Participation spectroscopy and entanglement Hamiltonian of quantum spin models

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PRL **112**, 057203 (2014)

PRB **89**, 165106 (2014)

Review
JSTAT, P08007 (2014)

PRB **90**, 125105 (2014)

CCQS, Évora, October 2014

Introduction

- Question : How much a wave-function is localized in a given (computational) basis ?

$$|\Psi\rangle = \begin{pmatrix} . \\ . \\ \vdots \\ . \end{pmatrix}_{\{|i\rangle\}}$$

- Various motivations :
- Localization physics : Anderson (single-particle, disorder), many-body localization
- Complexity theory : how many states needed to describe correctly phenomena ? (variational methods, computational complexity)
- Relation to multifractal analysis

  - Will concentrate on wave-functions ground-states of quantum many-body lattice problems

Part 1 : Introduction

1. Definitions & generalities
2. Methods to compute participation
3. Basis dependence ?

Definitions

$$|\Psi\rangle = \sum_i a_i |i\rangle$$

- Assume normalized wave-function $\sum_i |a_i|^2 = 1$
- Moments = typical tools for measuring localization
- Historically : Inverse Participation Ratio (IPR) $IPR^{-1} = \sum_i |a_i|^4$
- More generally, define basis state participation $\boxed{p_i = |a_i|^2}$

Participation entropies

$$\boxed{S_q = \frac{1}{1-q} \ln \sum_i p_i^q} \qquad q \neq 1$$

$$\boxed{S_1 = \lim_{q \to 1} S_q = -\sum_i p_i \ln(p_i)}$$

Simple expectations

- Denote by $\mathcal{H}$ the size of configuration space $|\Psi\rangle = \sum_i a_i |i\rangle$

- Consider the simple wave-function $a_i = \begin{cases} \frac{1}{\sqrt{\mathcal{N}}} & \forall i \in 1 \ldots \mathcal{N} \\ 0 & \text{otherwise} \end{cases}$

- One simply obtains $S_q = \ln(\mathcal{N})$

- Scaling : $S_q \propto \ln(\mathcal{H})$: delocalized

  $S_q = O(1)$: localized

- Remark 1 : Many-body problem : $\mathcal{H} = \alpha^N$, in general expect

$$S_q \propto N$$

- Remark 2 : Obviously, S_q is basis-dependent !

Is there something else beyond these remarks ?

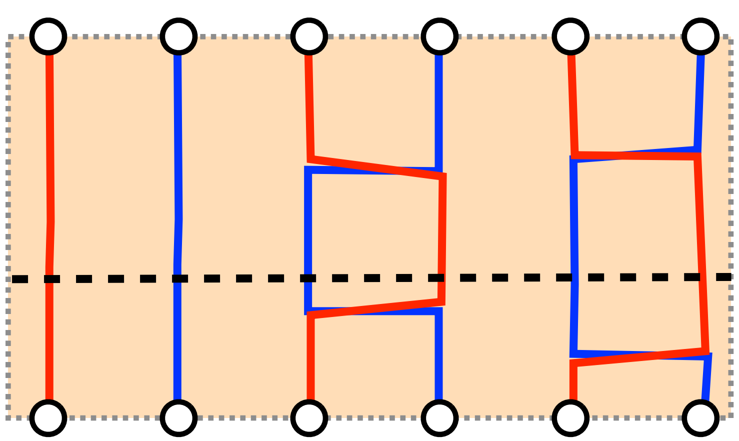
- Main Claim (part 2) $\boxed{S_q = a_q N + \text{universal term}_q + \cdots}$

Computing participation

- Analytics
  - Exact calculations difficult (even for free fermions !)
  - Field theory approach: replica+CFT, free-field

Stéphan *et al.*

- Numerics
  - Exact diagonalization, DMRG : easy (but exact enumeration!)
  - Quantum Monte Carlo: Importance sampling does the exact job !



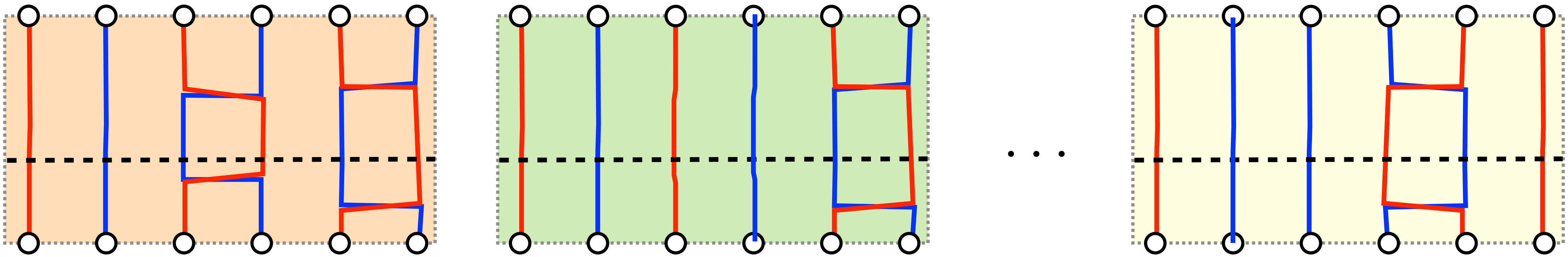
$$|i\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$$

$$p_i^{\mathrm{MC}} \propto \langle i|e^{-\beta H}|i\rangle \overset{\beta\to\infty}{=} a_i^2 = p_i = \langle |i\rangle\langle i|\rangle$$

- Measure Histogram $H(|i\rangle)$ and obtain all S_q
- S_∞ is easily measured as $S_\infty = -\ln(p_{\max})$ Most likely state

Computational replica trick

- Replica trick : Simulate q independent copies



$|i_1\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$ $|i_2\rangle = |\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\rangle$ $\cdots$ $|i_q\rangle = |\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\rangle$

Estimator for $\sum_i p_i^q = \langle \delta_{|i_1\rangle,|i_2\rangle,\cdots,|i_q\rangle} \rangle$

- S_q for integer $q \geq 2$

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Basis dependence & universality

- No generic proof
- Some arguments (to be continued) :
- Some «natural» bases are singled out:
  - Eigenbasis of operators in H (computational QMC basis)
  - Rokshar-Kivelson construction picks up one basis
- Relation between basis:

$$S^{x/z}_{q=1/2} = N \ln(2) - S^{z/x}_{q=\infty}$$ General

$$S^{(x)}_q(h) = S^{(z)}_q(1/h) + \ln(2)$$ 1d Ising

- 1d critical systems: Boundary CFT classifies basis dependence, verified by numerics
- Same basis, same results for systems in the same universality class
- Conjecture: Local unitary transforms does not change subleading terms (or only trivially)

Part II : Review of results

Catalog of universal subleading terms

Review
JSTAT, P08007 (2014)

1) Critical spin chains

2) 2d Spin systems

- Discrete symmetry breaking
- Continuous symmetry breaking

Scaling of participation entopies

- Numerical and analytical evidences for scaling

$$S_q = a_q N + \text{universal term}_q + O(1/N) + \cdots$$

Depends on details
Multifractality

Detects physics!

- Will be illustrated on two spin models

S=1/2 XXZ model $$H = J \sum_{\langle i,j \rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z$$

Transverse-field Ising model $$H = J \sum_{\langle i,j \rangle} \sigma_i^x \sigma_j^x - h \sum_i \sigma_i^z$$

Critical spin chains

Stéphan *et al.*

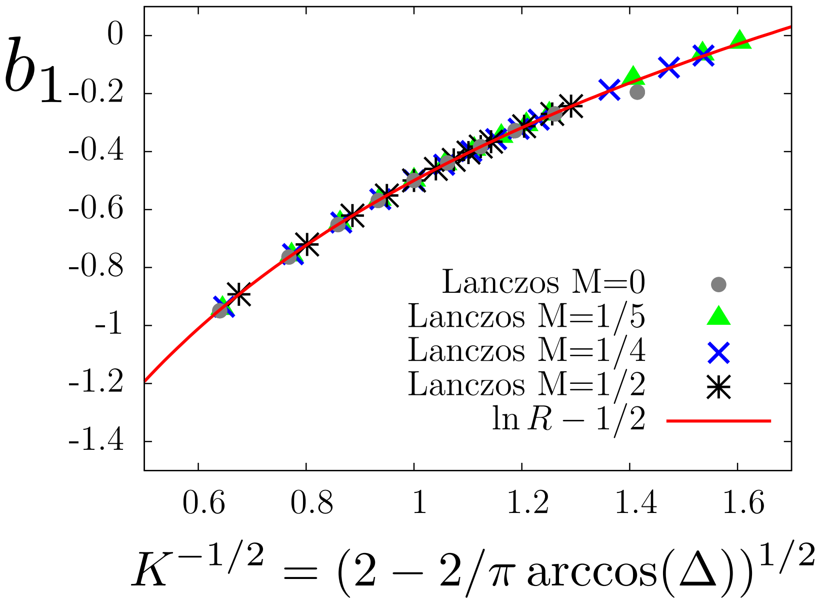
- Numerics + Analytics give strong evidence for universal scaling
- Periodic chains: $S_q = a_q N + b_q + c_q/N + \cdots$

Luttinger liquids

$$b_q = -\frac{1}{2}\left(\ln K + \frac{\ln q}{q-1}\right) \qquad q \le q_c = K\mathcal{D}^2$$

$$b_{q>q_c} = \frac{1}{1-q}\left(q \ln \sqrt{K} + \ln \mathcal{D}\right)$$

Easy way to compute Luttinger parameter !



Ising universality class

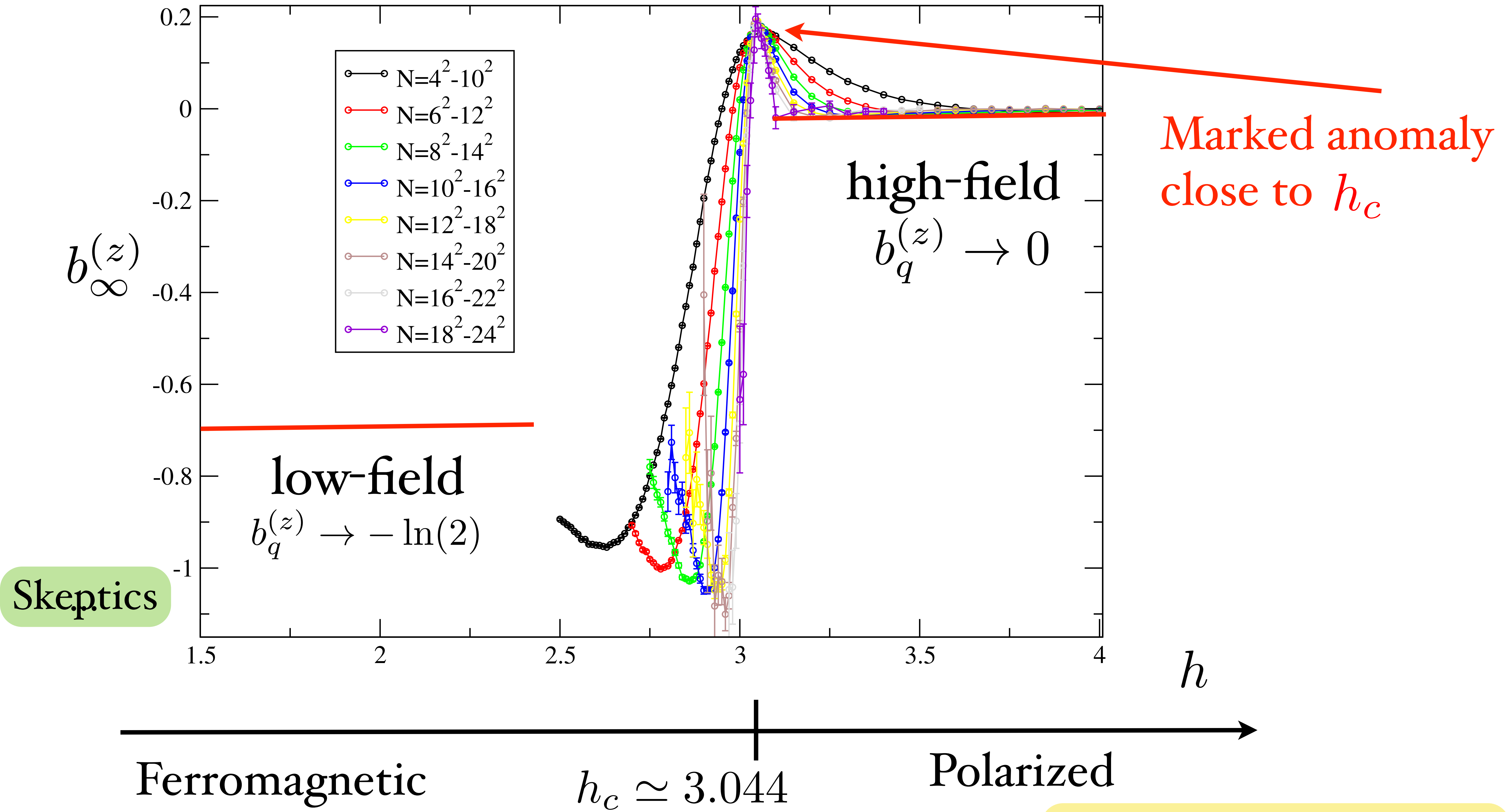
$$b_q^{*(x)} = \begin{cases} 0 & q < 1 \\ 0.25439\cdots & q = 1 \\ \ln(2) & q > 1 \end{cases}$$

- Open chains : $S_q = a_q N + l_q \ln(N) + \tilde{b}_q + c_q/N \cdots$

- How much survives beyond the 1d tractable (exact) cases ?

2d transverse-field Ising model

- QMC data well fitted by $S_q = a_q N + b_q + c_q/N + \cdots$



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2d transverse-field Ising model

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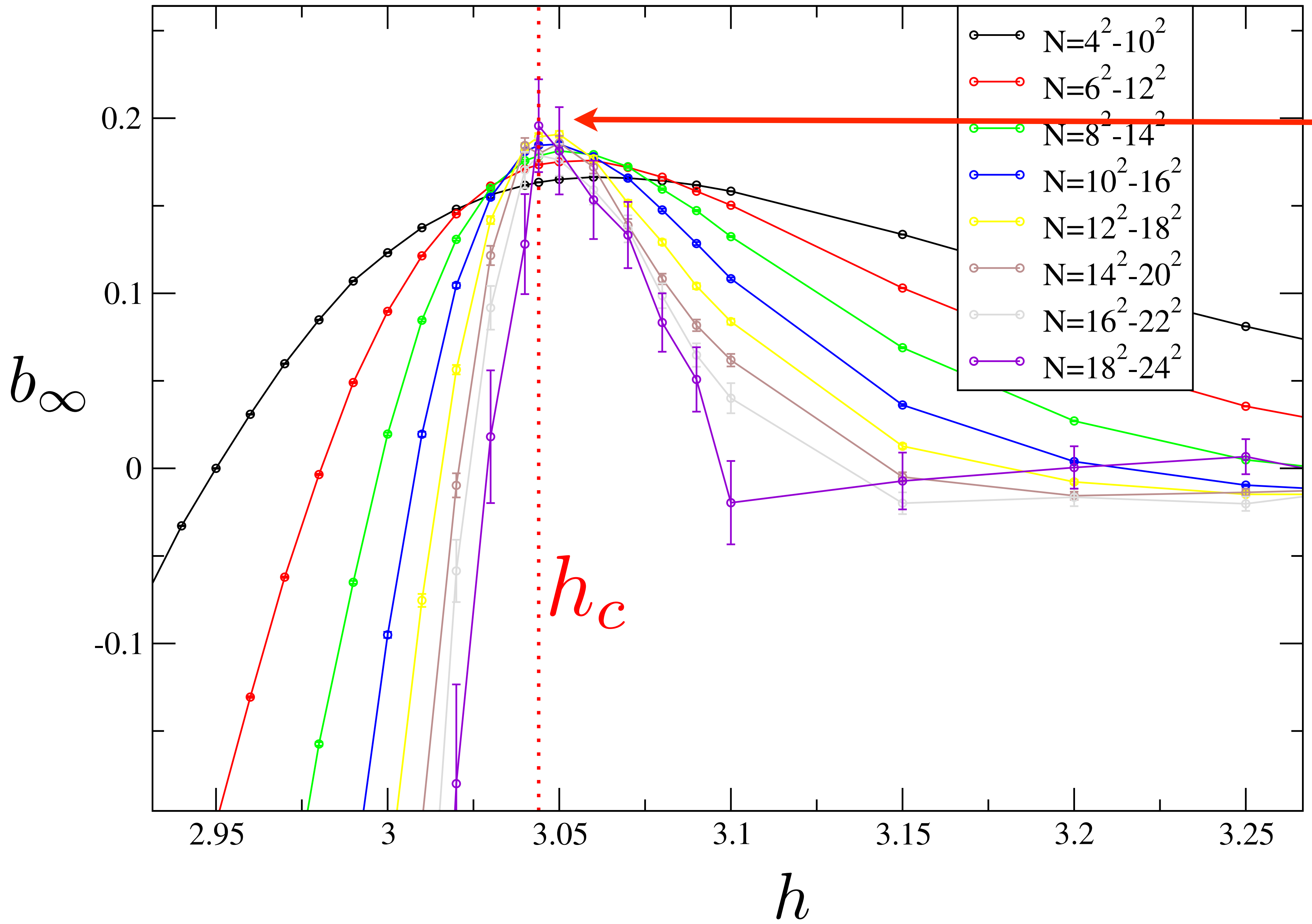
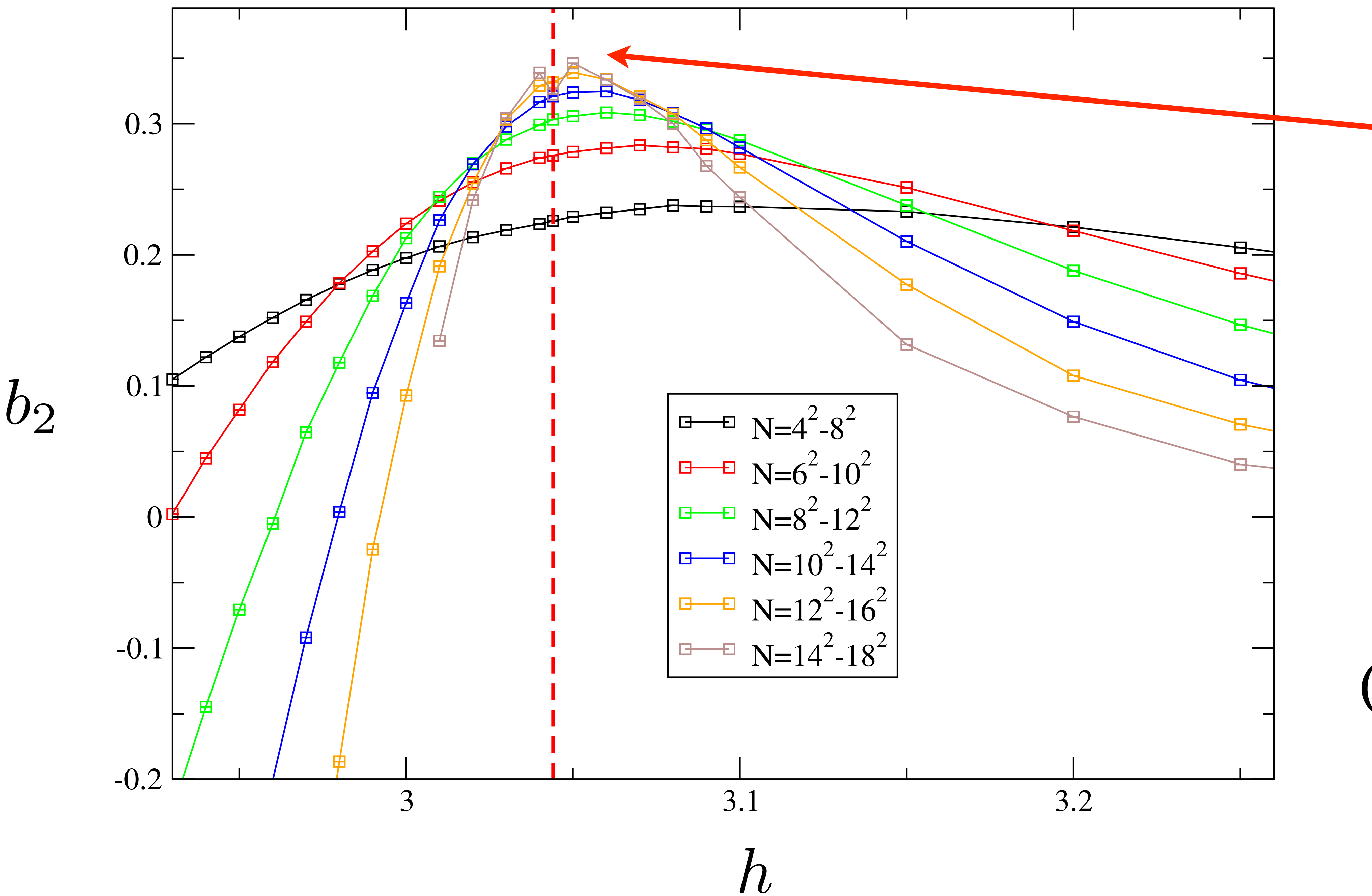


Convergence to a non-trivial value $b^*_\infty \simeq 0.18$

2d transverse-field Ising model

- QMC data well fitted by $S_q = a_q N + b_q + c_q/N + \cdots$

- Similar behavior for $b_2, b_3, b_4 \cdots$



$b_2^* \simeq 0.36$

$b_3^* \simeq 0.26$

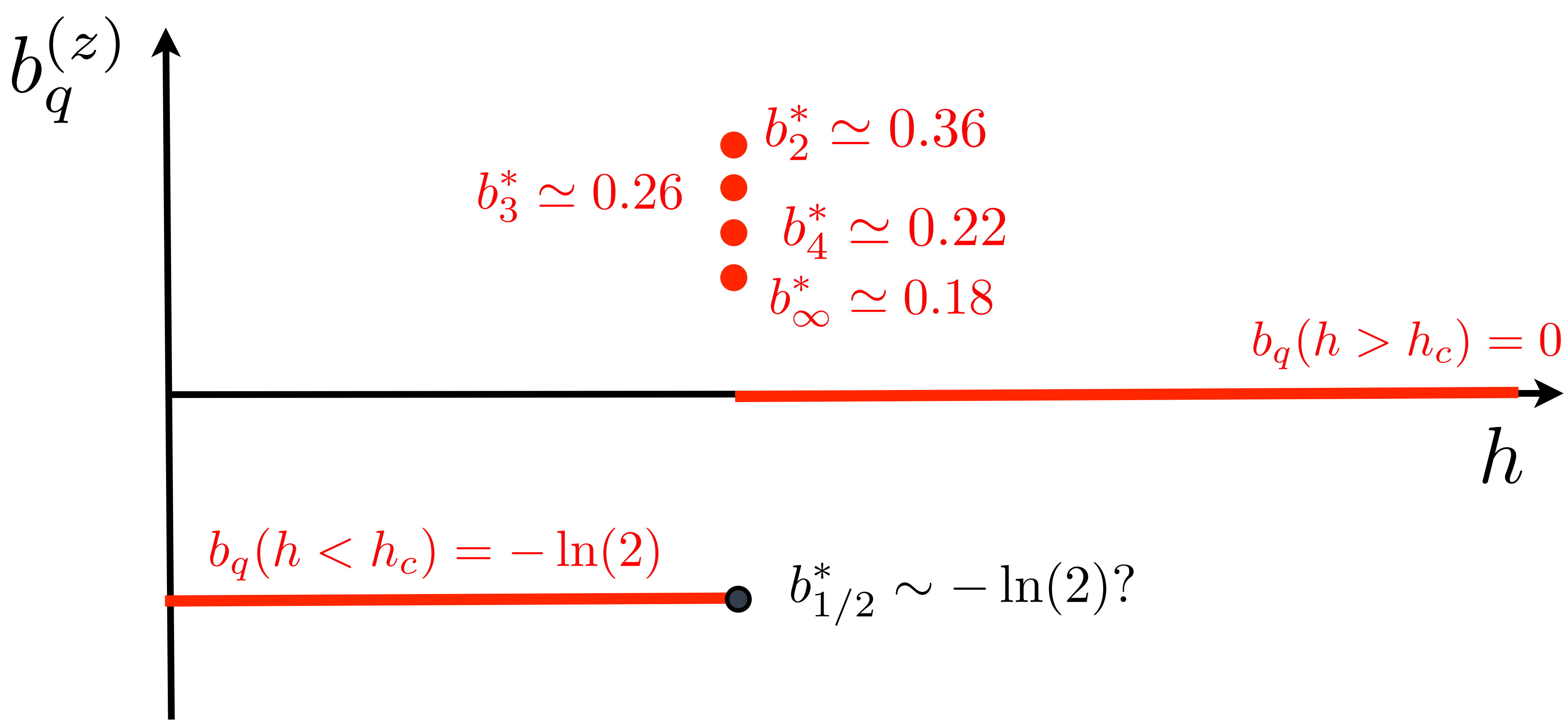
$b_4^* \simeq 0.22$

(not shown)

2d transverse-field Ising model

- QMC data well fitted by $S_q = a_q N + b_q + c_q/N + \cdots$

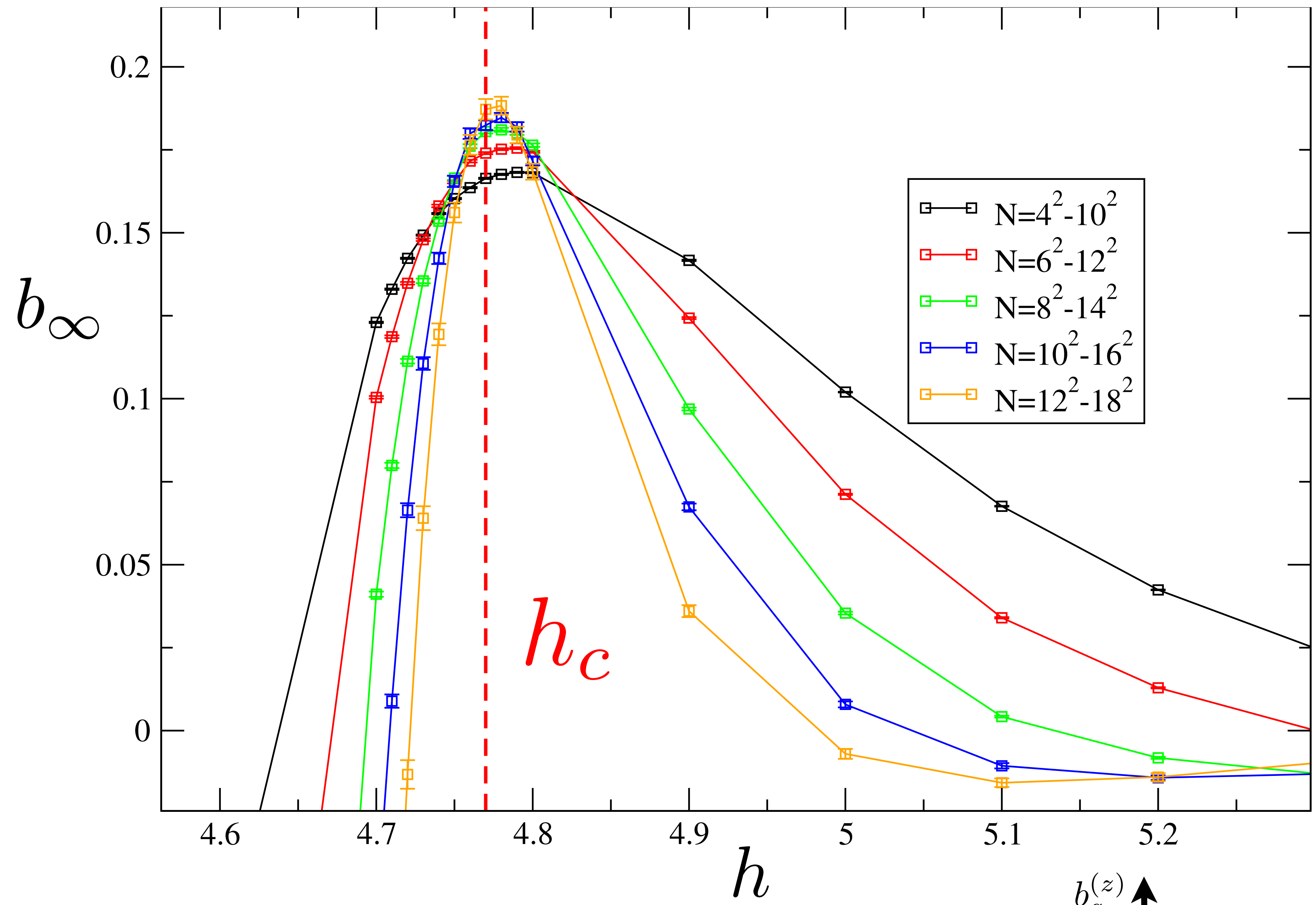
- Summary for $b_q^{(z)}$



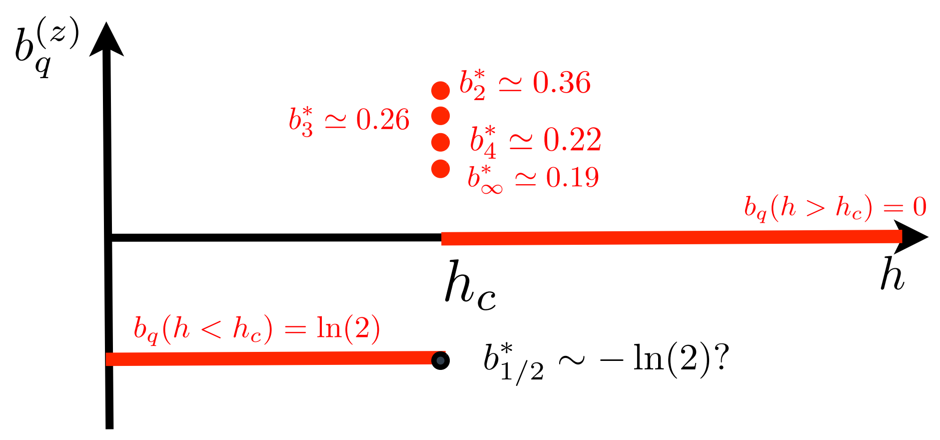
- Non-trivial (universal ?) values at h_c , different from 1d
- Speculation : boundary-induced phase transition at $0.5 \leq q_c \leq 1$?

Universality

- Same model on triangular lattice



- Same constants found at and out of criticality



2d XXZ antiferromagnetic model

$$H = J \sum_{\langle i,j \rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z$$

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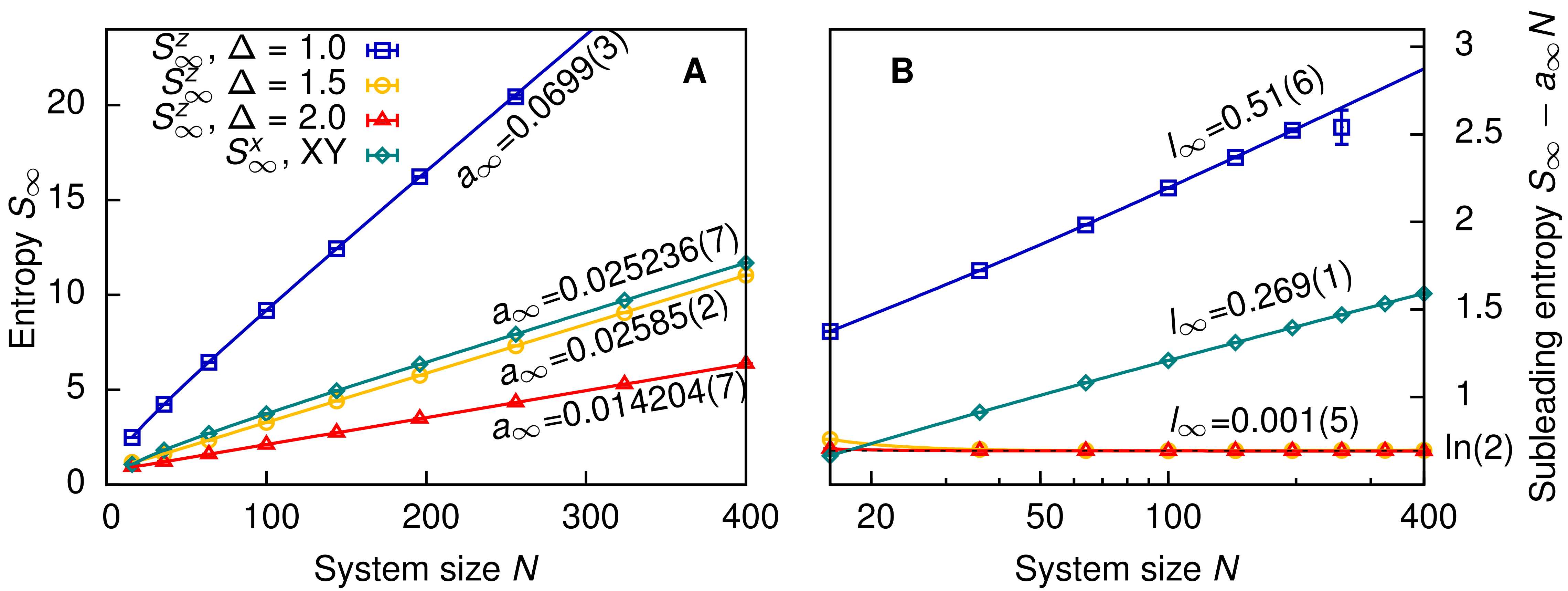
- Long range order in ground-state
  - $0 \leq \Delta \leq 1$ continuous symmetry breaking

QMC data well fitted by $S_q = a_q N + l_q \log(N) + b_q + \cdots$

  - $\Delta > 1$ discrete symmetry breaking : Log vanish



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Log and Goldstone modes

QMC data well fitted by $S_q = a_q N + l_q \log(N) + b_q + \cdots$

- Analytical prediction: Coefficient of log $\propto$ # Goldstone modes

Misguich, Oshikawa *et al.*

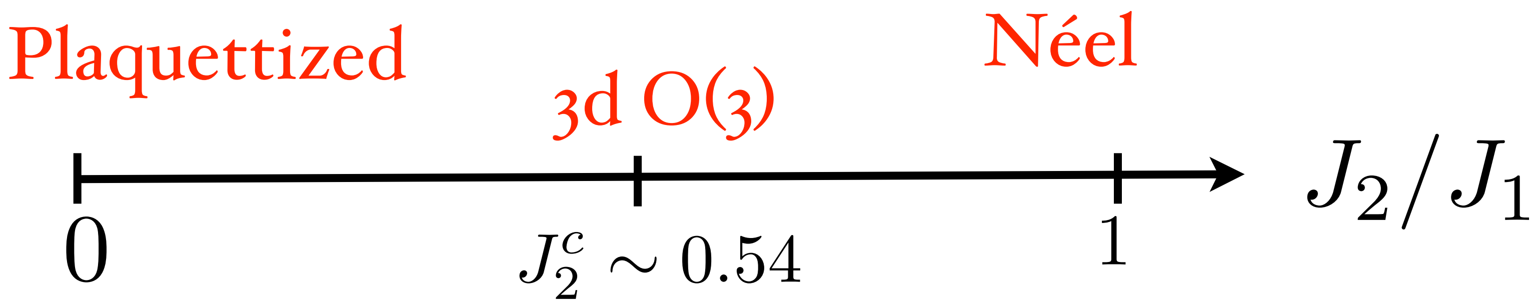
Model	n	$\log(N)$ coef. Ref. [4]	$\frac{N_{\rm NG}}{4}\frac{n+1}{n-1}$
Heisenberg			
$J_2 = 0$	∞	0.460(5)	0.5
$J_2 = -5$	∞	0.58(2)	0.5
$J_2 = 0$	2	1.0(2)	1.5
$J_2 = -5$	2	1.25(4)	1.5
$J_2 = -5$	3	1.06(3)	1
$J_2 = -5$	4	1.0(1)	0.8333

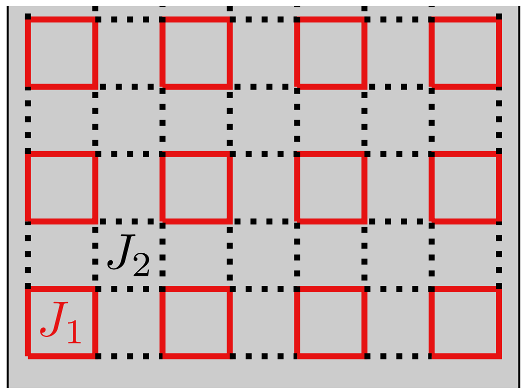
Model	n	$\log(N)$ coef. Ref. [4]	$\frac{N_{\rm NG}}{4}\frac{n+1}{n-1}$
XY			
$J_2 = 0$	∞	0.281(8)	0.25
$J_2 = -1$	∞	0.282(3)	0.25
$J_2 = 0$	2	0.585(6)	0.75
$J_2 = -1$	2	0.598(4)	0.75
$J_2 = 0$	3	0.44(2)	0.5
$J_2 = -1$	3	0.432(7)	0.5
$J_2 = 0$	4	0.35(8)	0.4166
$J_2 = -1$	4	0.38(2)	0.4166

- Numerical simulations on larger systems ongoing...

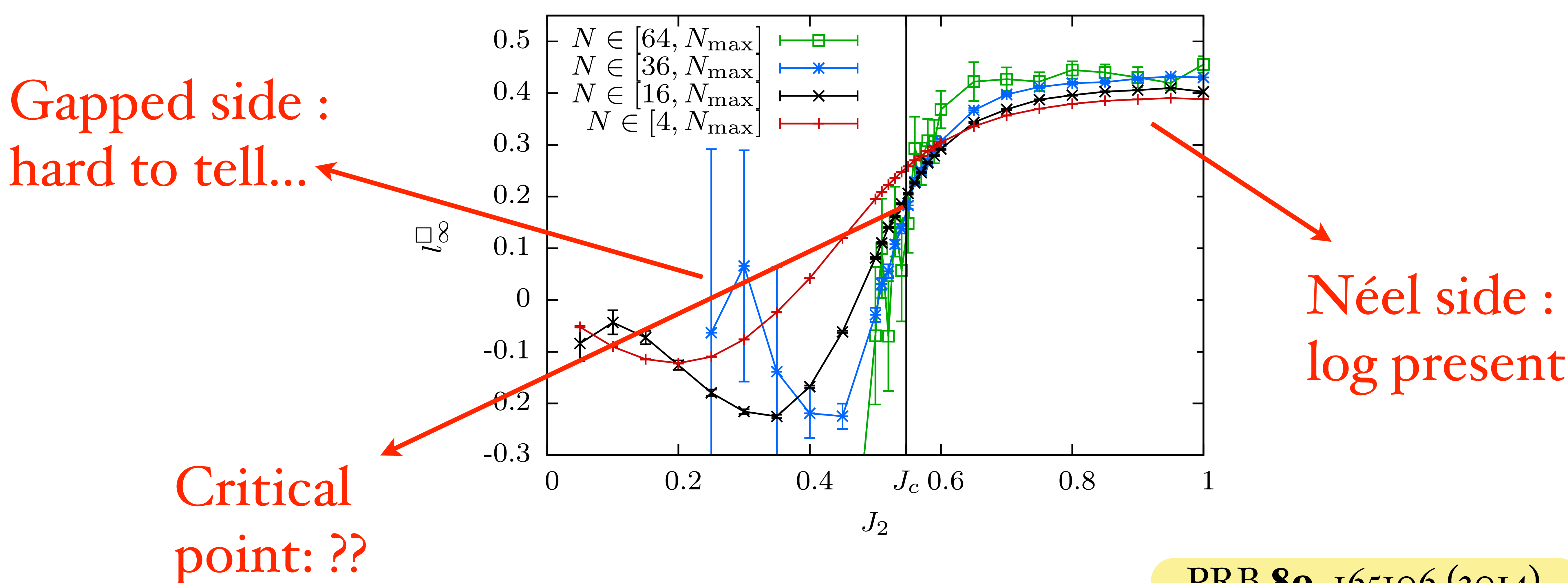
2d quantum phase transition

- Plaquettized 2d Heisenberg Hamiltonian





$$S_q = a_q N + l_q \log(N) + b_q + \cdots$$



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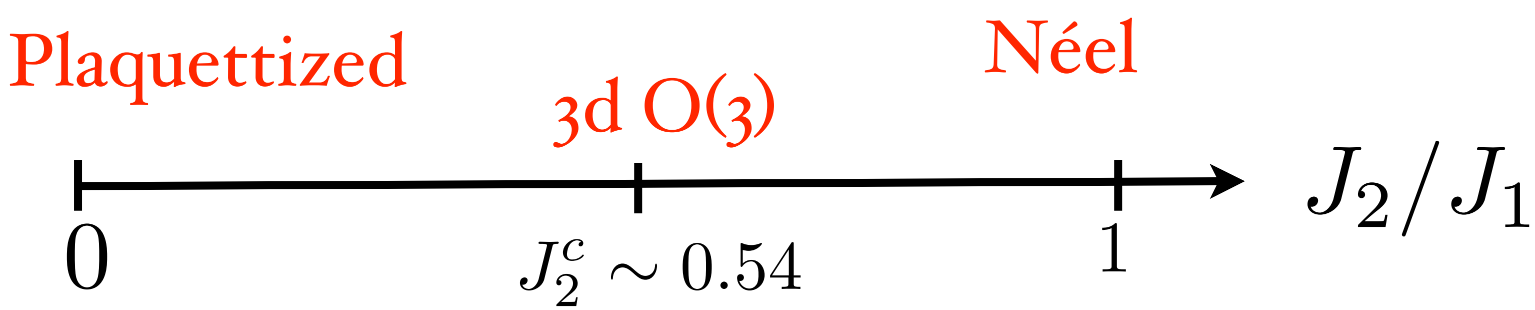
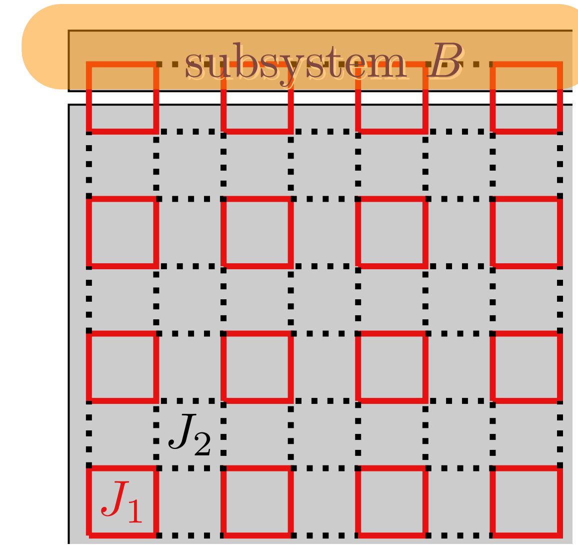
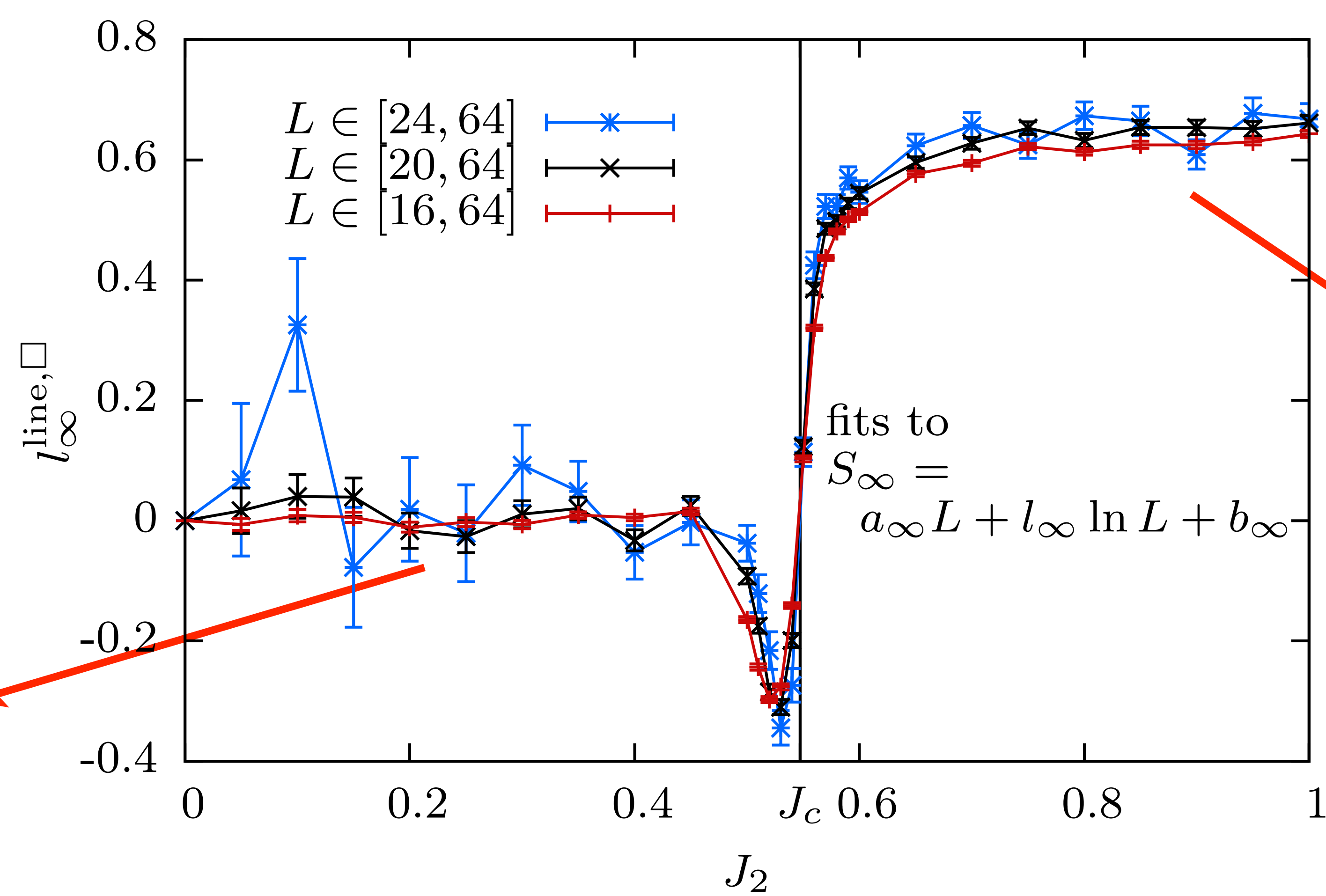
Line subsystem





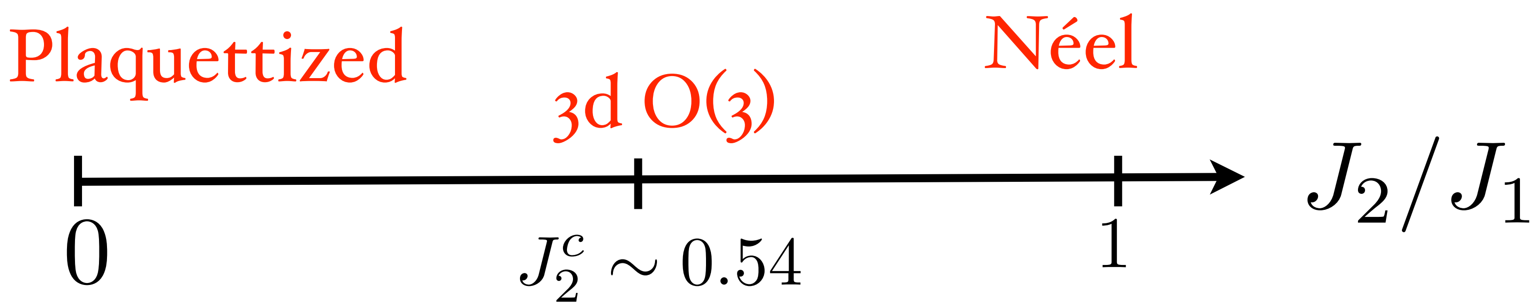
$$S_q^{\text{line}} = a_q^{\text{line}} L + l_q^{\text{line}} \log(L) + b_q^{\text{line}} + \cdots$$

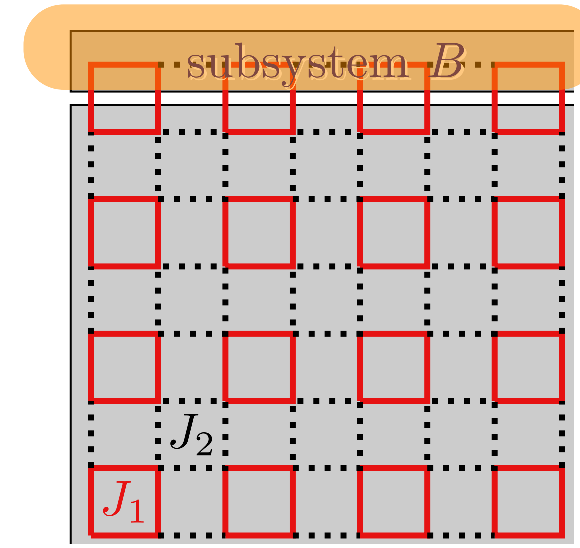


Gapped side : log vanish

Néel side : log present

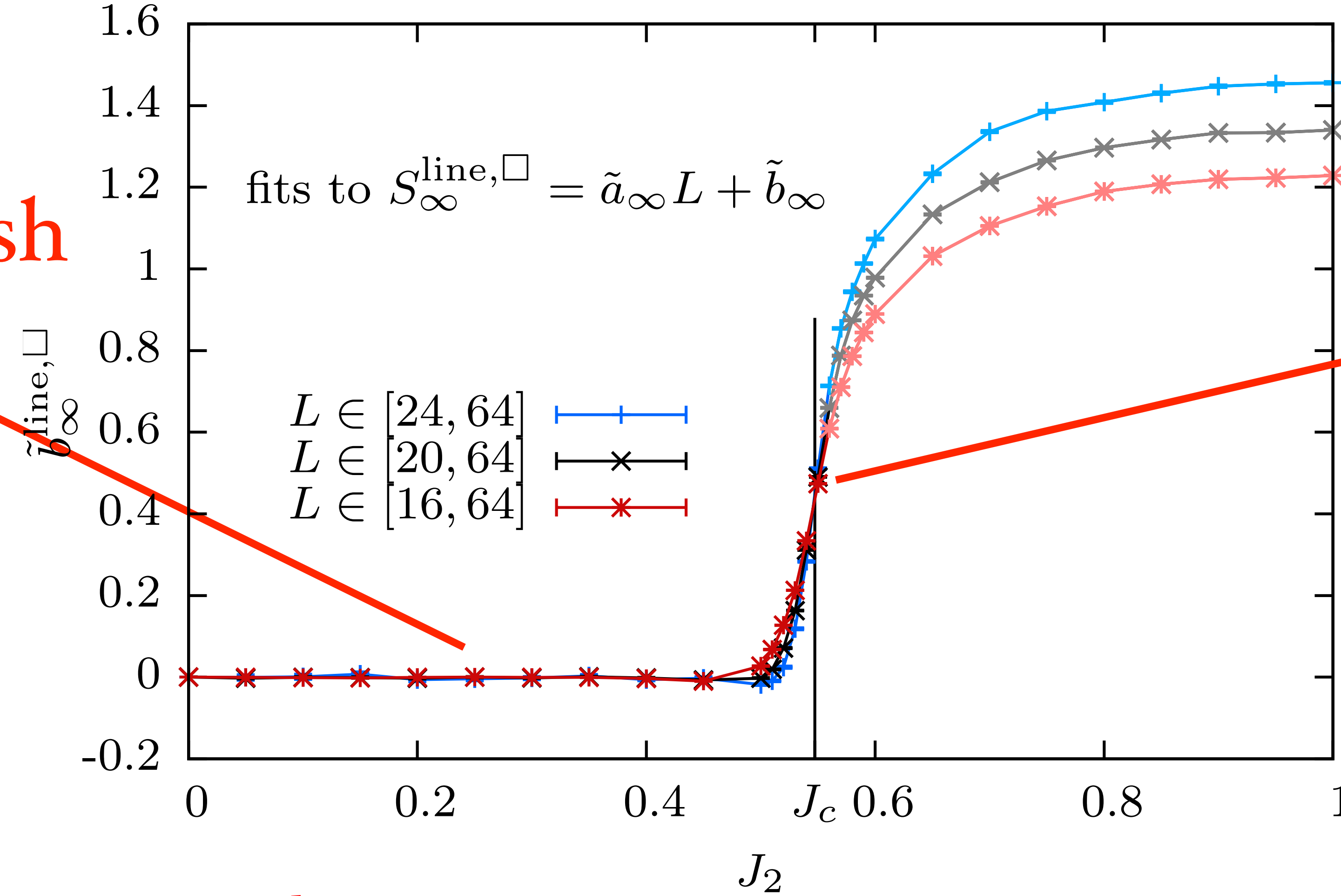
Line subsystem





$$S_q^{\mathrm{line}} = a_q^{\mathrm{line}} L + l_q^{\mathrm{line}} \log(L) + b_q^{\mathrm{line}} + \cdots$$

Gapped side : constant vanish



Critical point: universal constant $b_\infty^{\mathrm{line},*} \simeq 0.41$

- Universal constant $b_\infty^{\mathrm{line},*}$ characteristic of 3d O(3) universality class
- Likely similar universal constant b_q^* (but can't prove it)

Summary of 2d results + Speculations

- Gapped (broken-symmetry) phases

$$S_q = a_q N + b_q + c_q/N + \cdots$$

$b_q = \ln(\mathrm{deg})$ captures ground-state degeneracy

- Continuous symmetry-broken phases

$$S_q = a_q N + l_q \log(N) + b_q + \cdots$$

l_q proportional to # Goldstone modes

- Quantum critical points

$$S_q = a_q N + b_q^* + c_q/N + \cdots$$

b_q^* characteristic of universality class

- Could universal terms arise for spin liquids ?

$S_q = a_q N - b_q + \cdots$ topological order ?

$S_q = a_q N + ?? + \cdots$ critical spin liquids ??

Part 3 : Relation to entanglement

1. Definitions & differences
2. Testing entanglement Hamiltonian

Participation ≠ entanglement

Participation entropy

- Characterizes localization
- Consider full system (in general)

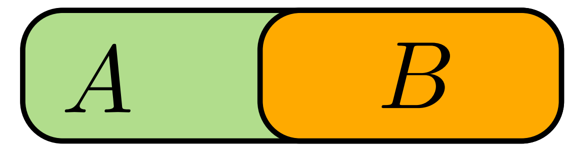
- Diagonal elements of the density matrix

$$S_q = \frac{1}{1-q} \ln \sum_i \rho_{ii}$$

- Volume law $S_q \propto N = L^d$

Entanglement entropy

- Characterizes entanglement
- Consider bipartition of the system

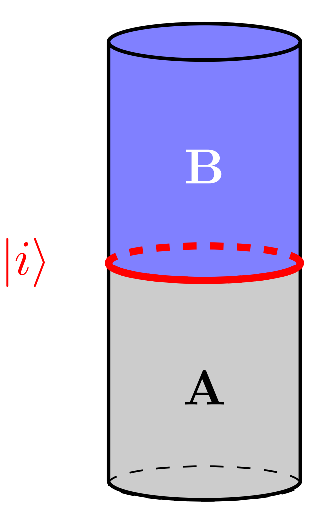


- Eigenvalues of the reduced density matrix

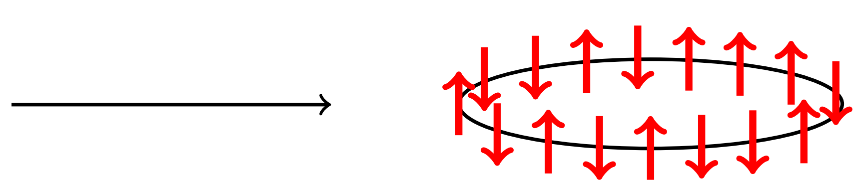
$$S_q^{\mathrm{ent}} = \frac{1}{1-q} \ln \sum_i \lambda_i^q$$

- Area law $S_q^{\mathrm{ent}} \propto L^{d-1}$

- BUT can be related in some cases



$$|RK\rangle_d \rightarrow |\Psi_0\rangle_{d-1}$$

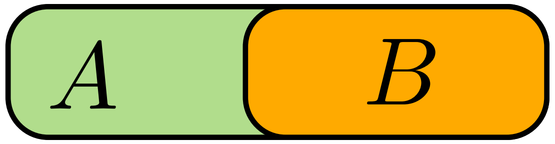


Stéphan *et al.*

Entanglement entropy of a Rokshar-Kivelson wave-function in dim. d = participation entropy of a ground-state in d-1

Entanglement Hamiltonian

- Entanglement Hamiltonian lives in A



$$\rho_A \equiv \exp(-\beta_{\text{ent}} H_{\text{ent}}(A))$$

- Useful to understand what is H_{ent} and its properties (range, gap…)
  - 1d critical states : H_{ent} determined by CFT
  - Topological phases: FQH states, topological order, topological / Chern insulators
  - Li-Haldane conjecture : H_{ent} characterize edge modes
  - Continuous symmetry breaking: Tower-of-states in H_{ent}

- In rare cases, H_{ent} is known (exactly or pertubatively)

- In general : Numerical determination of H_{ent} is very hard !
- Usually : comparison of spectra

Testing entanglement Hamiltonian

- Participation spectroscopy cannot find entanglement Hamiltonian, but can test educated guess

$$\rho_A \equiv \exp(-\beta_{\text{ent}} H_{\text{ent}}(A))$$

$$\langle i|\rho_A|i\rangle \equiv \langle i|\exp(-\beta_{\text{ent}} H_{\text{ent}}(A))|i\rangle \quad \text{in any basis } \{|i\rangle\}$$

Participation spectrum of subsystem A in the ground-state

Participation spectrum of the (test) entanglement Hamiltonian at finite T

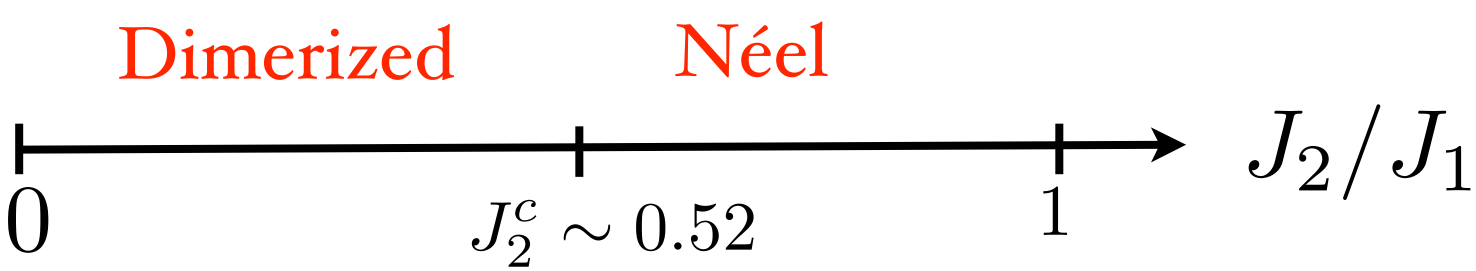
- Idea: Measure true participation spectrum of A, compare with the one of test entanglement Hamiltonian at some finite temperature

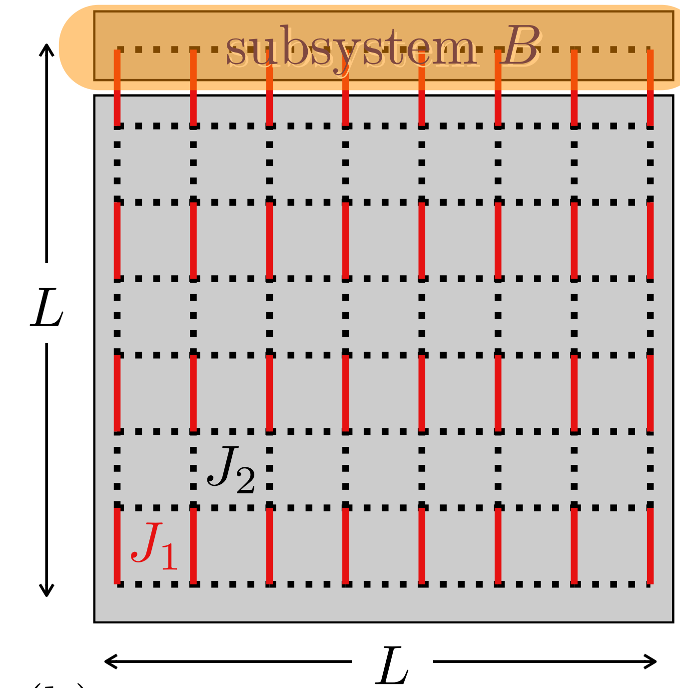
- How to have an educated guess ? Entanglement Hamiltonian should have at finite T the same physics than the subsystem

Concrete example

JSTAT (2014)

- Dimerized 2d Heisenberg Hamiltonian





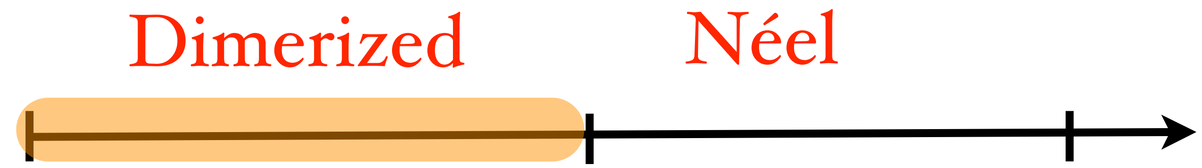
- What is the entanglement Hamiltonian of a line sub-system ?

→ 1d S=1/2 Hamiltonian with SU(2) symmetry

→ Must have extensive entropy, therefore finite T

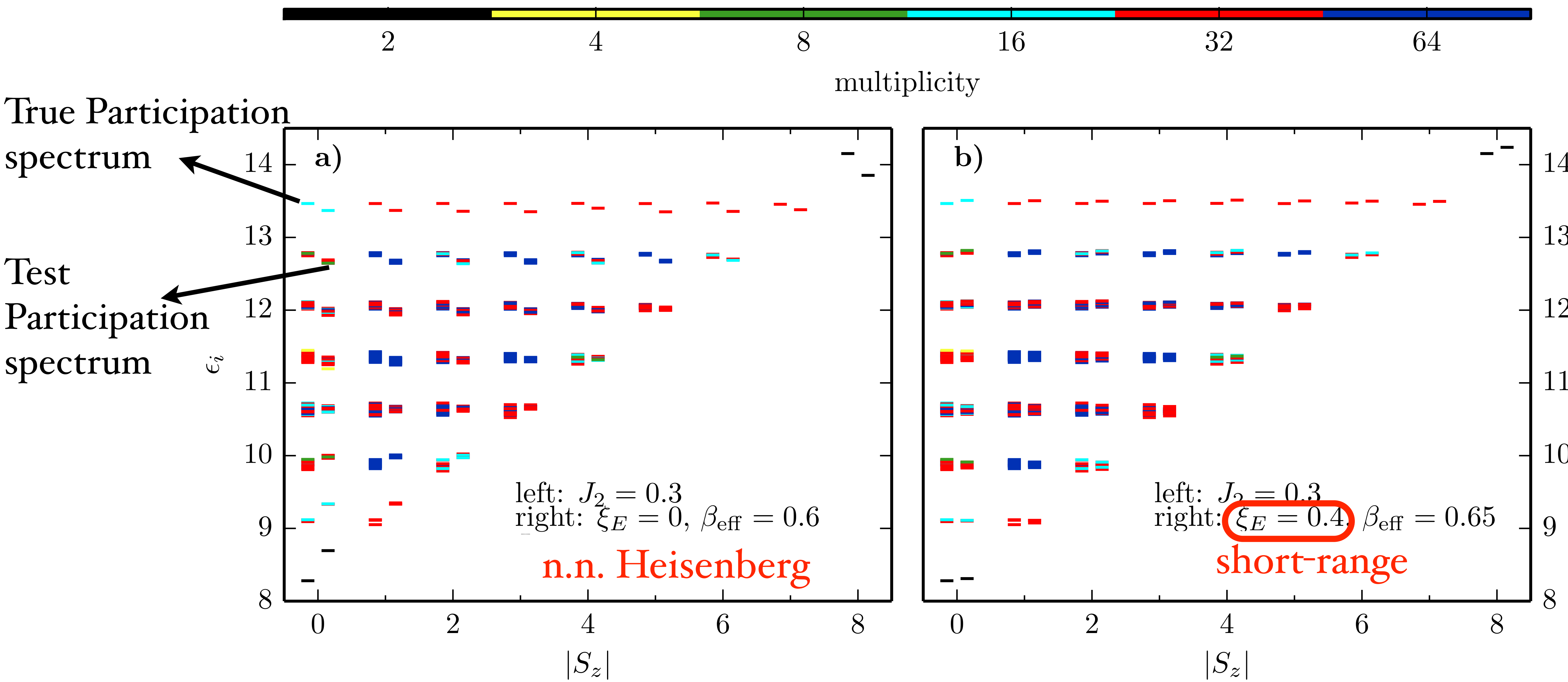
→ Disordered at finite T in the disordered phase, long-range at finite T in the ordered phase

Disordered phase



- Perturbation theory at small J2 : $H_{\text{ent}} = \sum_{i \in A} \mathbf{S}_i . \mathbf{S}_{i+1}$ $\quad \beta_{\text{ent}} = 2J_2$
- For (slightly) larger J2 : test short-range entanglement Hamiltonian

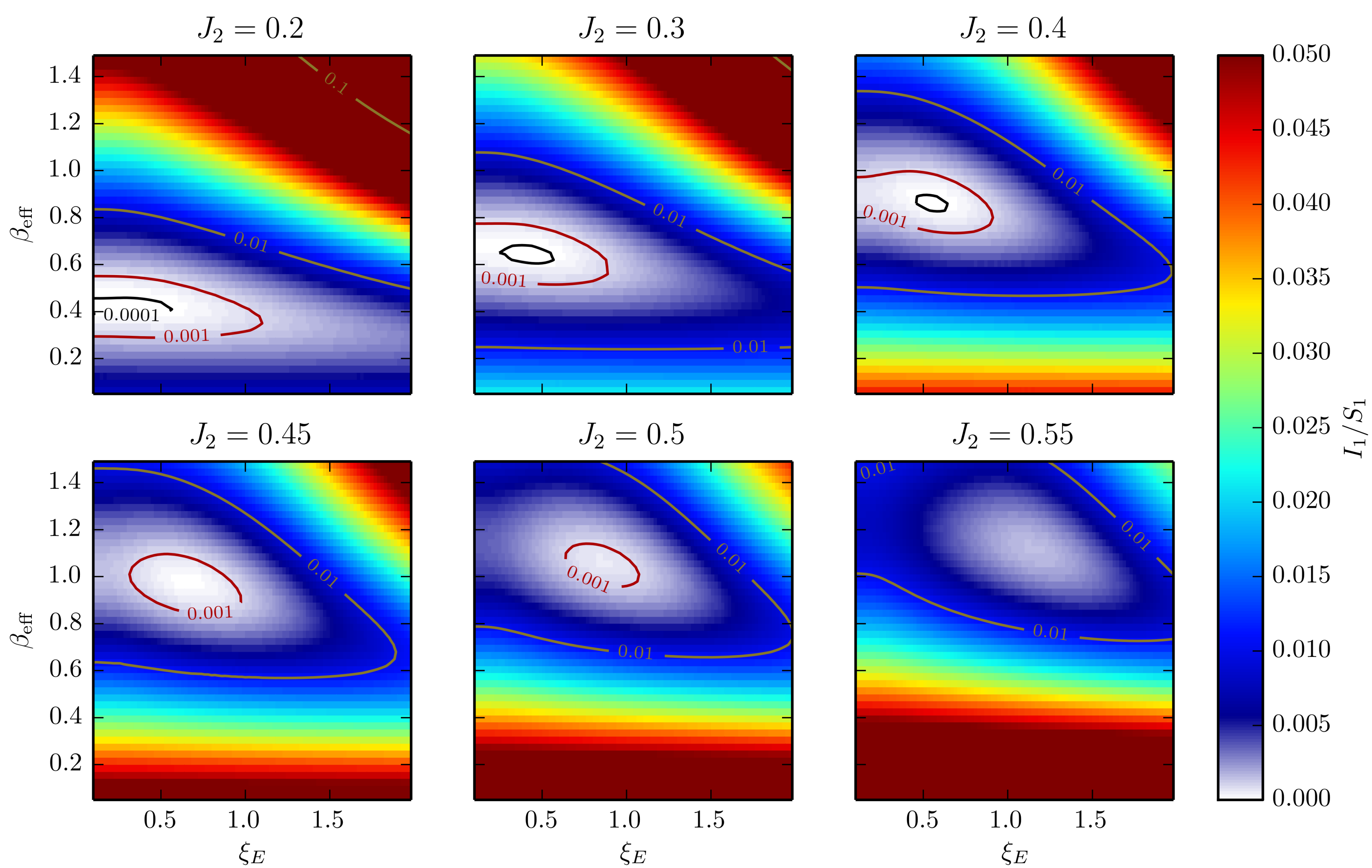
$$H_{\text{ent}} = - \sum_{i,j \in A} (-)^{|i-j|} J_{ij} \mathbf{S}_i . \mathbf{S}_j \qquad J_{ij} = \exp(-(|i-j|-1)/\xi_{\text{ent}})$$



Finding optimal test Hamiltonian

- Want to compare two probability sets (two participation spectra)
- Kullback-Leibler divergence $I_1(Q|P) = \sum_i Q_i \ln \frac{Q_i}{P_i}.$

Small if participation spectra similar, large if not



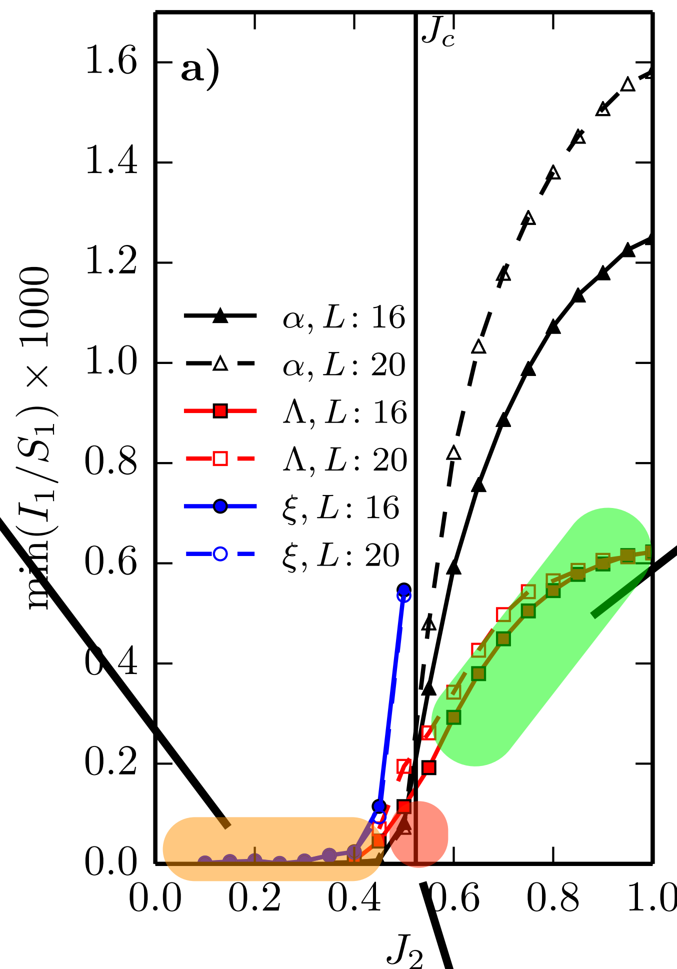
Final results: «Best» entanglement Hamiltonian

Dimerized $J_2^c \sim 0.52$ Néel J_2/J_1

Disordered phase

Short-range

$$J_{ij} = \exp(-(|i-j|-1)/\xi_{\text{ent}})$$



Néel-ordered phase

Long-range + power-law

$$J_{ij} = \Lambda/L + |i-j|^{-3}$$

LRO

Spin-waves $\omega \propto k$

Quantum critical point

Power-law ?

$$J_{ij} = |i-j|^{-\alpha}$$

JSTAT (2014)

NB: 4+ spins interactions neglected but likely in Néel phase

Conclusions & outlooks

- Message 1 : Universality sits in subleading terms of participation entropies
- Message 2 : QMC is well suited when wave-function is "reasonably" localized.
- Message 3 : In some cases, knowledge of participation entropy helps in understanding / measuring entanglement entropy

- Outlooks :
  - Check universality for different phases of matter (topological phases ?, critical spin liquids ?)
  - Extension of localization at finite temperature is possible (many-body localization ?)