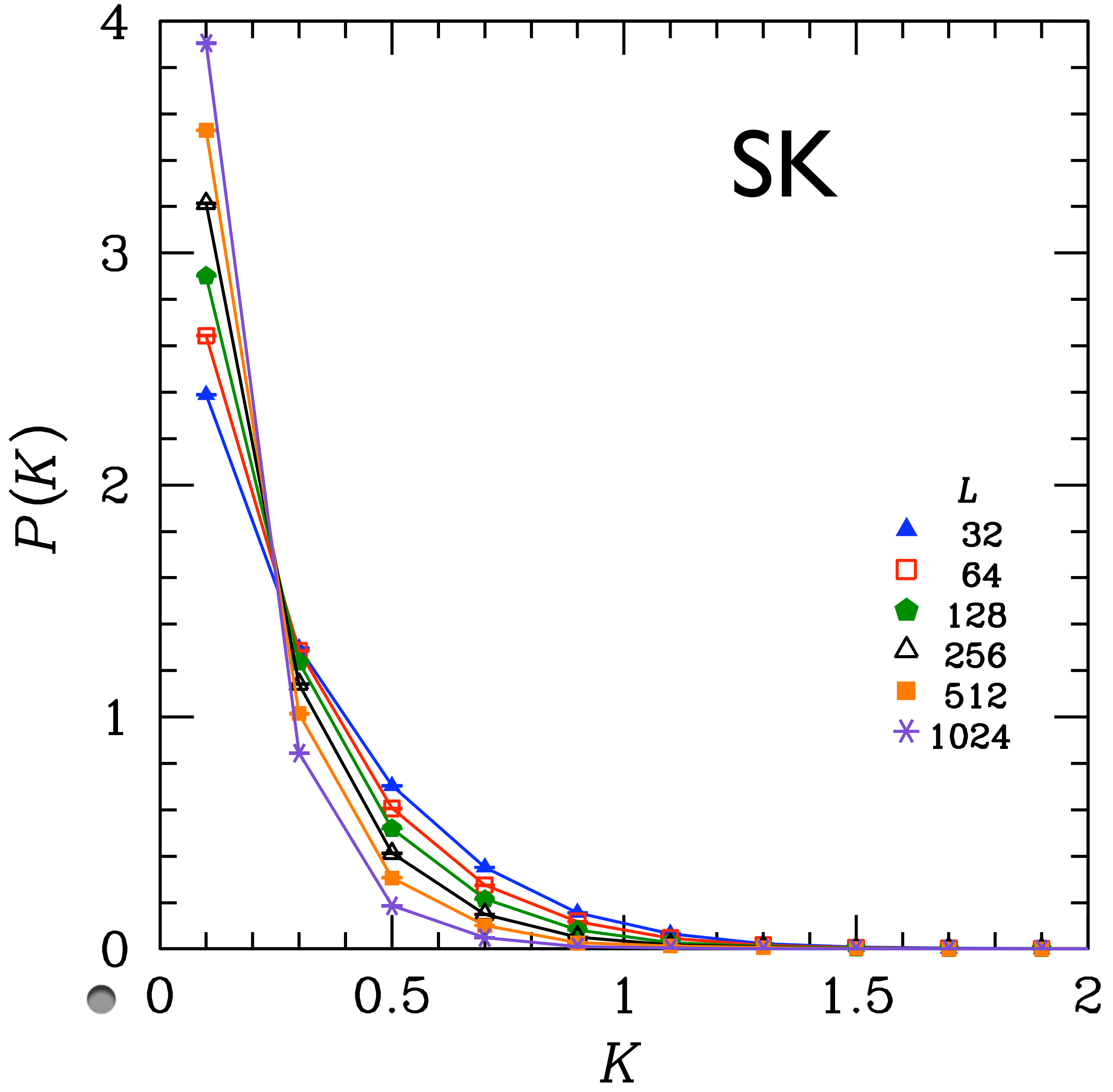
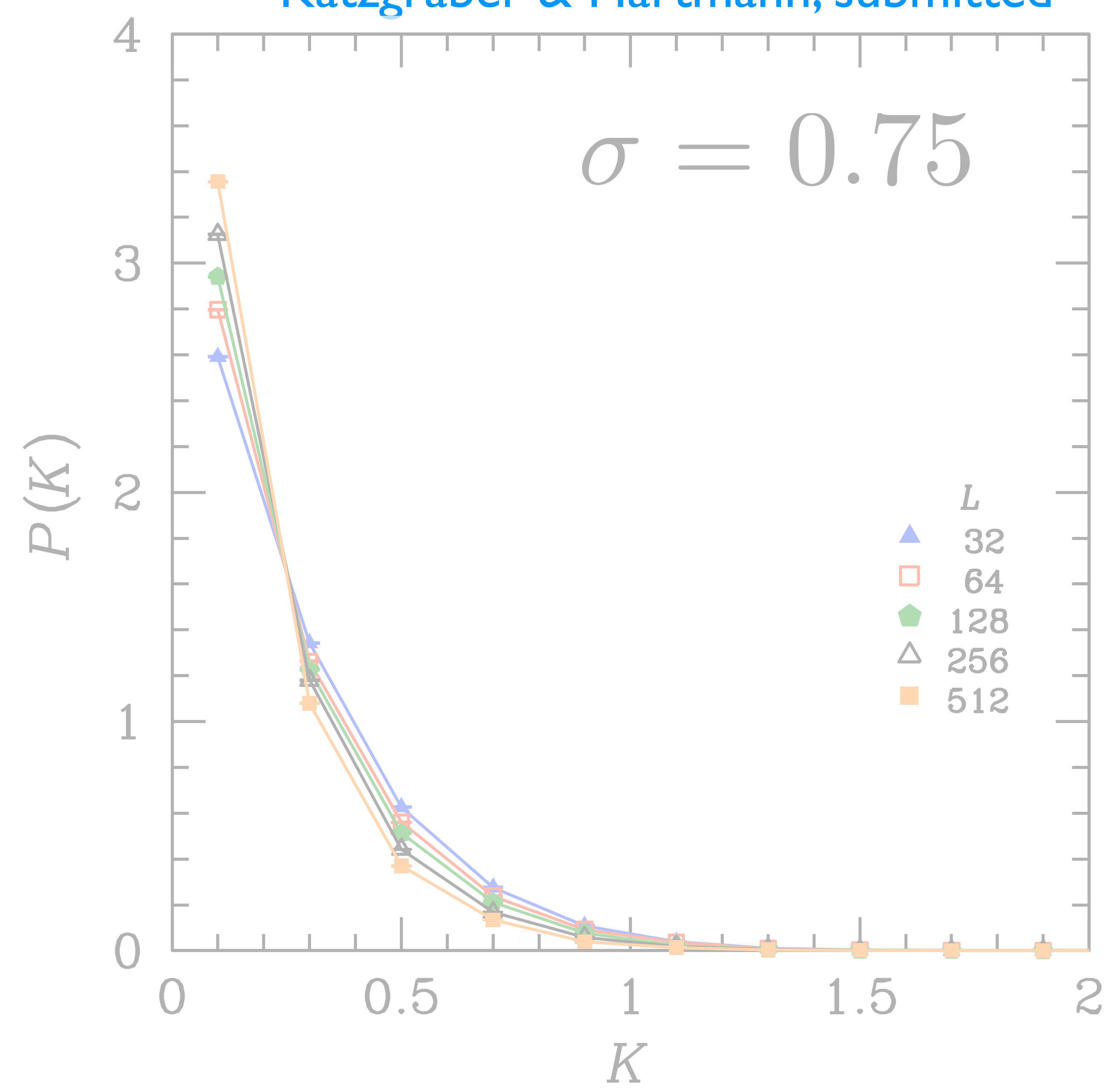
Distributions $P(K)$ at $T = 0.4T_c$

Katzgraber & Hartmann, submitted





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- Similar results for other values of σ.

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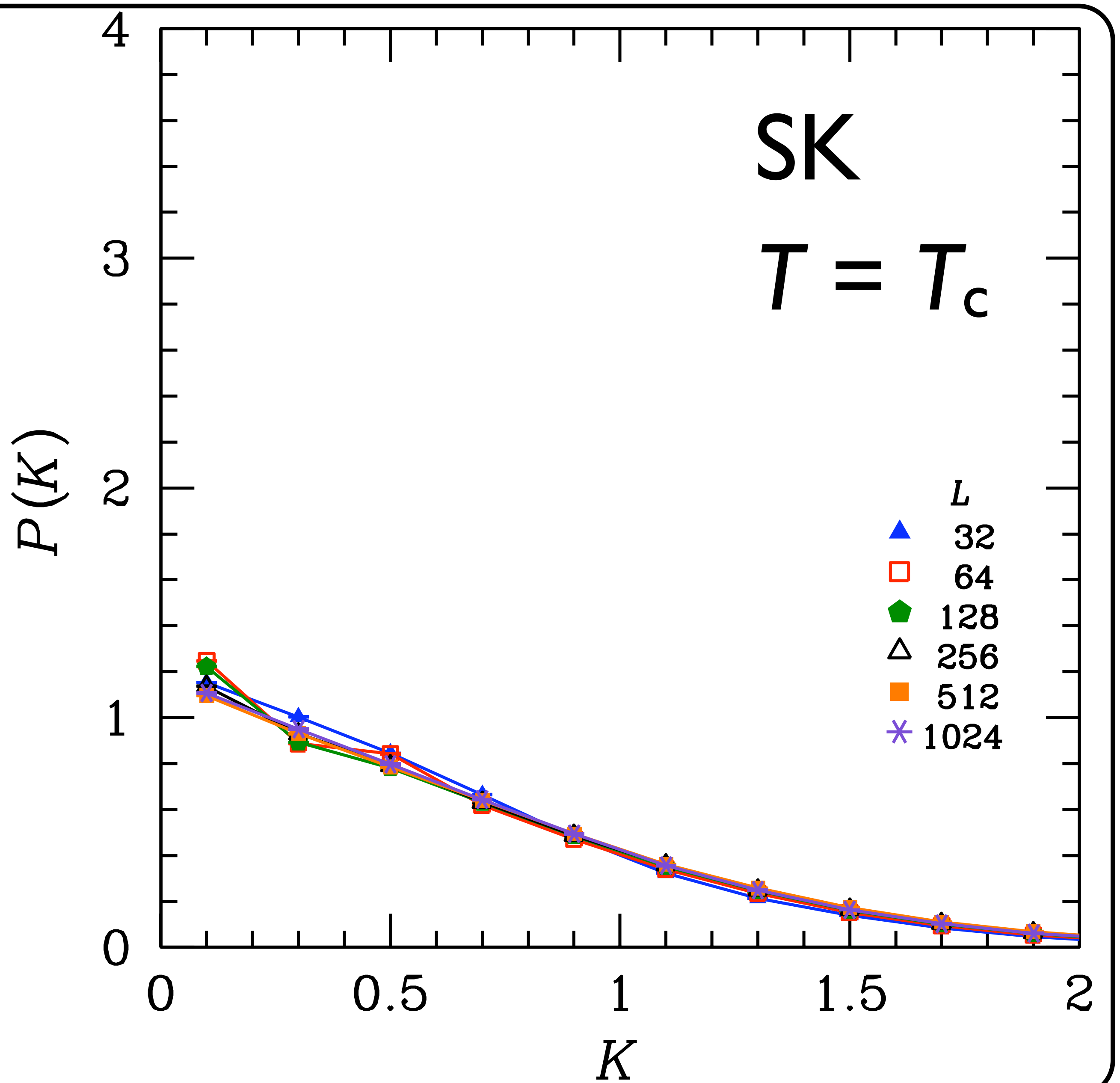

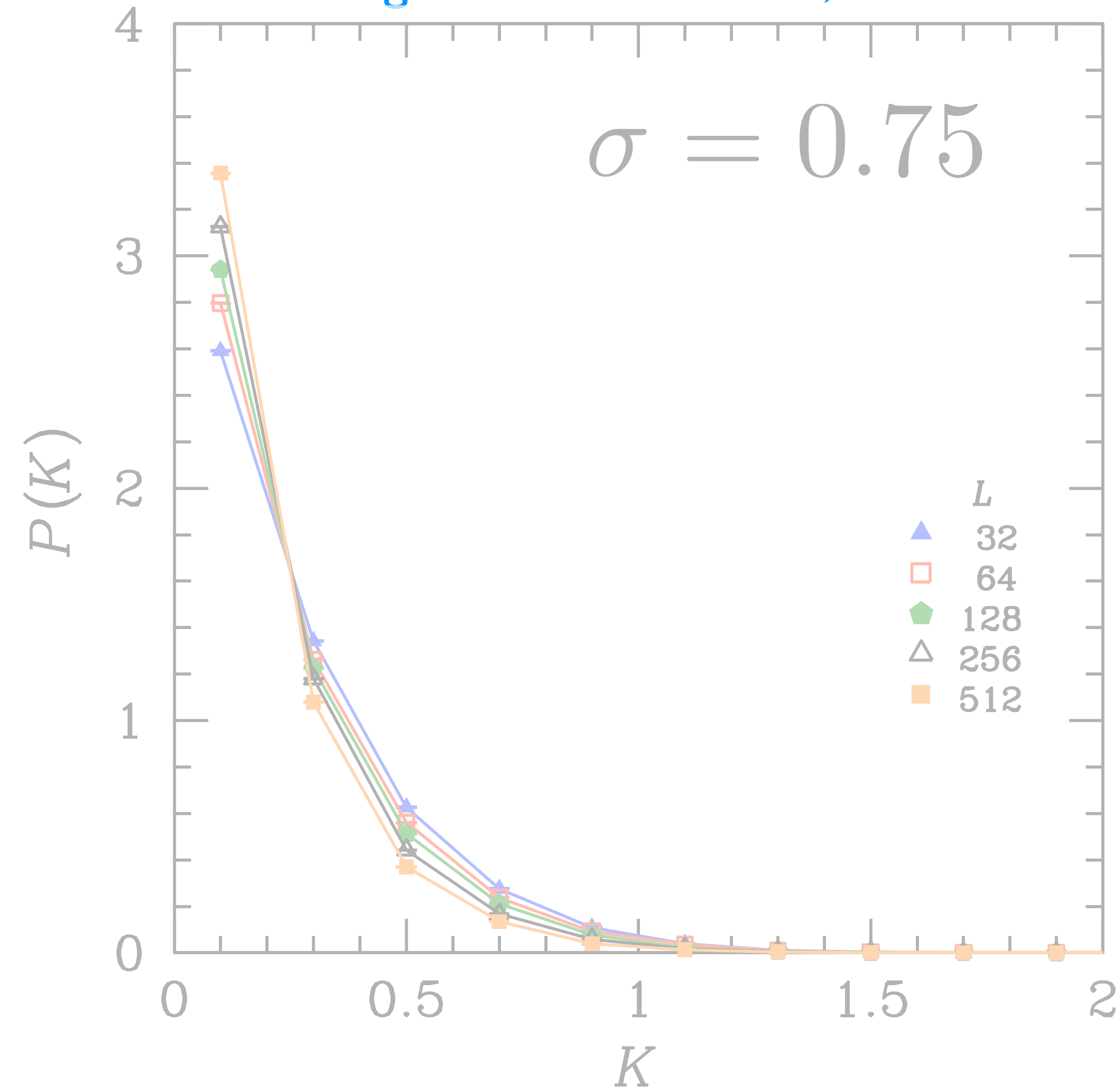

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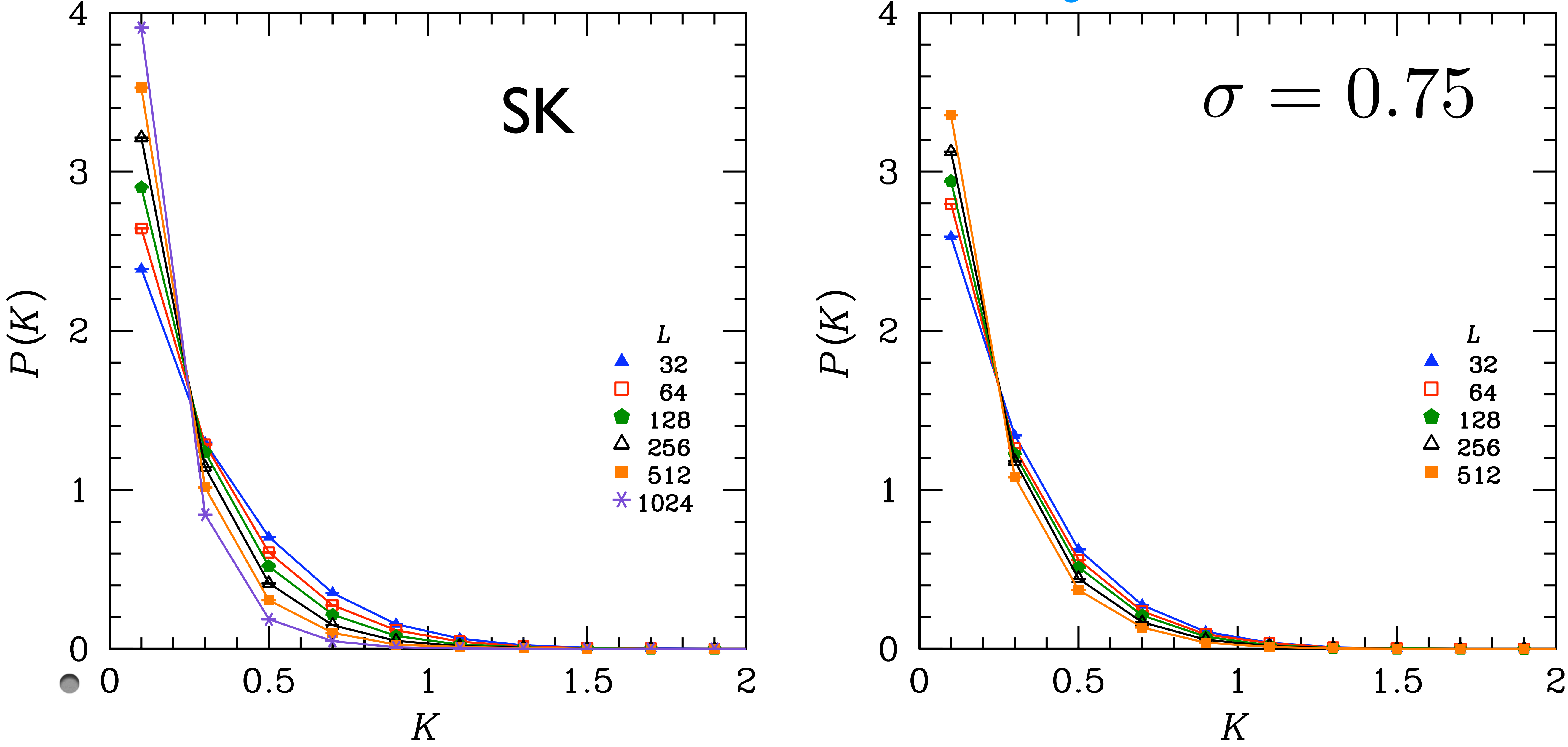

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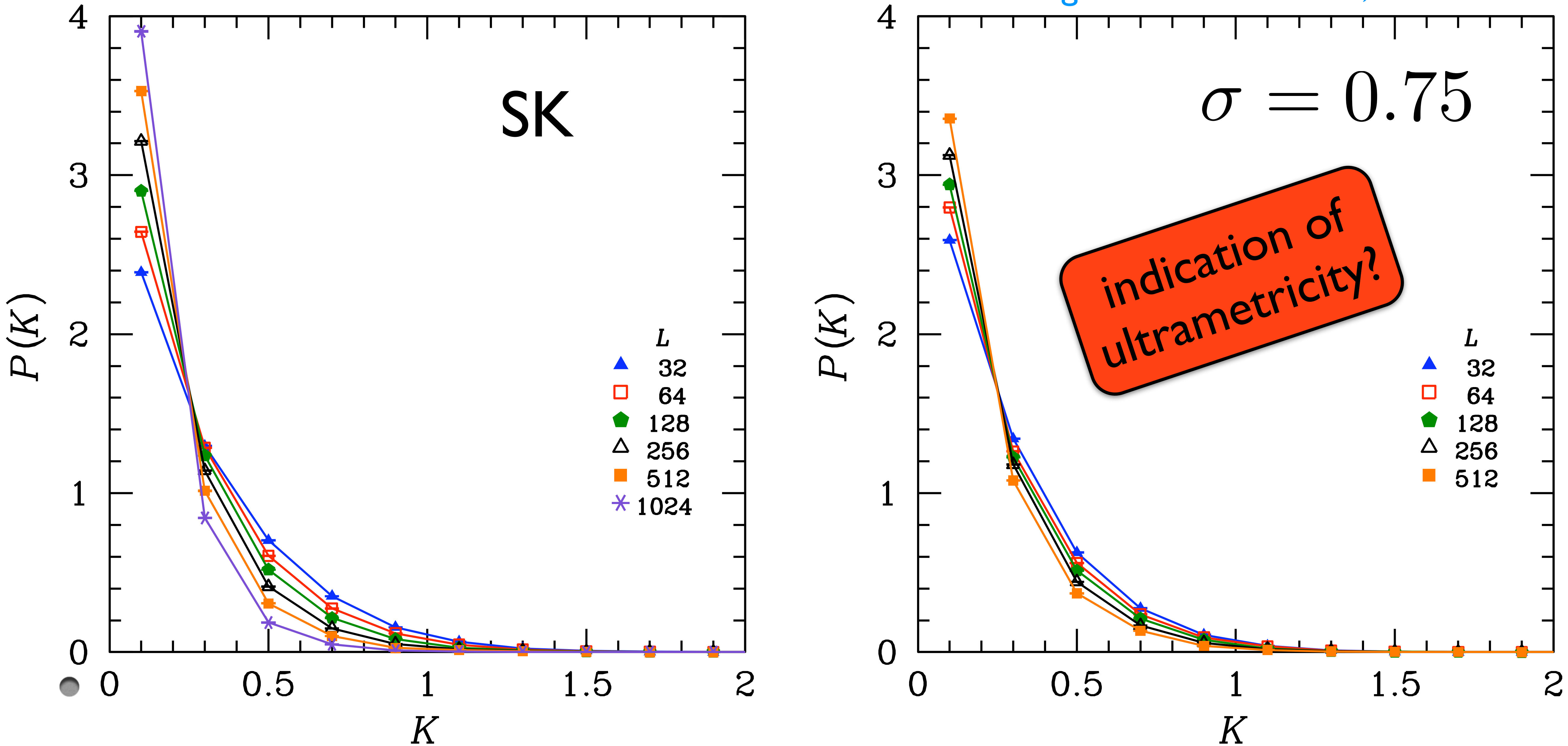

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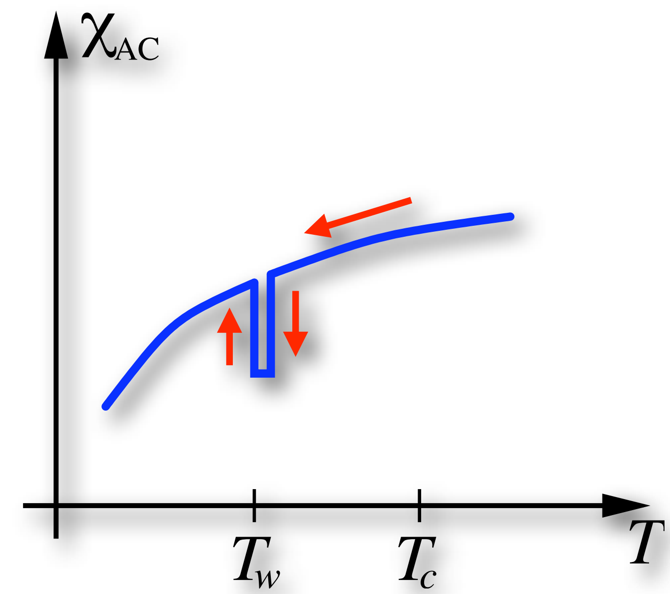
3.

What else can we do with the 1D chain?

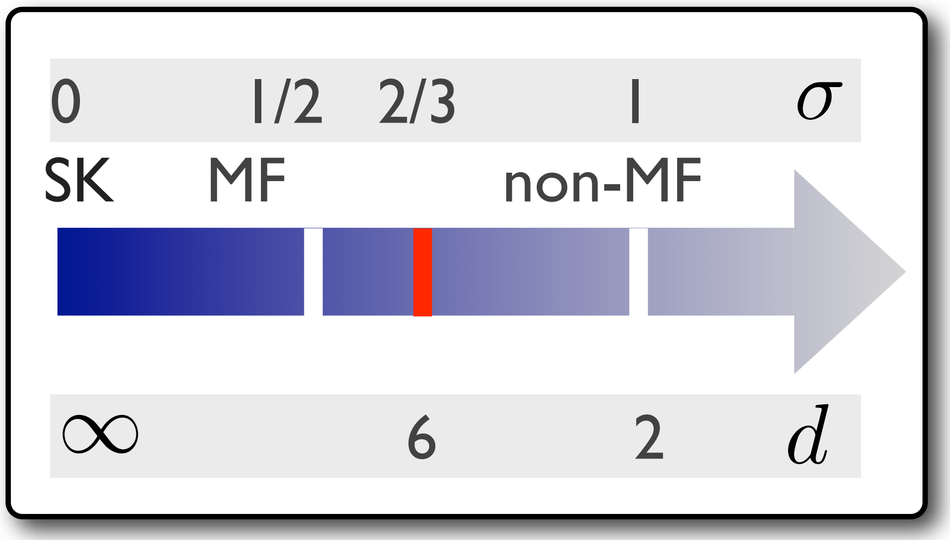
Other ideas currently explored

- Study open problems in spin glasses:
  - Chaos, aging, universality, memory effect, …



Matsuda et al. (07)

- Modifications of the model:
  - Spin symmetries (Potts, Heisenberg, …).
  - p-spin model for structural glasses.
  - Power-law probability-diluted chain (huge systems).



- Benchmarking algorithms:
  - How does the algorithm scale with the size of the input (N)?
  - How does the scaling of the algorithm depend on the complexity/connectivity?
  - 1D chain: range of the interactions (universality class) can be changed.

Other ideas currently explored

Examples:
1. diluted model
2. benchmarks

- Study open problems in spin glasses:
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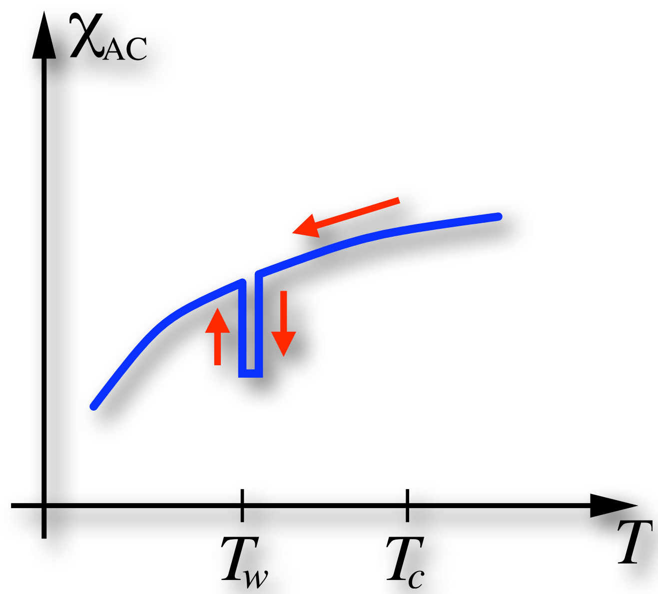

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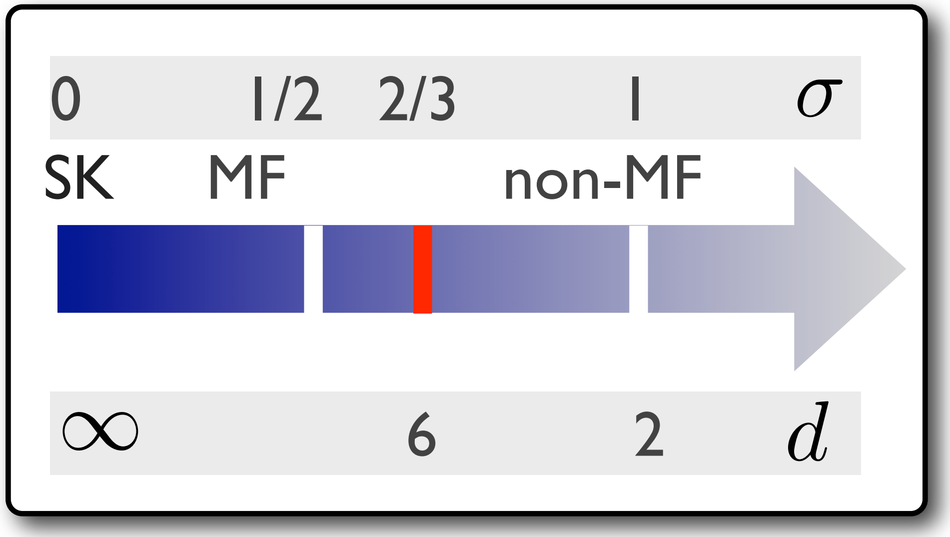
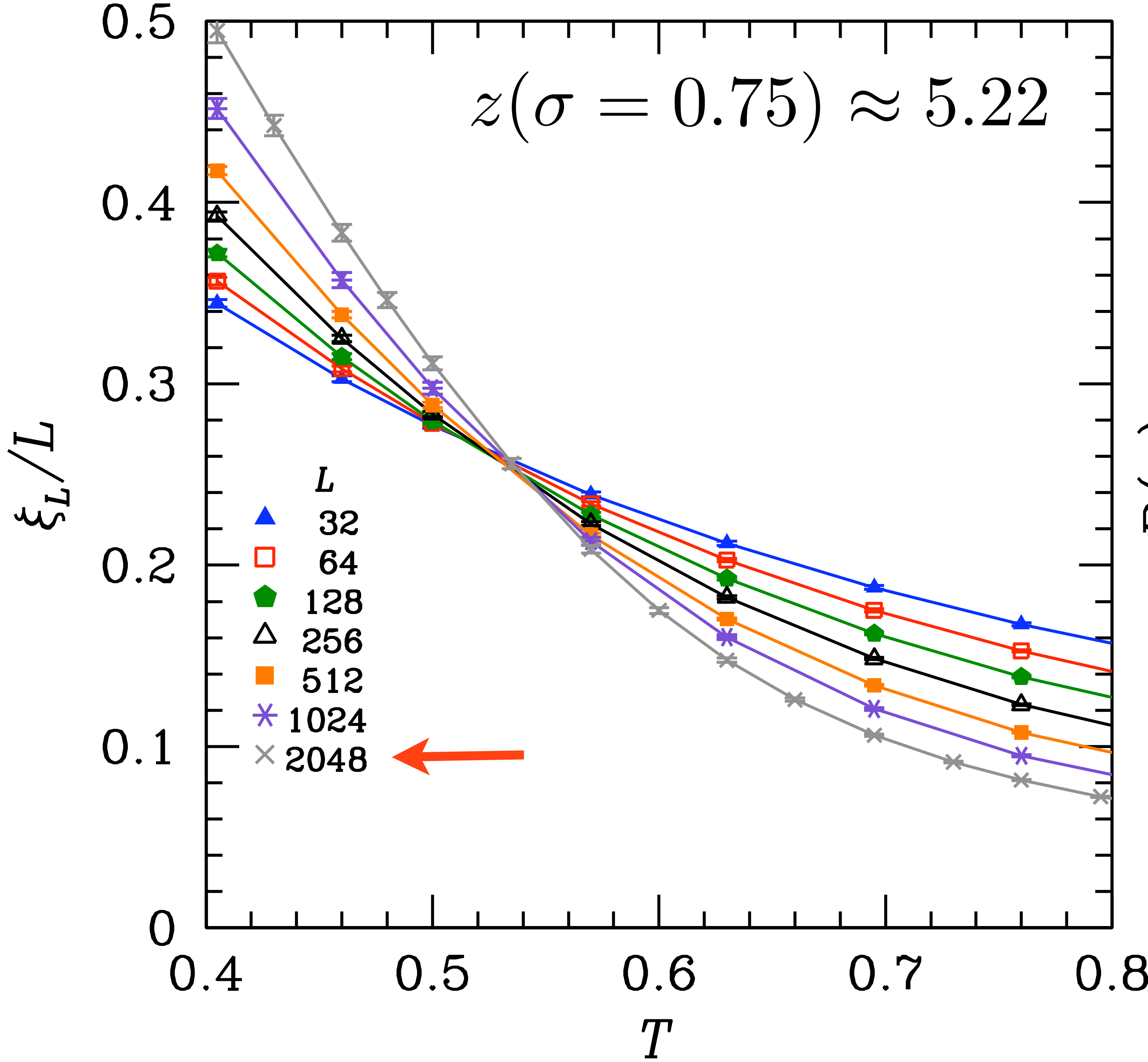


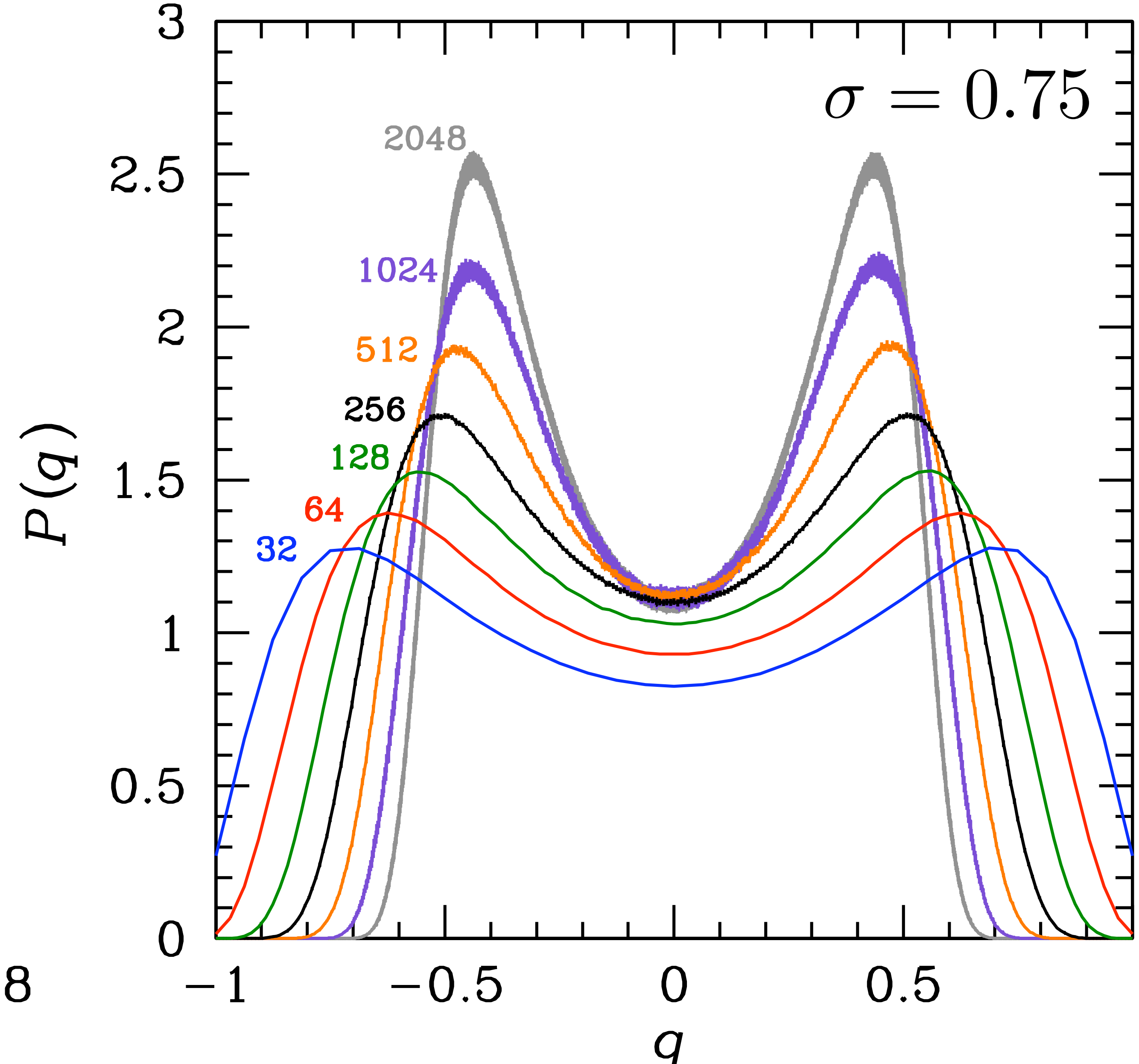
Probability-diluted Gaussian Ising chain

- Place a Gaussian random bond with $\mathcal{P}(J_{ij} \neq 0) \sim r^{-2\sigma}$
- Same behavior as the regular 1D chain, but $[z]_{\rm av} = 2\zeta(2\sigma)$.

$$\mathcal{H} = -\sum_{i<j} J_{ij} S_i S_j$$

Leuzzi, et al. (08)





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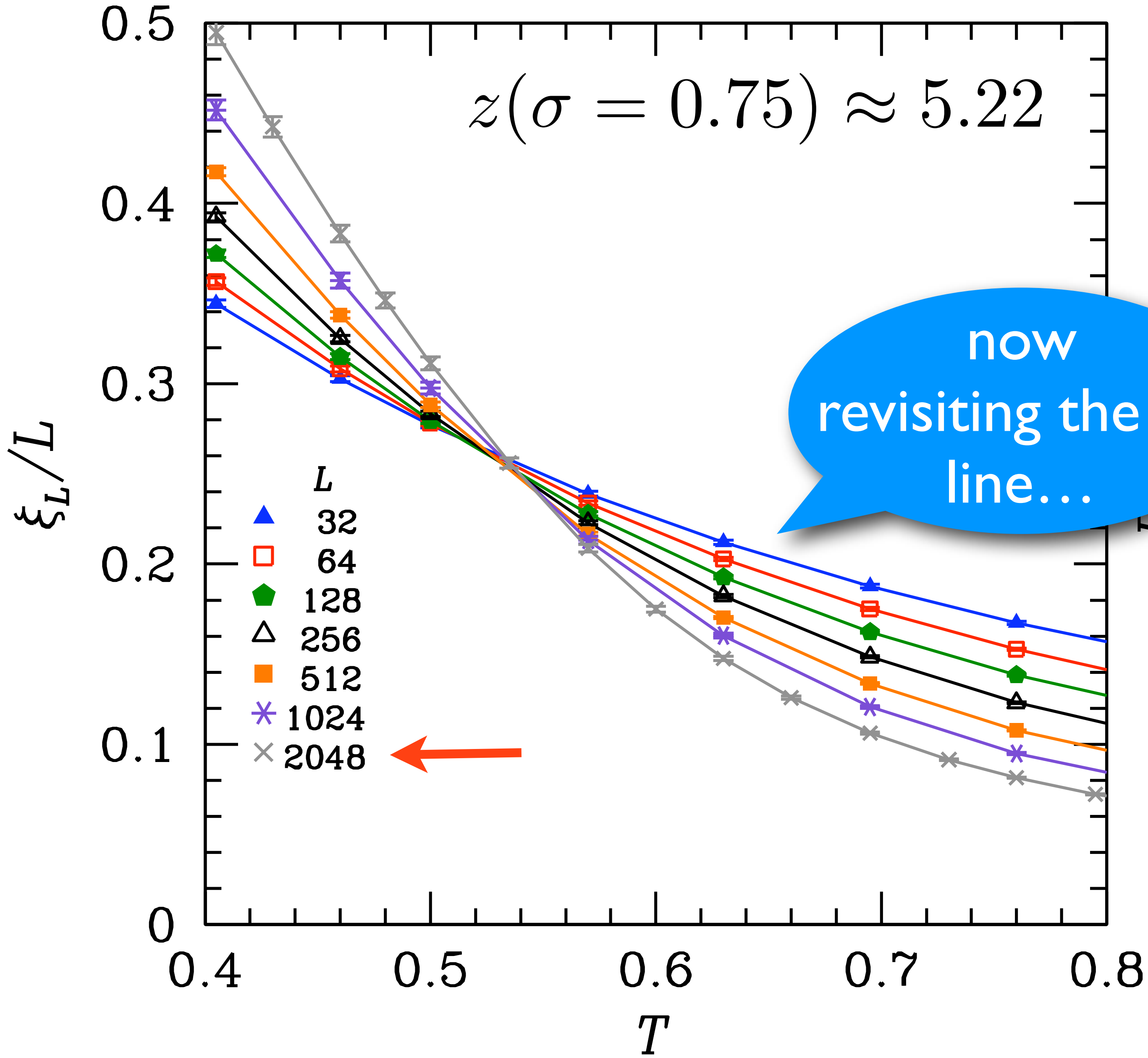
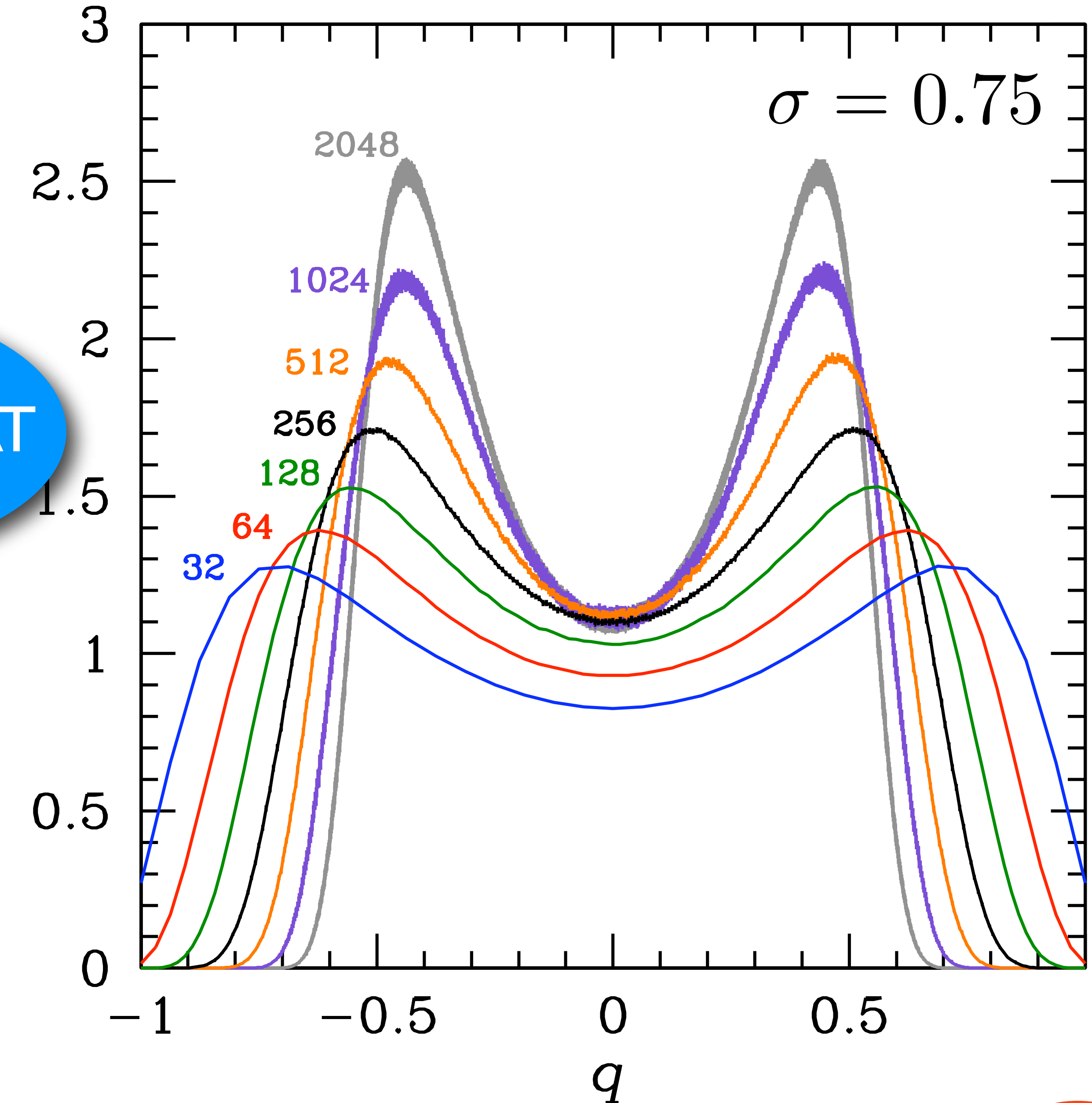


now revisiting the AT line…



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I.

Example: Hysteretic optimization

Zarand et al., PRL (02)

- Experiment:
  - Do you have a CRT monitor or a non-LCD TV at home?
  - Take a magnet and hold it to the screen.
  - You are in trouble.

- Solution:
  - Call the technician.
  - Make a degaussing coil and slowly do circles around the TV increasing the radius and distance.
- You have just hysteretically (and possibly also hysterically) demagnetized the TV screen.

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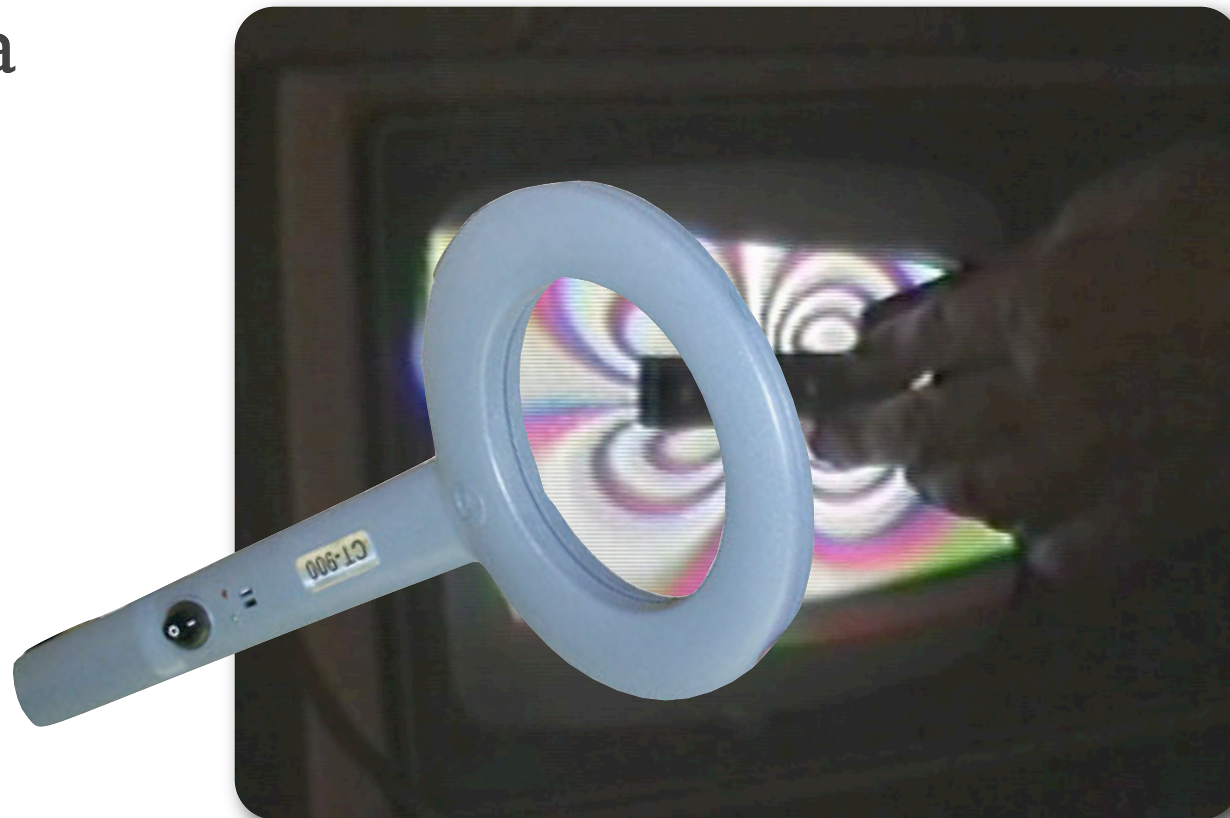

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Benchmarking: Hysteretic optimization

Zarand et al., PRL (02)

- Idea: Minimize the energy of a system by successive demagnetization.
- Example: Ising spin glass

$$\mathcal{H} = -\sum_{ij} J_{ij} S_i S_j - H \sum_i \xi_i S_i$$

$\xi_i = \pm 1$ random

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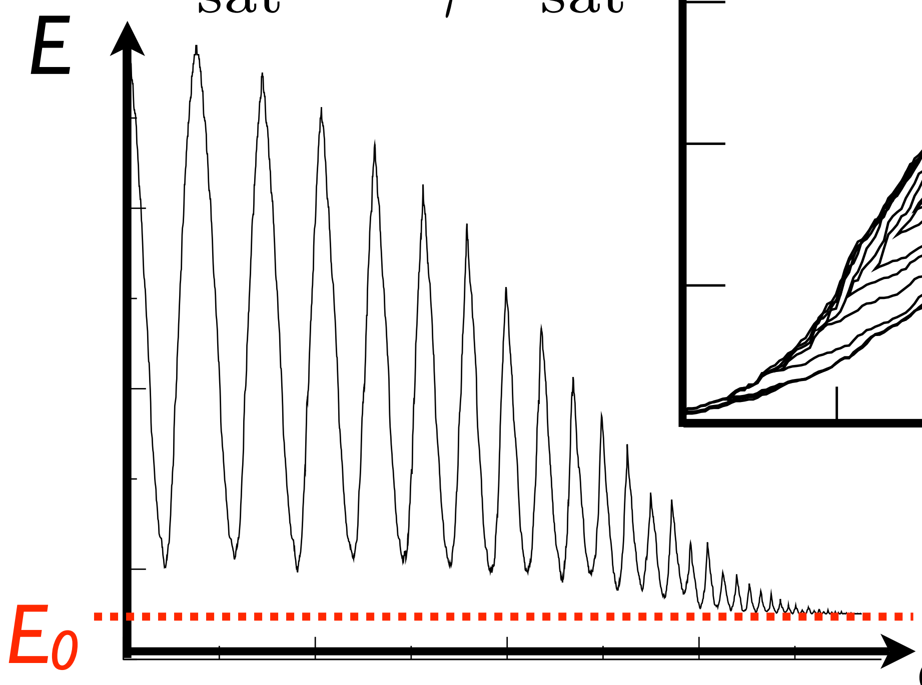
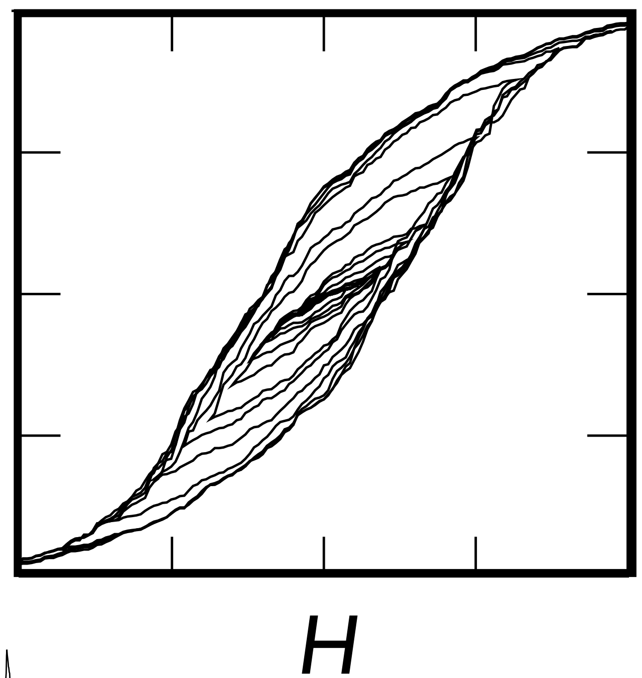
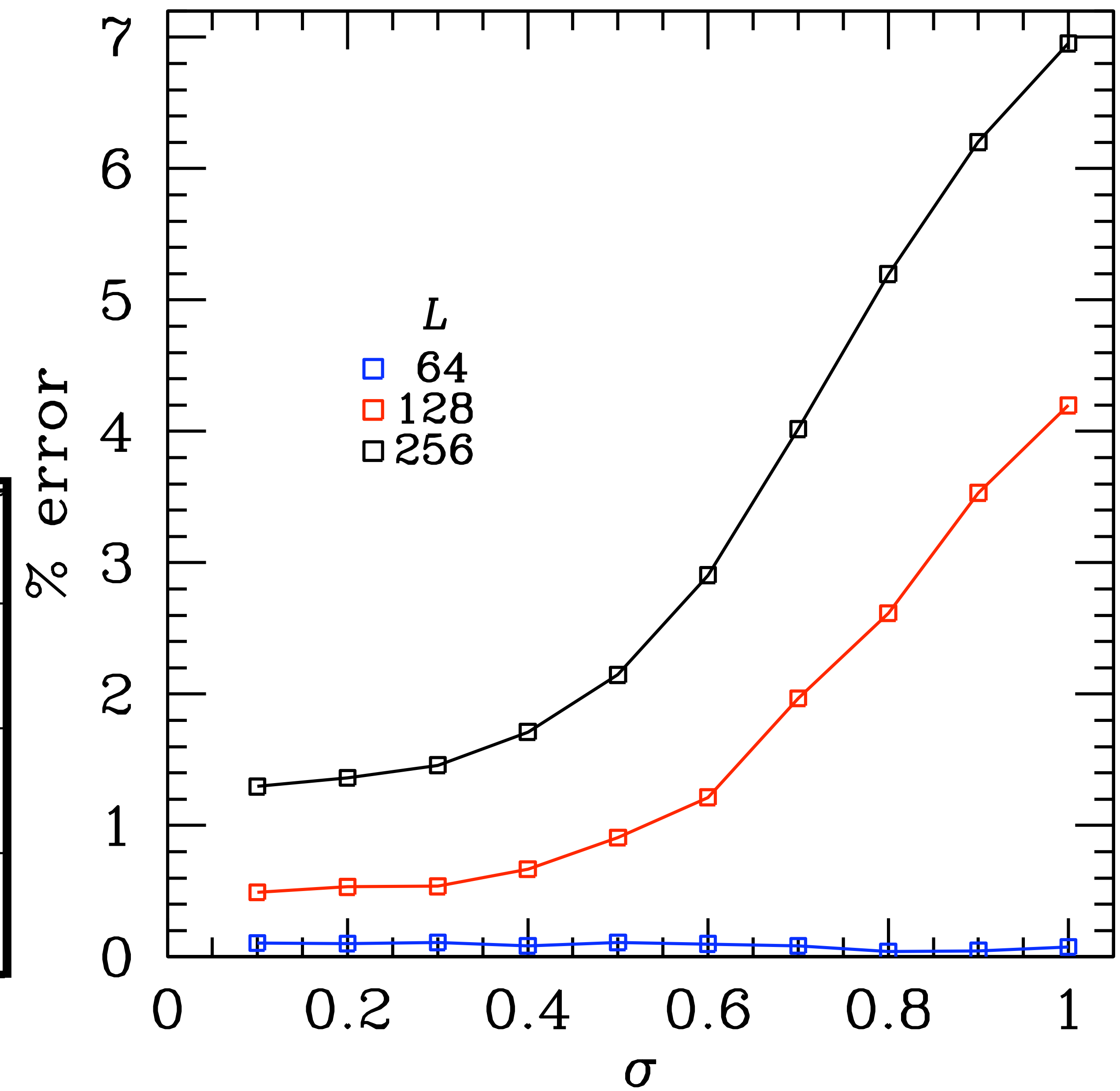
$$H_{\text{sat}} \to \gamma H_{\text{sat}}$$







adapted from Gonçalves & Boettcher (08)

for details see Hartmann & Rieger book (04)

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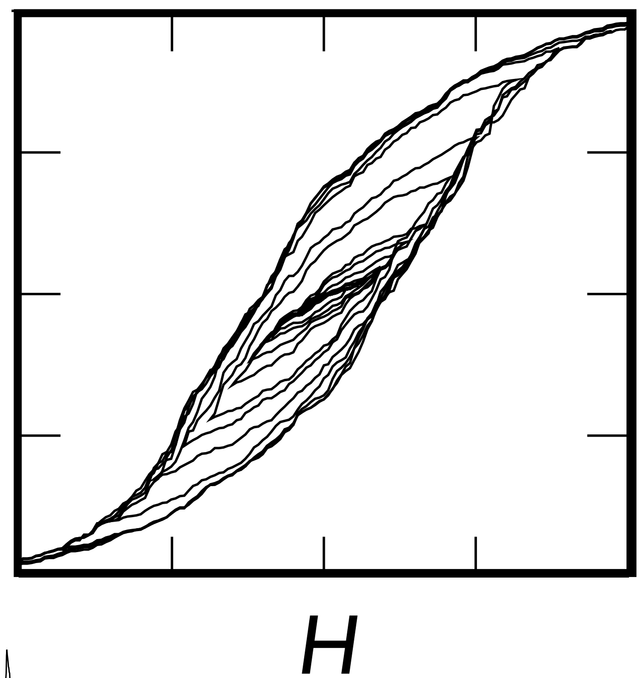

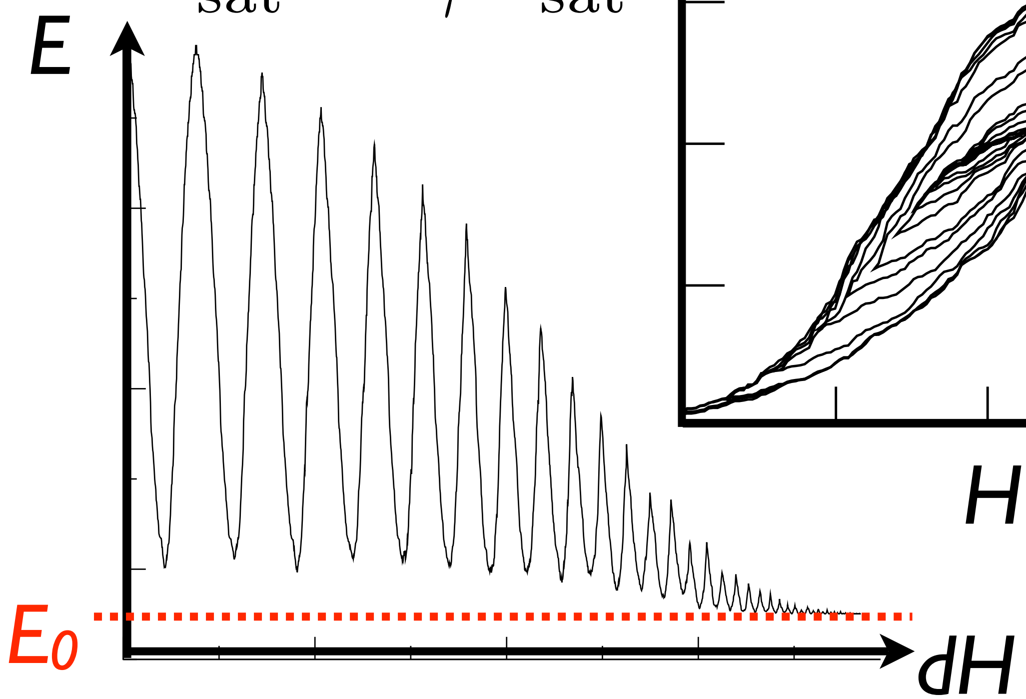

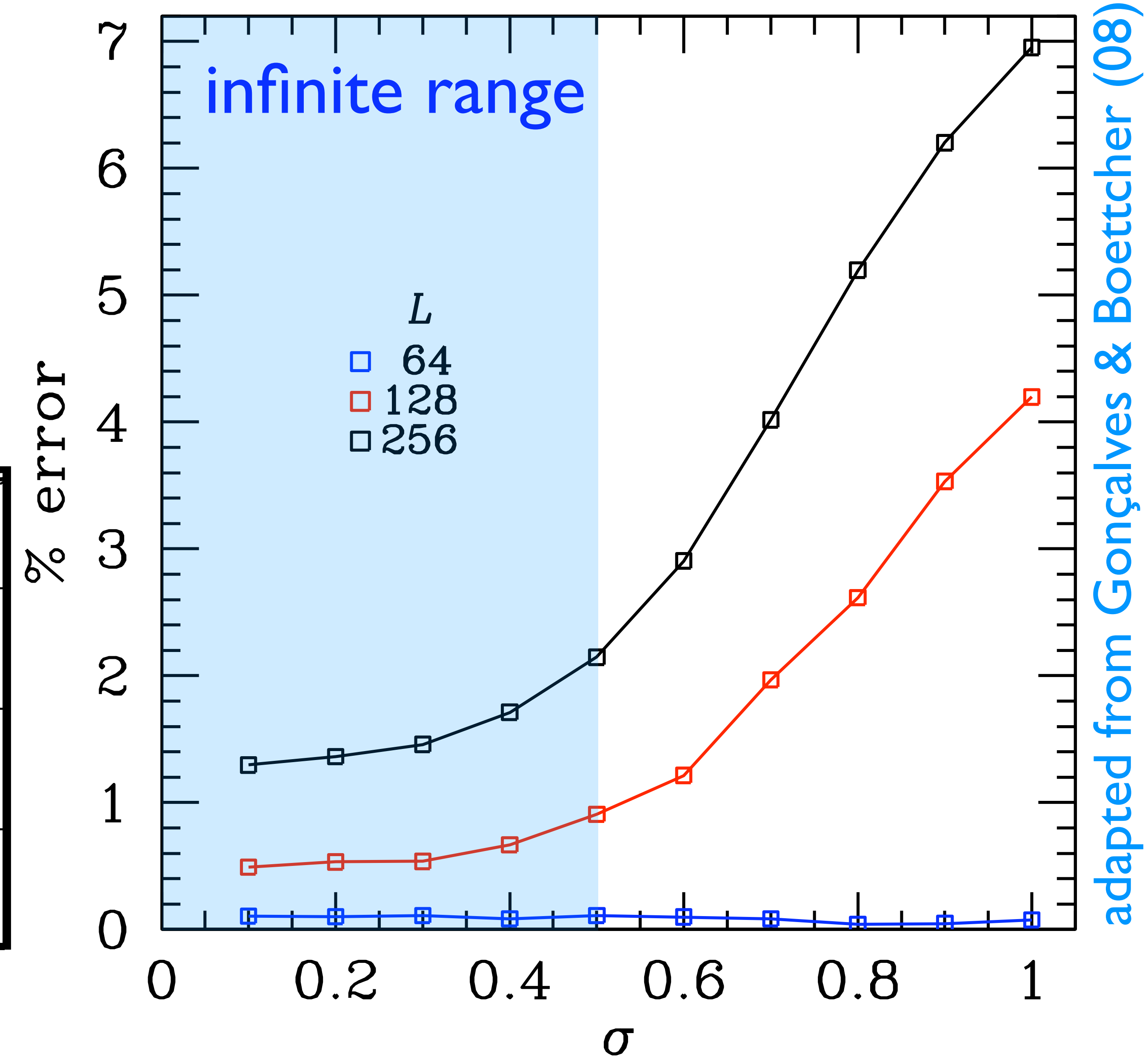

- The algorithm works best in the infinite-range regime.

for details see Hartmann & Rieger book (04)

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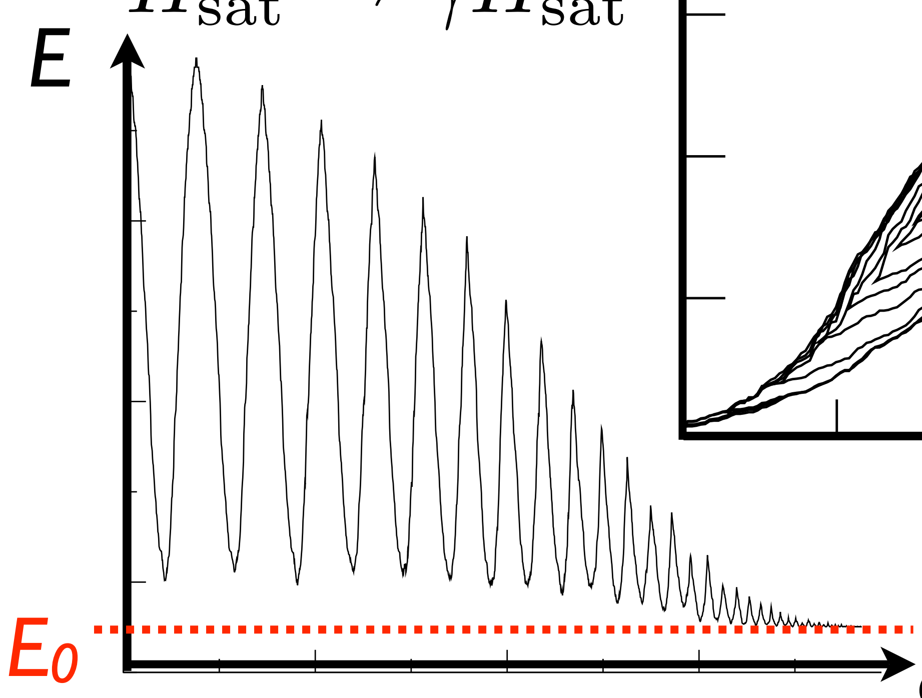

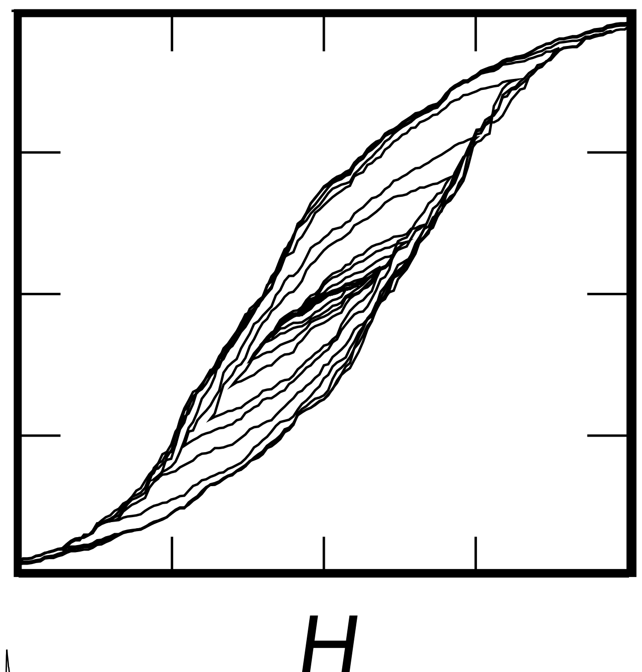

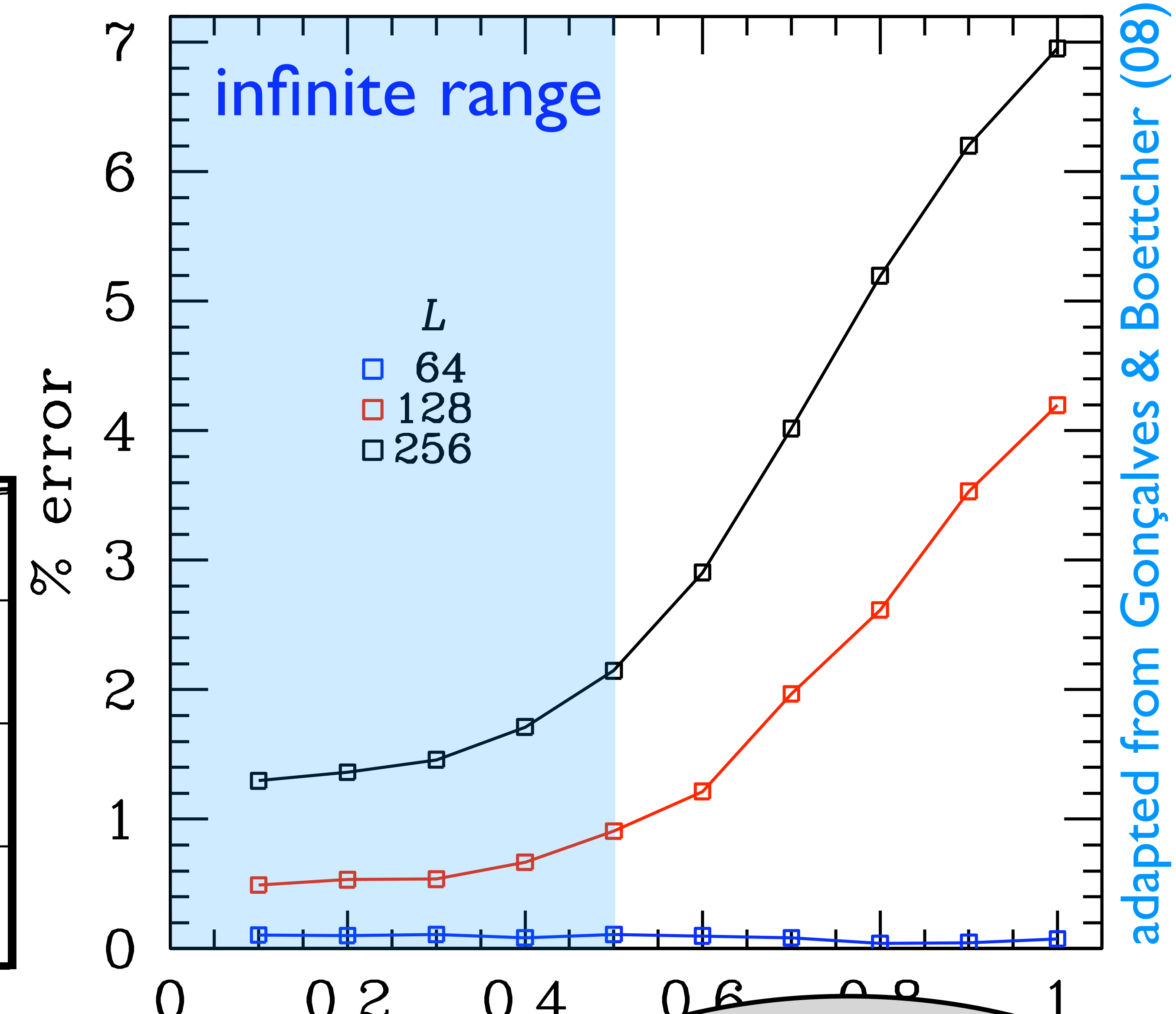

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- The algorithm wo[…] range regime.

Other algorithms tested: PT, hBOA, BCP, ...

New insights from one-dimensional spin glasses

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- Summary:
  - Do short-range spin glasses order in a field? No.
  - Are short-range spin glasses ultrametric? Seems like it.
  - What does this mean? The mean-field solution works only for certain aspects.
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