Baxter-Wu model in transverse magnetic field

Sylvain Capponi

Laboratoire de Physique Théorique - IRSAMC
Université Paul Sabatier Toulouse 3

UNIVERSITÉ TOULOUSE III PAUL SABATIER

Université de Toulouse

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Outline

- Introduction
  - Multi-spin interactions
  - Reminders about some classical models
- Adding quantum fluctuations
  - perturbative approach
  - exact quantum Monte-Carlo (QMC) approach
  - Quantum/thermal phase transitions
  - Global phase diagram

Collaborators

- Fabien Alet (Toulouse)
- Saeed Jahromi (Teheran)
- Kai Schmidt (Dortmund)

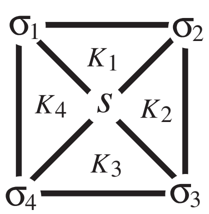
Ref: S. Capponi, S.S. Jahromi, F. Alet, and K. P. Schmidt, arXiv:1403.1406

Multispin interactions in Statistical Mechanics

Relevant for adsorbed atoms on graphite

Could be implemented with trapped ions Bermudez et al. PRA 2009

Rather natural extension:

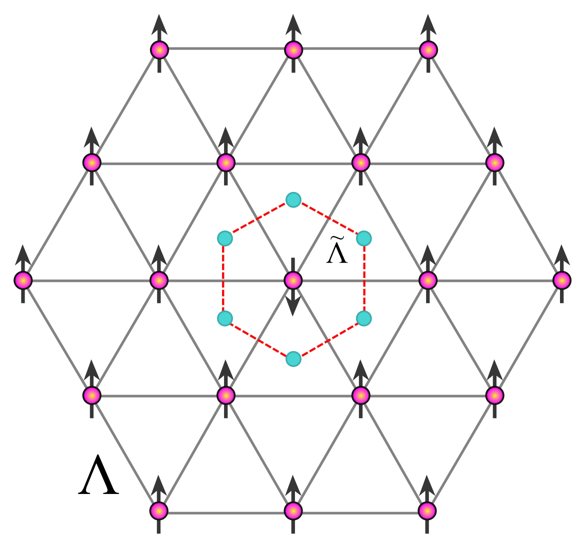


Ising model with 3-spin interaction on the union-jack lattice can be solved using 8-vertex model results Hinterman & Merlini, 1972

Baxter-Wu model

Baxter & Wu , 1973

$$\mathcal{H} = -J \sum_{\langle ijk \rangle} \sigma_i^z \sigma_j^z \sigma_k^z$$



ground-state has deg. 4 $|\uparrow\uparrow\uparrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\rangle$

same universality class as 4-state Potts model *without* log corrections

Recent generalization to arbitrary 3-colorable graph

Huang et al., Nucl. Phys. B 2013

Multispin interactions in Statistical Mechanics

BW is related to 2d Ising with m-spin interaction in 1 (space) dimension and 2-spin in 1 (time) dimension

Debierre-Turban, Penson, Igloi,…, 80's

$$\mathcal{H} = -\sum_{(i,j)} \left(J_y \sigma^z_{i,j} \sigma^z_{i+1,j} + J_x \prod_{\ell=0}^{m-1} \sigma^z_{i,j+\ell} \right)$$

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equivalently 1d Ising with multi-spin interactions in transverse field

$$\mathcal{H} = -\lambda \sum_i \sigma_i^z \sigma_{i+1}^z \ldots \sigma_{i+m-1}^z - h \sum_i \sigma_i^x$$

self-dual at $h = \lambda$ with 2nd (resp. 1st) order phase transition for $m \leq 3$ (resp. >3)

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Many results have been obtained on Ashkin-Teller like models too

$$\mathcal{H}_{\mathrm{AT}} = -\sum_{\langle ij \rangle} \left(\sigma_i^z \sigma_j^z + \tau_i^z \tau_j^z + K \sigma_i^z \sigma_j^z \tau_i^z \tau_j^z \right)$$

Ashkin & Teller, 1943

deep relations between them

Huang et al., Nucl. Phys. B 2013

Baxter-Wu model

- **Duality relation** $$T_c = 2J/\log(\sqrt{2}+1) \simeq 2.269J$$

- **exact solution** (using coloring problem + Bethe ansatz technique)

Phase transition at T_c in the same universality class as **4-state Potts model**

$$\alpha = 2/3 \quad \nu = 2/3 \quad \eta = 1/4 \quad \beta = 1/12$$

without logarithmic corrections !

- numerically **difficult** to simulate/analyze

- **Our goal: include quantum fluctuations**

Add a transverse field →

$$\mathcal{H} = -J \sum_{\langle ijk \rangle} \sigma_i^z \sigma_j^z \sigma_k^z - h \sum_i \sigma_i^x$$

Methods

- T=0 series expansion for large/small field
- large-scale quantum Monte-Carlo simulations

About large h:
unique ground-state with spins polarised along field

About small h: use duality ! New model on honeycomb lattice

$$\mathcal{H}_{\mathrm{dual}} = -J \sum_{i \in \tilde{\Lambda}} \tau_i^z - h \sum_{p \in \tilde{\Lambda}} \tau_1^x \tau_2^x \tau_3^x \tau_4^x \tau_5^x \tau_6^x$$

Series expansion

see also Jahromi et al. 2013

$$e_0^{\mathrm{hf}} = -1 - \frac{1}{3}J^2 - \frac{19}{216}J^4 - \frac{5359}{34020}J^6 - \frac{500690327}{1371686400}J^8 - \frac{74305313819}{72013536000}J^{10}$$

$$e_0^{\mathrm{lf}} = -2 - \frac{1}{12}h^2 - \frac{1}{864}h^4 - \frac{19}{155520}h^6 - \frac{1133}{238878720}h^8 - \frac{12026279}{2708884684800}h^{10}$$

hints toward a first order phase transition,
however series expansion becomes less reliable there…

What about thermal fluctuations too ?

QMC implementation

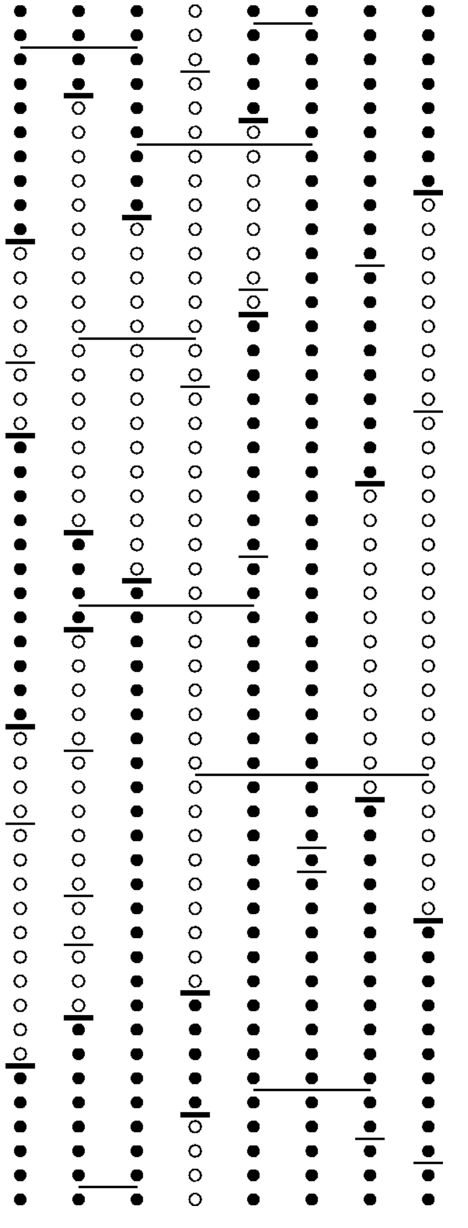
- Based on Stochastic Series expansion (Sandvik 90's)

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | \mathcal{H} | \alpha_{n-1} \rangle \ldots \langle \alpha_2 | \mathcal{H} | \alpha_1 \rangle \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle$$

- Cluster update similar to the one used for Ising model in transverse field (Sandvik 2003), although here we do not have the usual Z_2 symmetry $\sigma^z \rightarrow -\sigma^z$

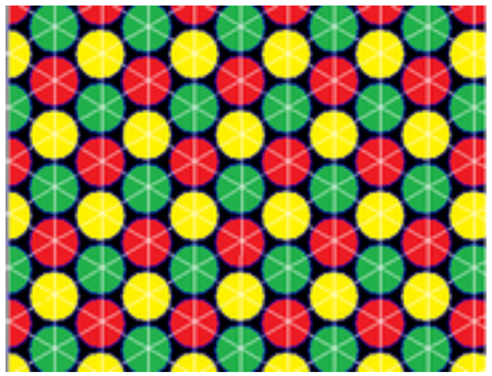
- Defining 3 sublattices A,B,C, we have instead the following symmetry:

If one sub lattice is "frozen" then we can reverse the spins on the 2 others



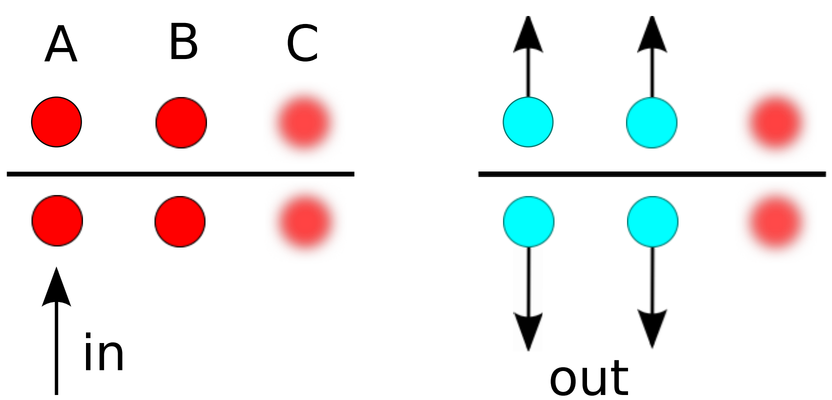
Sandvik PRE 2003

QMC implementation



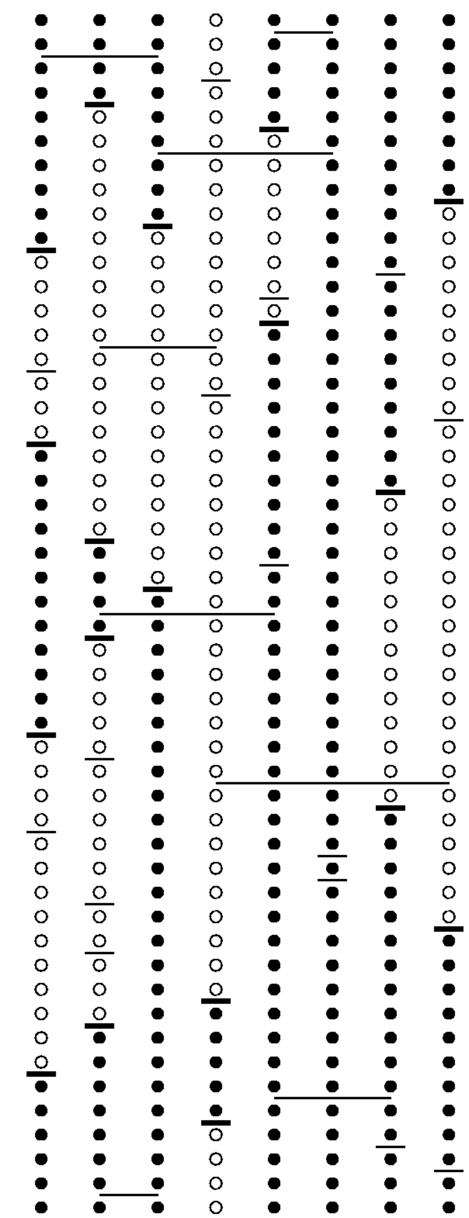
Use 3-sublattice decomposition

If one sub lattice is “frozen” then we can reverse the spins on the 2 others

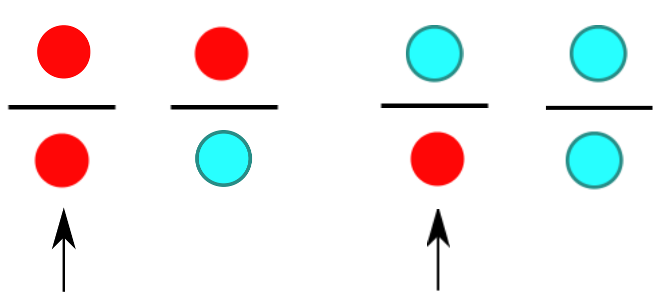


same weight !

flip with proba 1



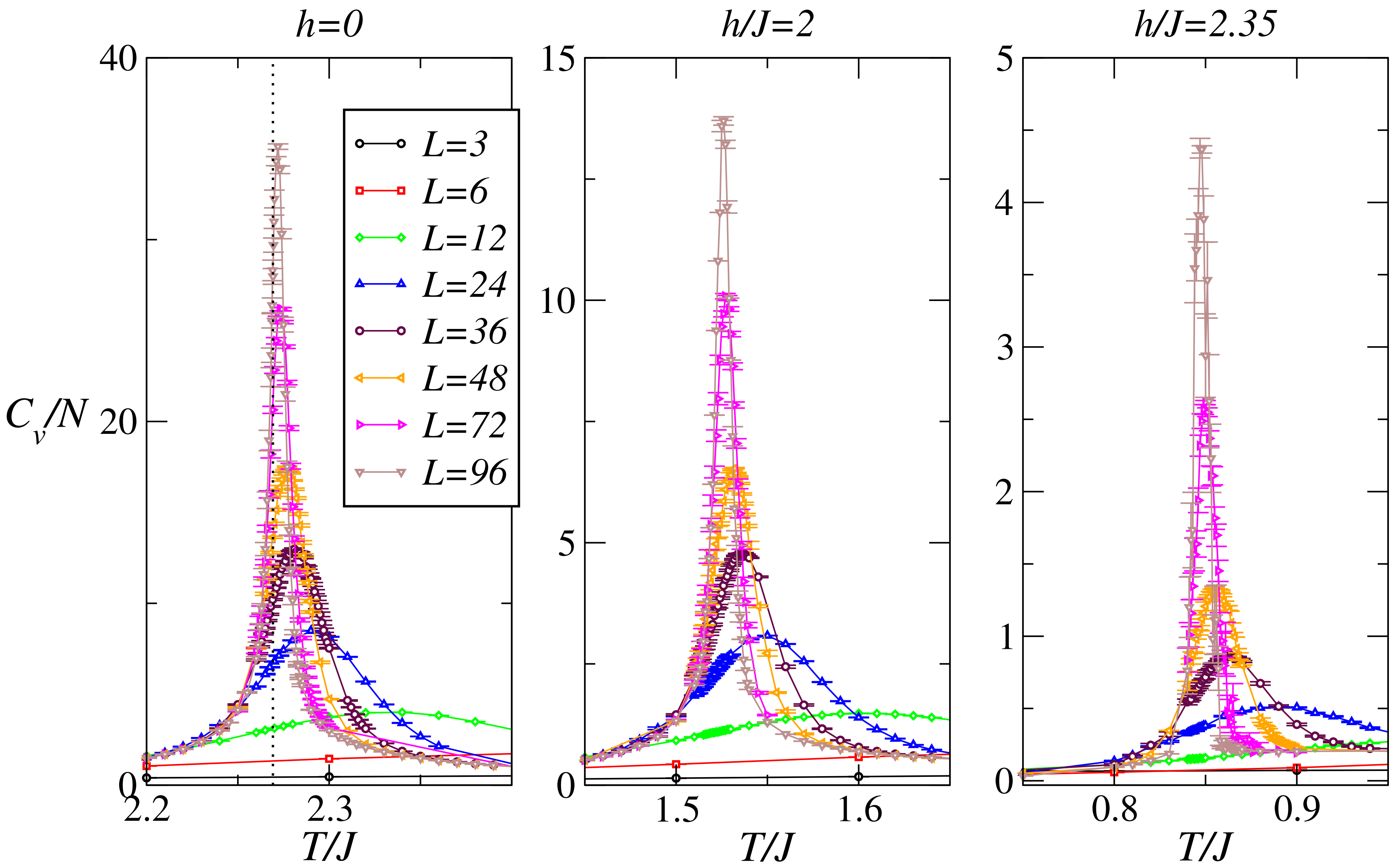
Cluster update using worms can be implemented
~ Evertz-Novotny for BW model



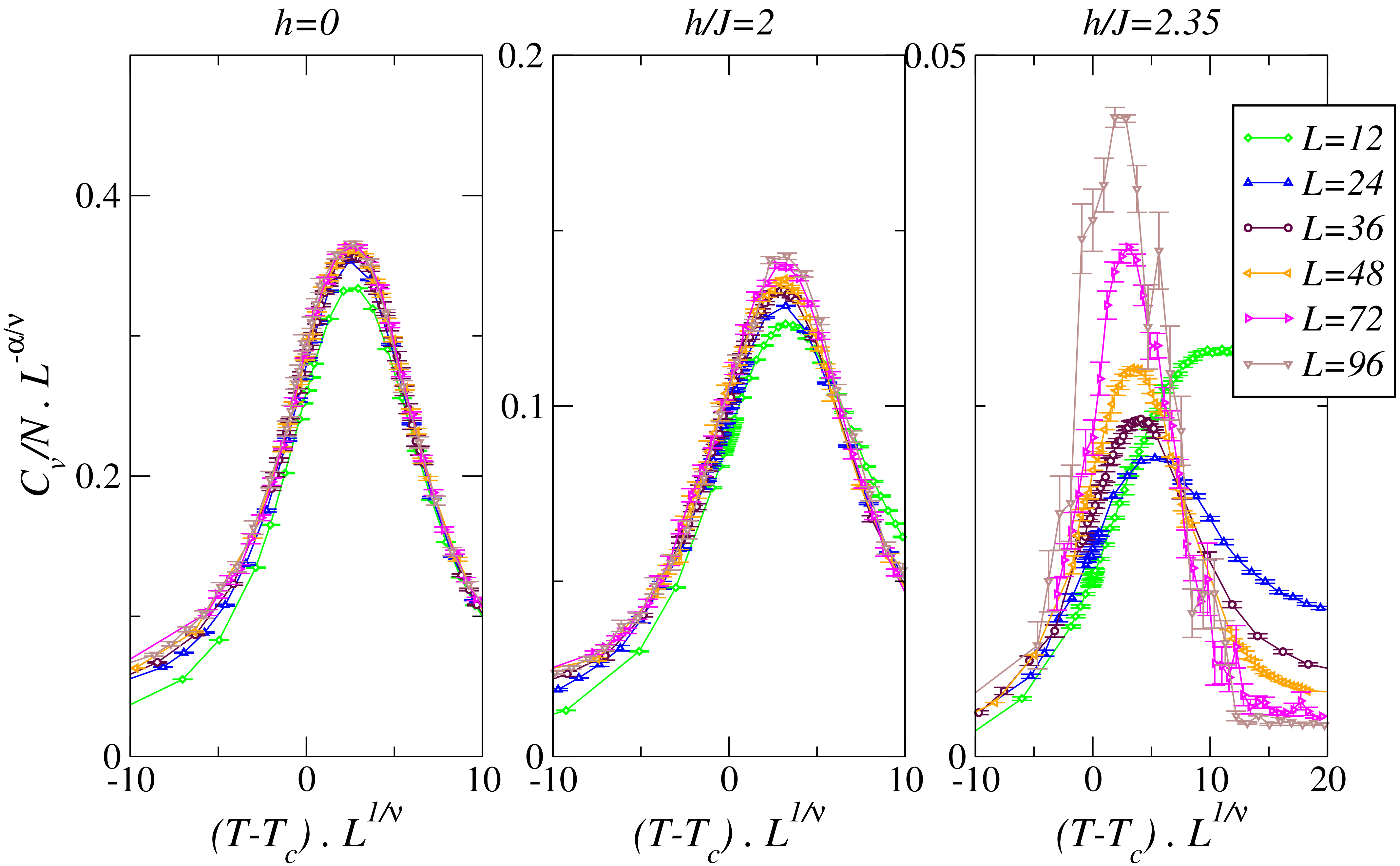
Sandvik PRE 2003

Switching on h: finite-T results

Specific heat data: allows to extract $T_c(h)$



Specific heat collapse using BW critical exponents

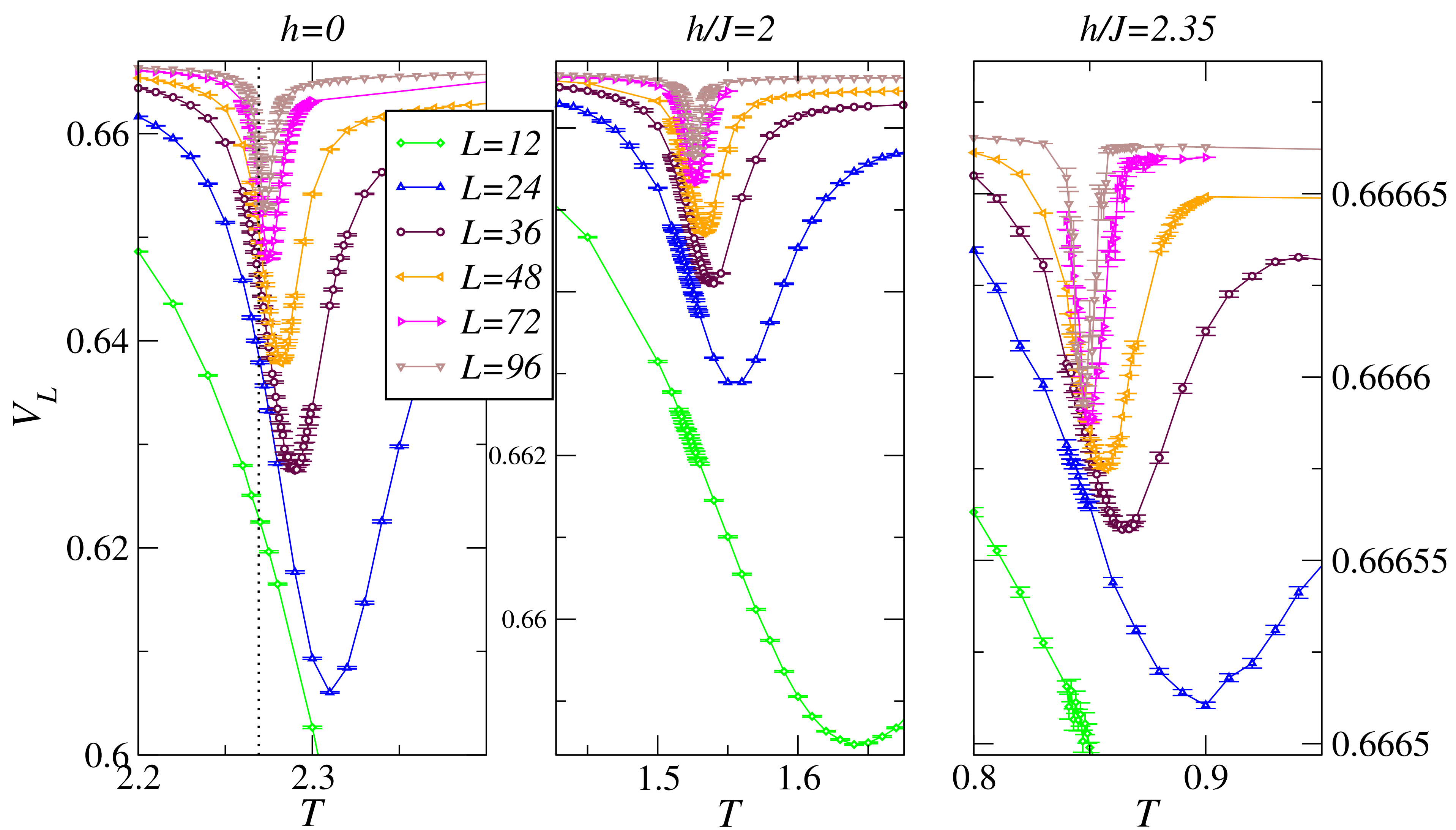


In this case, L^2 divergence: first order ?

Energy Binder cumulant

$$V_L = 1 - \frac{\langle \mathcal{H}^4 \rangle}{3\langle \mathcal{H}^2 \rangle^2}$$

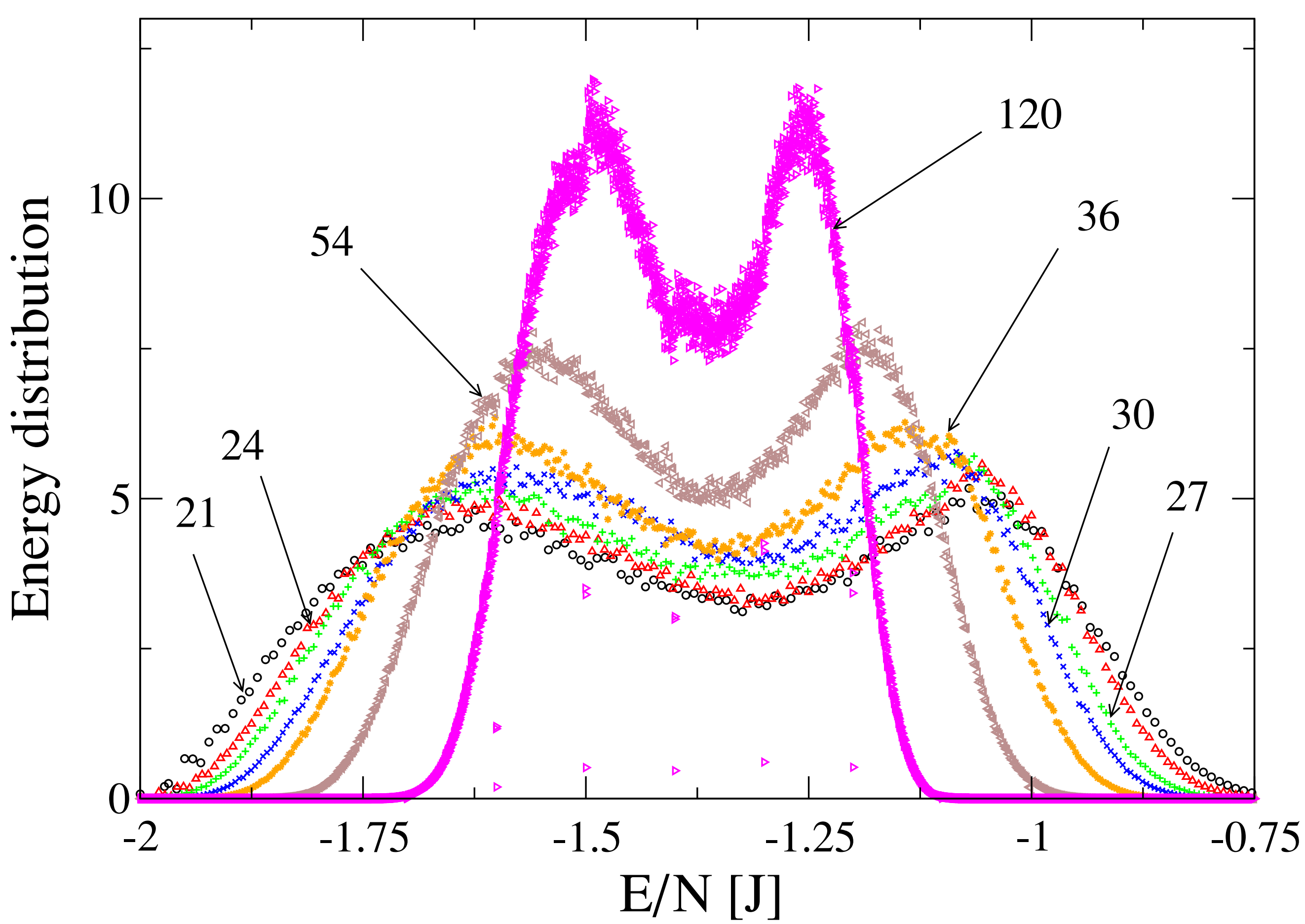
equals 2/3 away from criticality
and also for 2nd order



finite dip: 1st order ?

Energy histograms: classical Baxter-Wu

Schreiber & Adler, J. Phys. A 2005



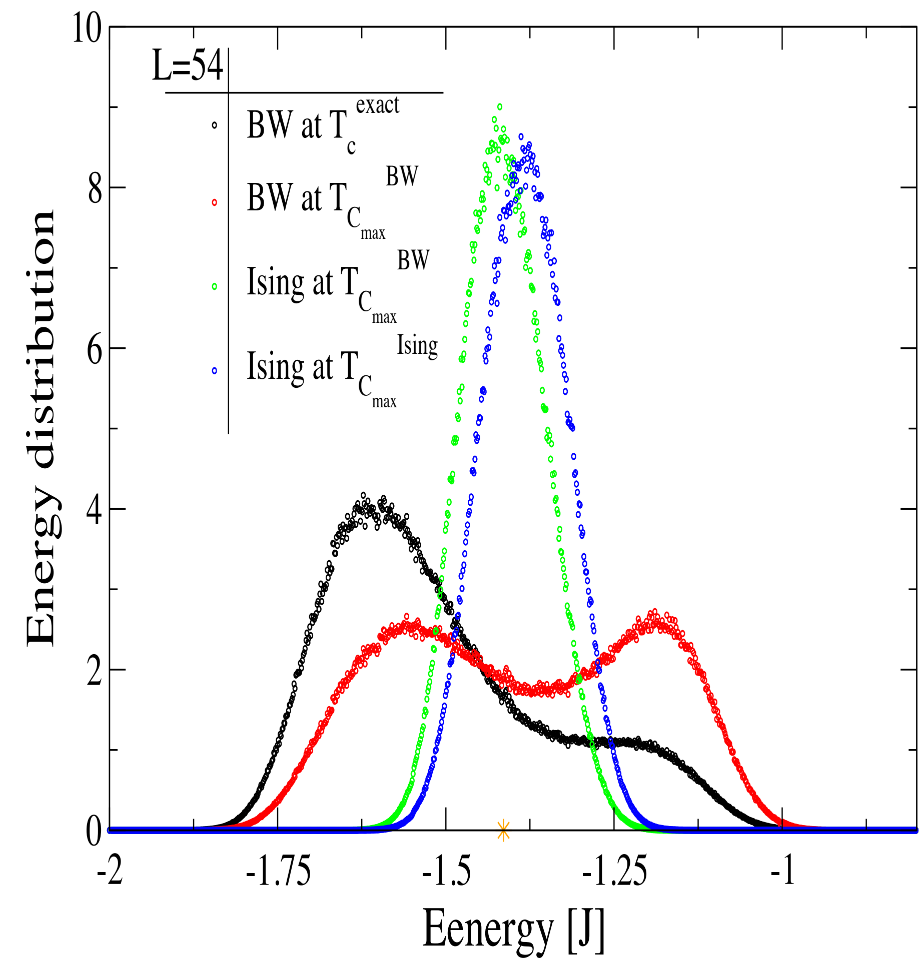
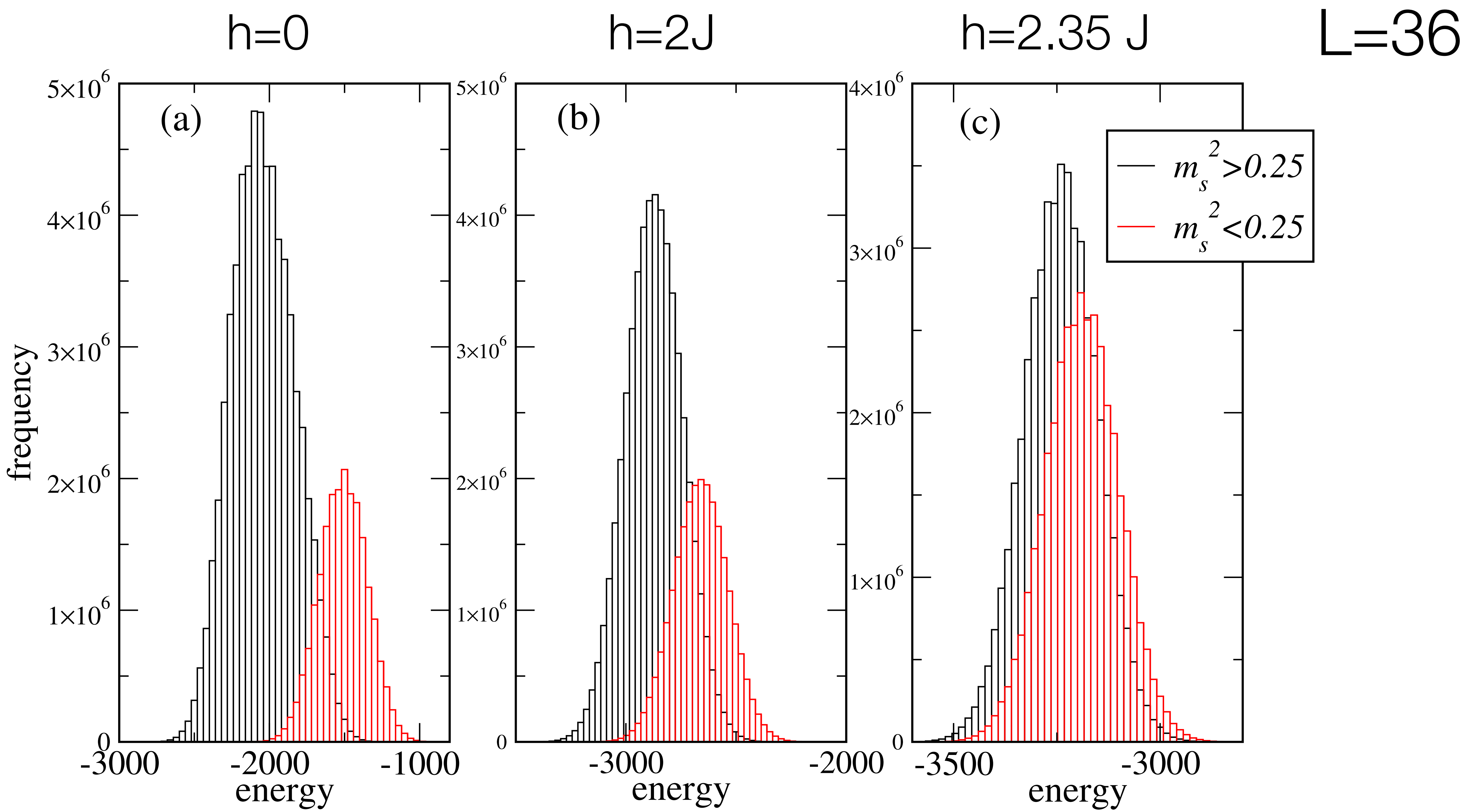


Figure 5. Critical distribution calculated at $T_{C_{\max}}$ for the pure BW model. The lattice sizes are denoted by arrows. The $L = 120$ data suffers from the systematic errors resulting from the DOS calculations for large systems.

Energy histograms



Order parameter

Sublattice magnetization $m_\alpha = 1/(N/3) \sum_{i \in \alpha} \sigma_i^z \,, \quad \alpha = A, B, C$

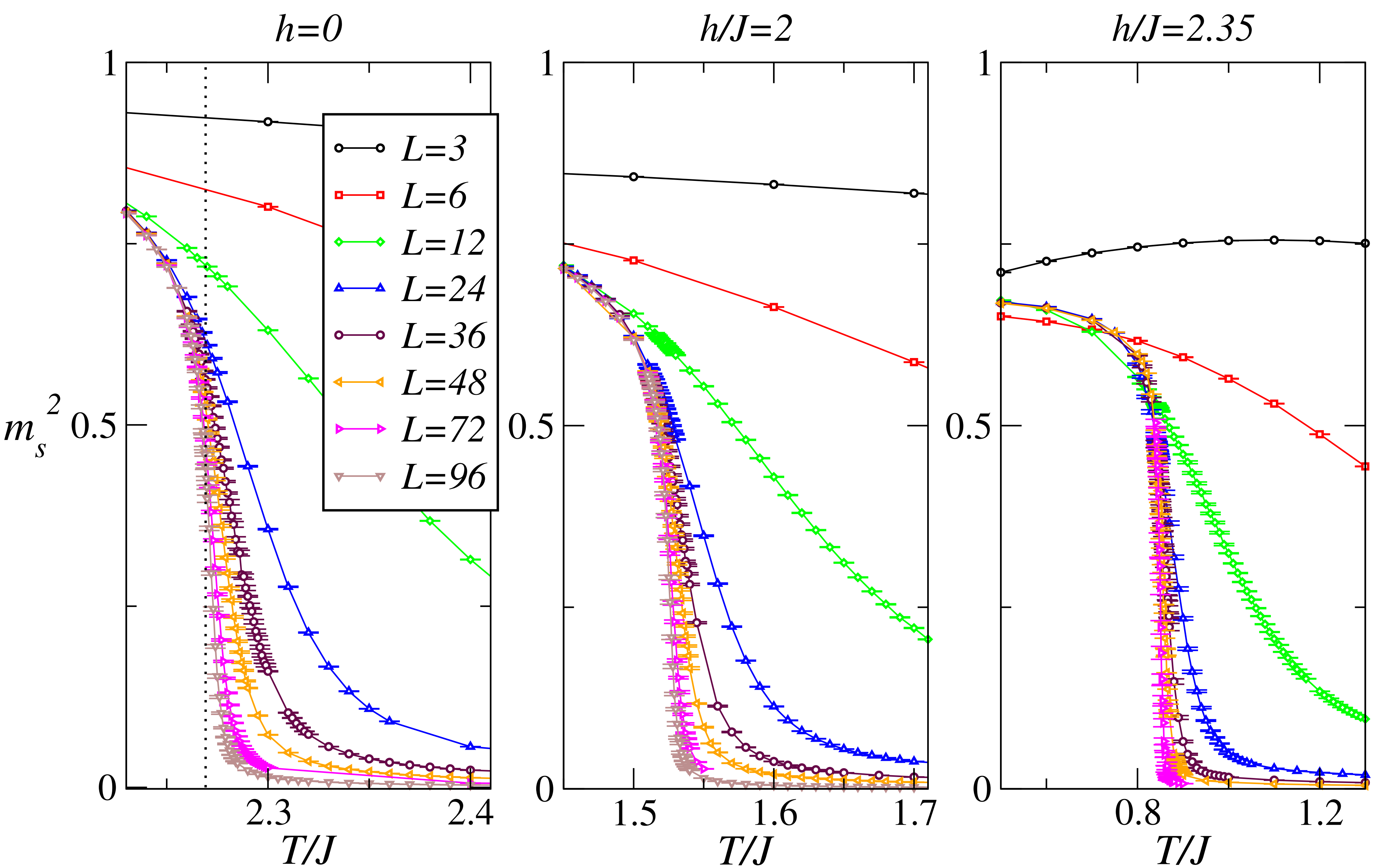
vanishes by symmetry for any finite system

→ $$m_s^2 = \frac{m_A^2 + m_B^2 + m_C^2}{3}$$

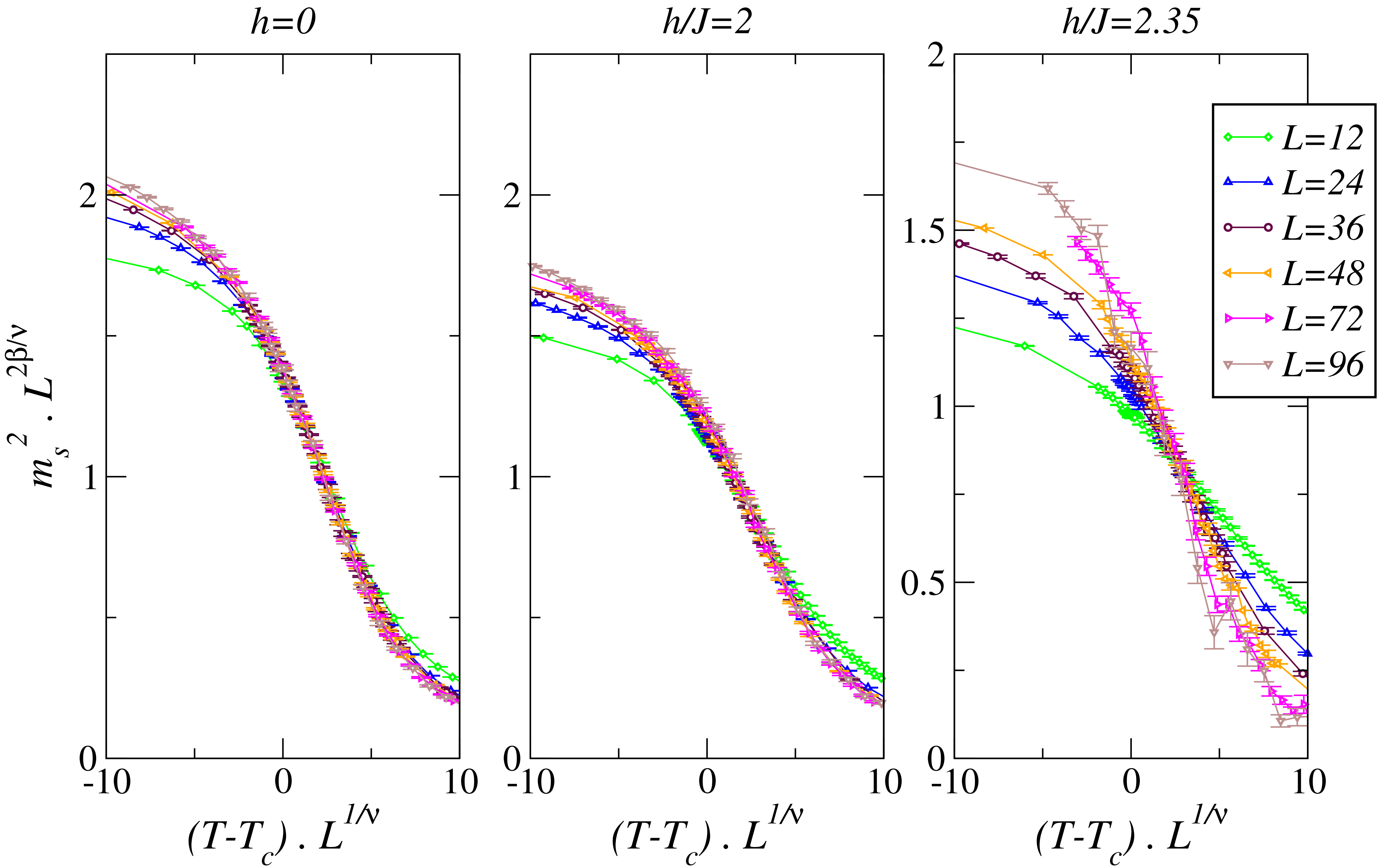
scaling form $\langle m_s^2 \rangle = L^{-2\beta/\nu} f((T - T_c)\, L^{1/\nu})$

usual Binder cumulant $U_L = 1 - \frac{3}{5} \frac{\langle m_s^4 \rangle}{\langle m_s^2 \rangle^2}$

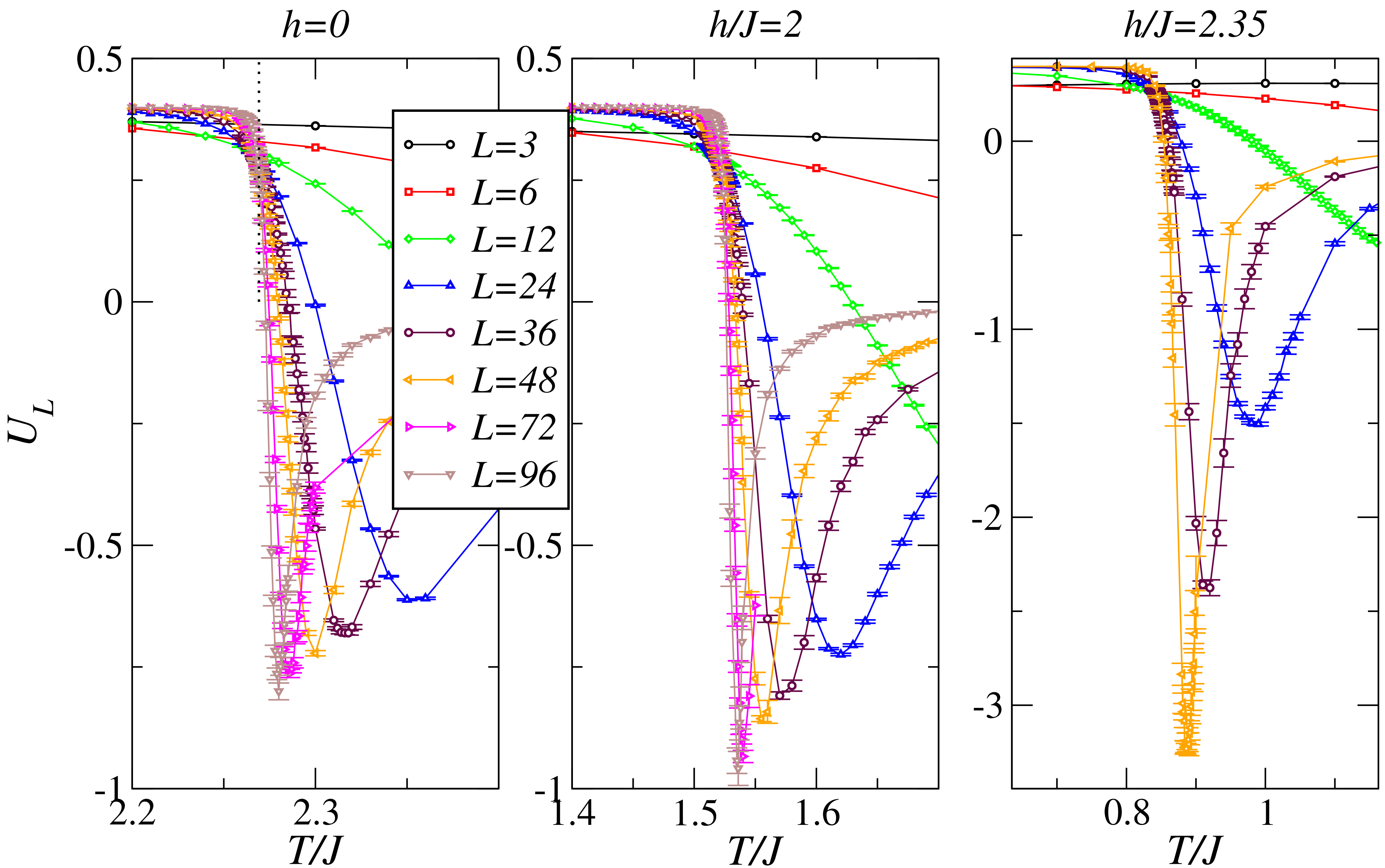
Numerical data



Scaling analysis using BW exponents



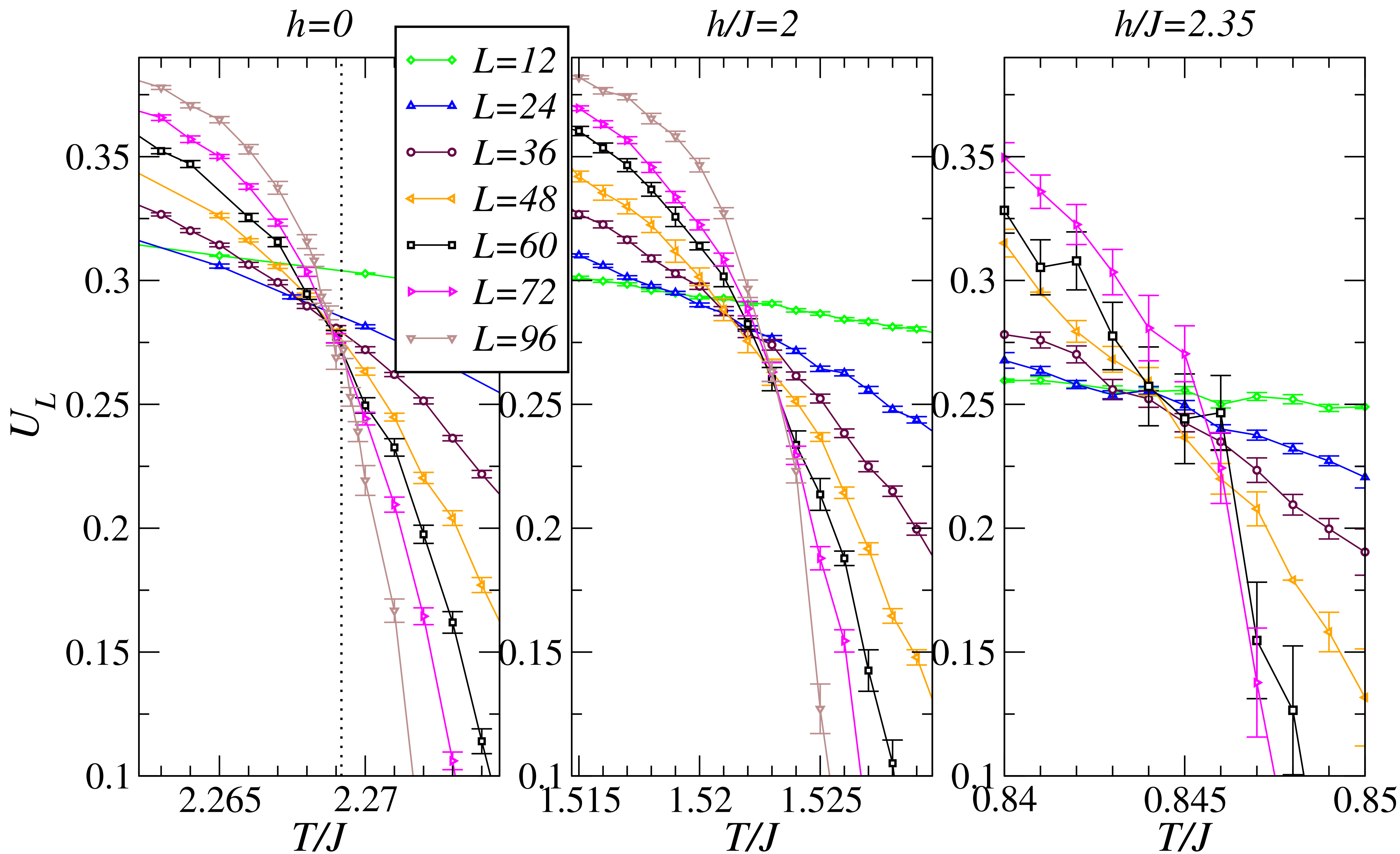
Order parameter Binder cumulant



Negative values even for the pure BW !?

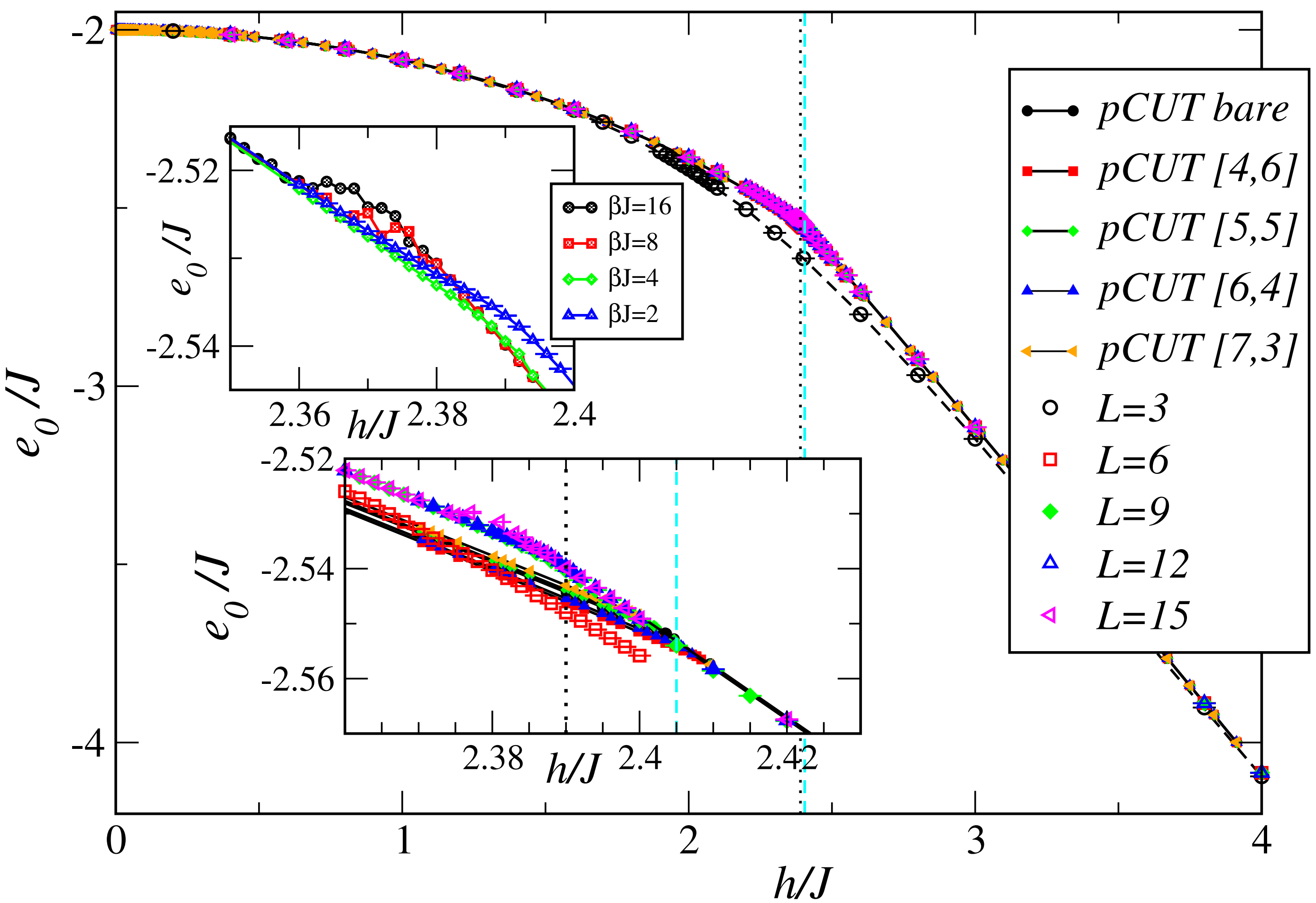
Schreiber and Adler, J. Phys. A 2005

Order parameter Binder cumulant



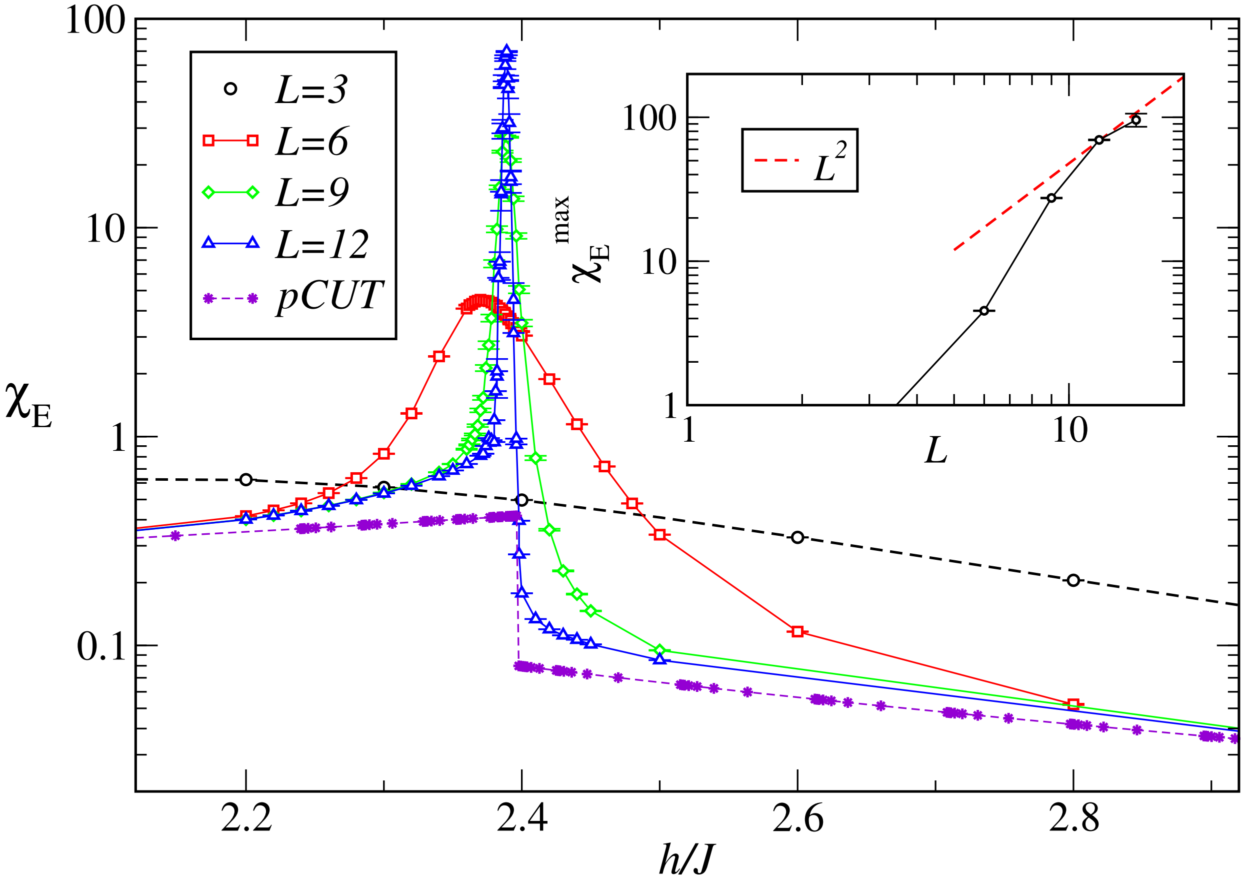
Different crossing values = different universality class

T=0 results: energetics



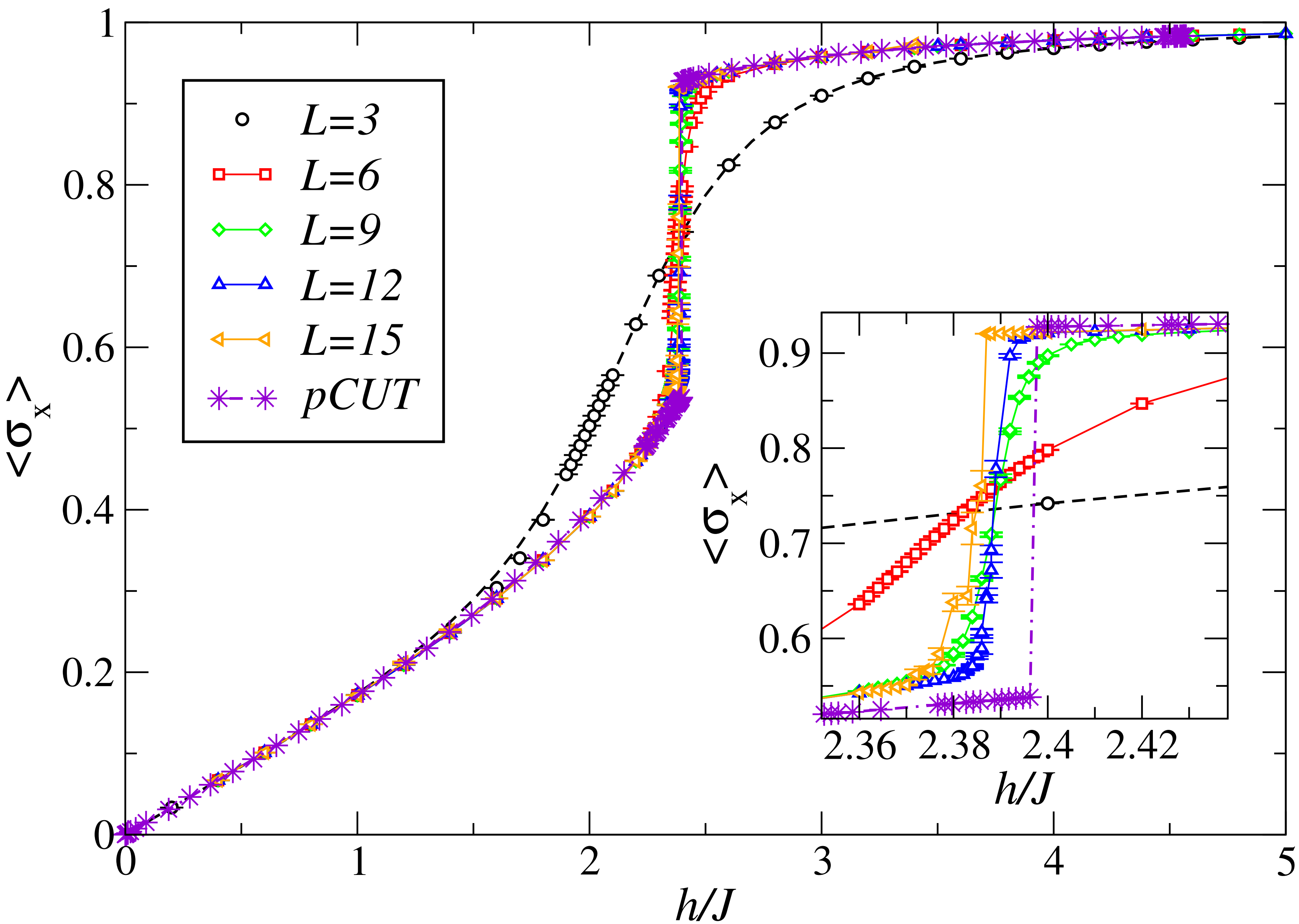
$$\chi_E = -\frac{\partial^2 e_0}{\partial h^2}$$

$$\sim \begin{cases} L^{2/\nu-(d+z)} & \text{for 2nd order} \\ L^d & \text{for 1st order} \end{cases}$$



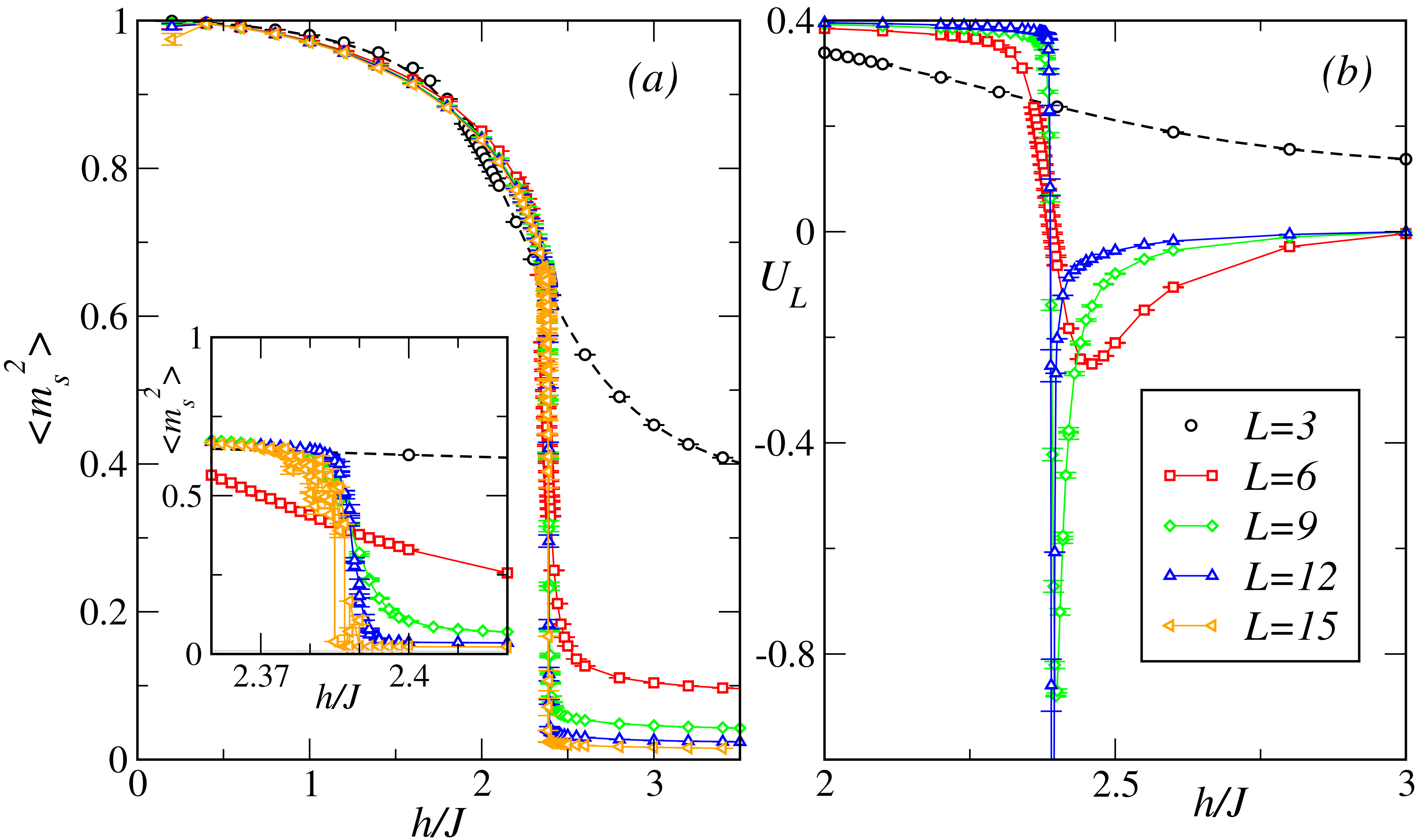
hard simulations,
hysteresis ...

T=0: magnetization along field



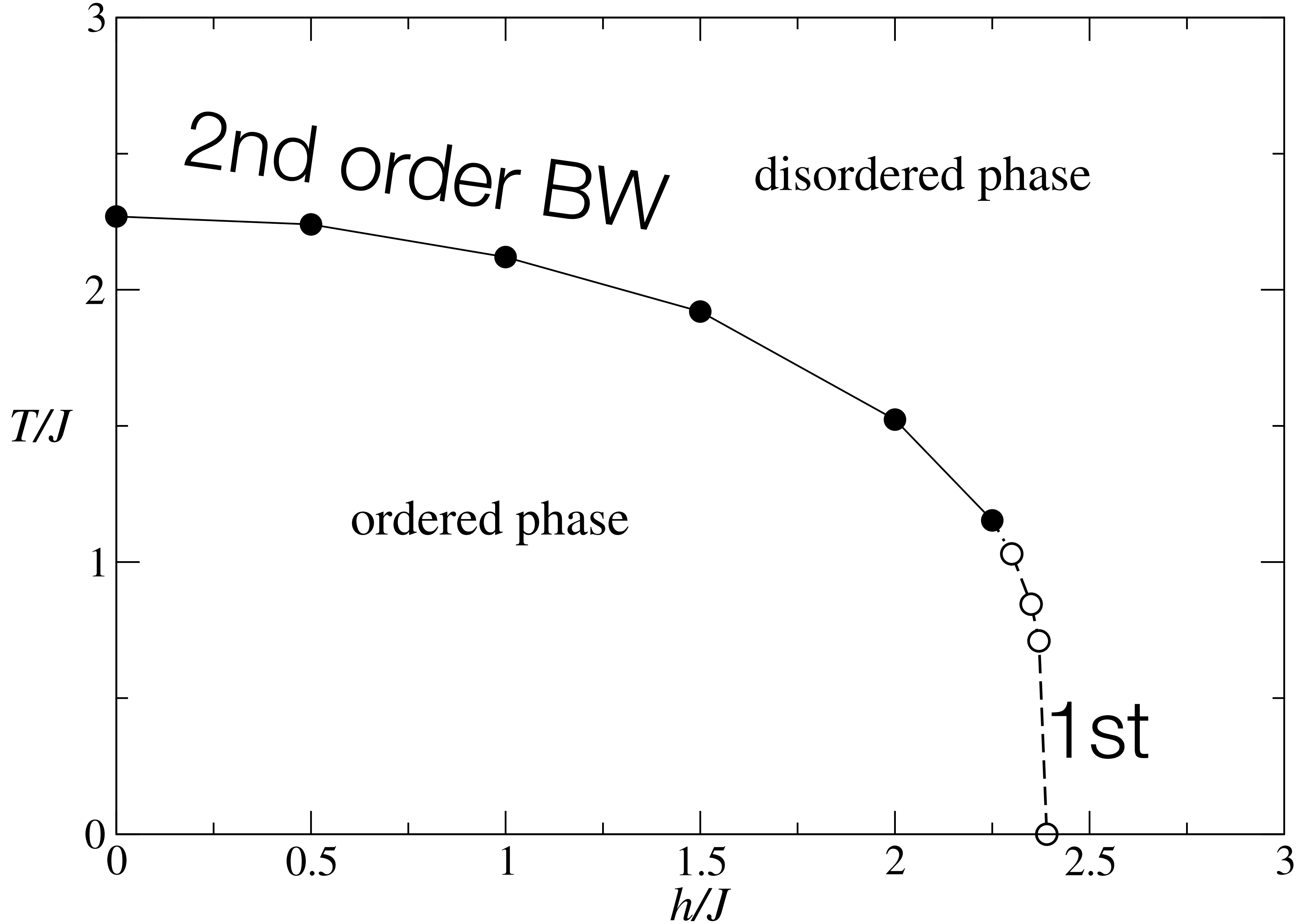
Clear jump forming at the QPT $h \simeq 2.39J$

T=0: order parameter



Binder cumulant has large negative values: 1st order

Global phase diagram: tricritical point ?



Conclusions

- Study of a minimal model with 3-spin interactions, thermal and quantum fluctuations
- Large region of **2nd order** phase transition in the same universality class as the classical model (different from the longitudinal field that breaks symmetry)
- At and close to T=0 QPT, **1st order** behaviour instead → **tricritical point !**
- Efficient large-scale numerical algorithm

Perspectives:

- Characterize this tricritical point
- Models with competing 2-spin and *m*-spin interactions + *h*
- Model is isospectral to topological color code with magnetic field

Jahromi et al. 2013