

# Quantum-Monte-Carlo Approach to the Thermodynamics of Highly Frustrated Spin- $\frac{1}{2}$ Antiferromagnets

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UNIVERSITY



# Take-home message



*Efficient Quantum Monte-Carlo simulations can be performed for certain highly frustrated quantum magnets using a suitable computational basis.*

## References:

1. A.H., S.Wessel, R. Kerkdyk, T. Pruschke, F. Mila, B. Normand, Phys. Rev. B **93**, 054408 (2016)
2. S.Wessel, B. Normand, F. Mila, A.H., SciPost Phys. **3**, 005 (2017)
3. J. Stapmanns, P. Corboz, F. Mila, A.H., B. Normand, S.Wessel,  
[arXiv:1805.11017](https://arxiv.org/abs/1805.11017)
4. S.Wessel, I. Niesen, J. Stapmanns, B. Normand, F. Mila, P. Corboz, A.H.,  
[arXiv:1807.1????](https://arxiv.org/abs/1807.1????)

## See also:

5. F.Alet, K. Damle, S. Pujari, Phys. Rev. Lett. **117**, 197203 (2016)
6. K.-K. Ng, M.-F.Yang, Phys. Rev. B **95**, 064431 (2017)

# Outline

- 1 **Motivation:** thermodynamics of the spin- $\frac{1}{2}$  Shastry-Sutherland magnet  $\text{SrCu}_2(\text{BO}_3)_2$
- 2 **Quantum-Monte Carlo:**  
**sign problem** + dimer basis
- 3 Application to **fully frustrated bilayer**
- 4 Application to the **2D Shastry-Sutherland model**
- 5 **Summary**



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# Shastry-Sutherland model

Physica 108B (1981) 1069-1070

North-Holland Publishing Company

EXACT GROUND STATE OF A QUANTUM MECHANICAL ANTIFERROMAGNET

B. Sriram Shastry and Bill Sutherland

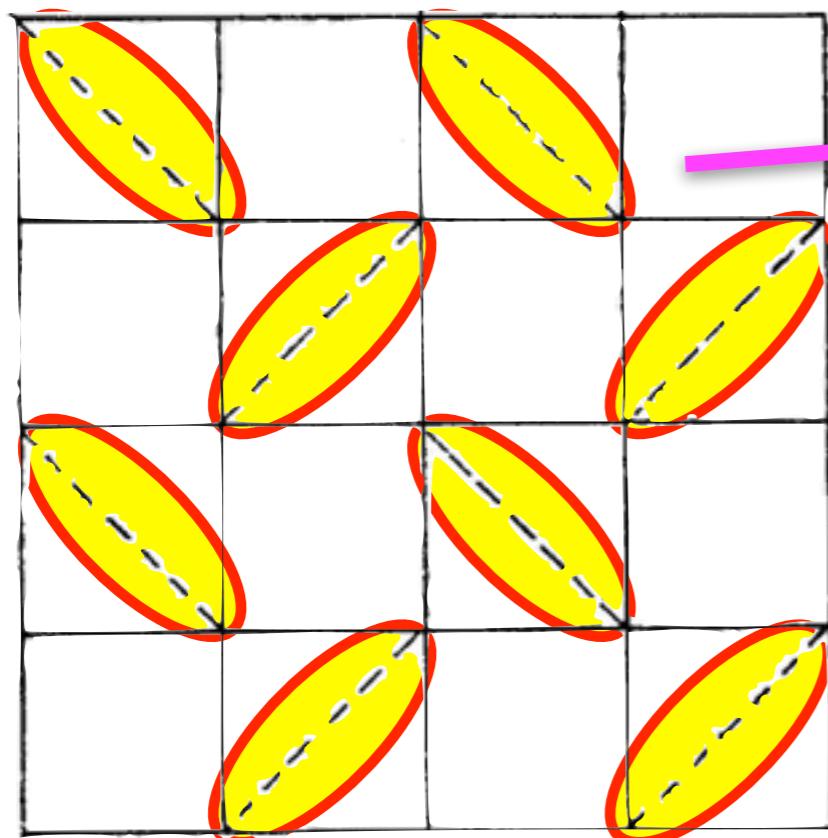


Fig. 1. The Lattice

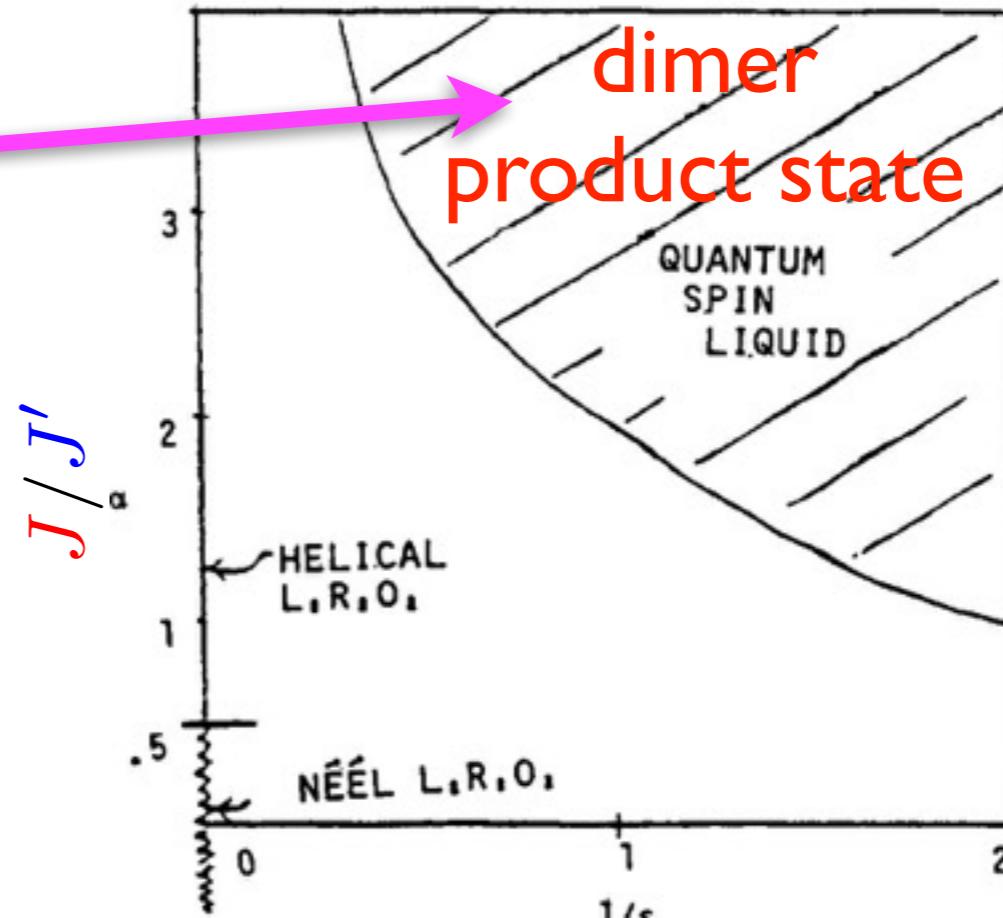


Fig. 2. The Phase Diagram

$$\mathcal{H} = \sum_{\text{square lattice}} J' \vec{S}_i \cdot \vec{S}_j + \sum_{\text{dimers}} J \vec{S}_i \cdot \vec{S}_j$$

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SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>

structure of a layer

B. Sriram Shastry an

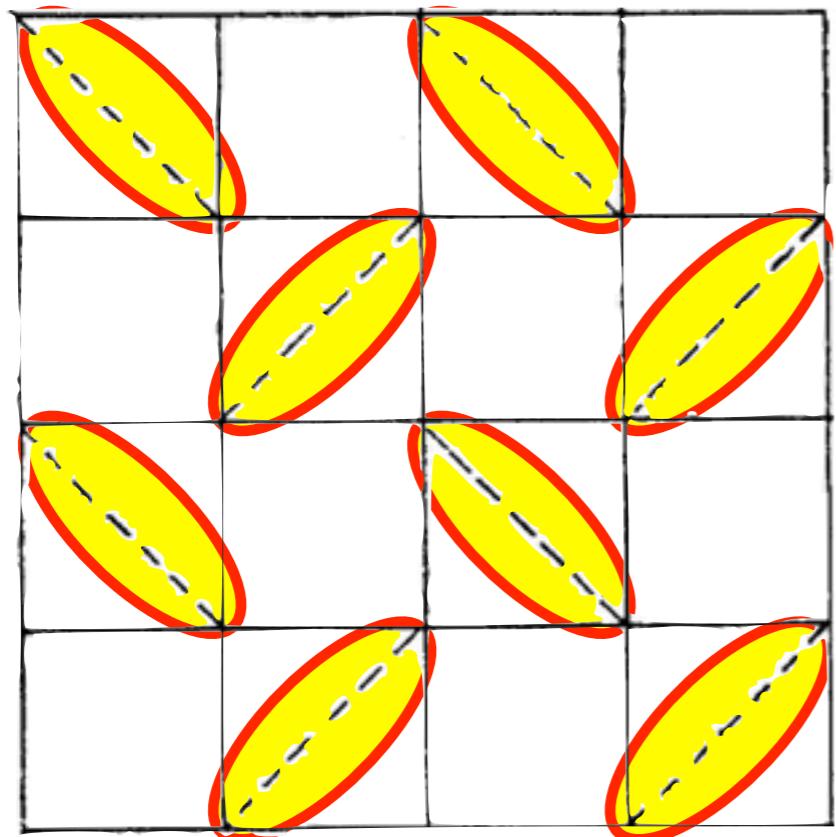
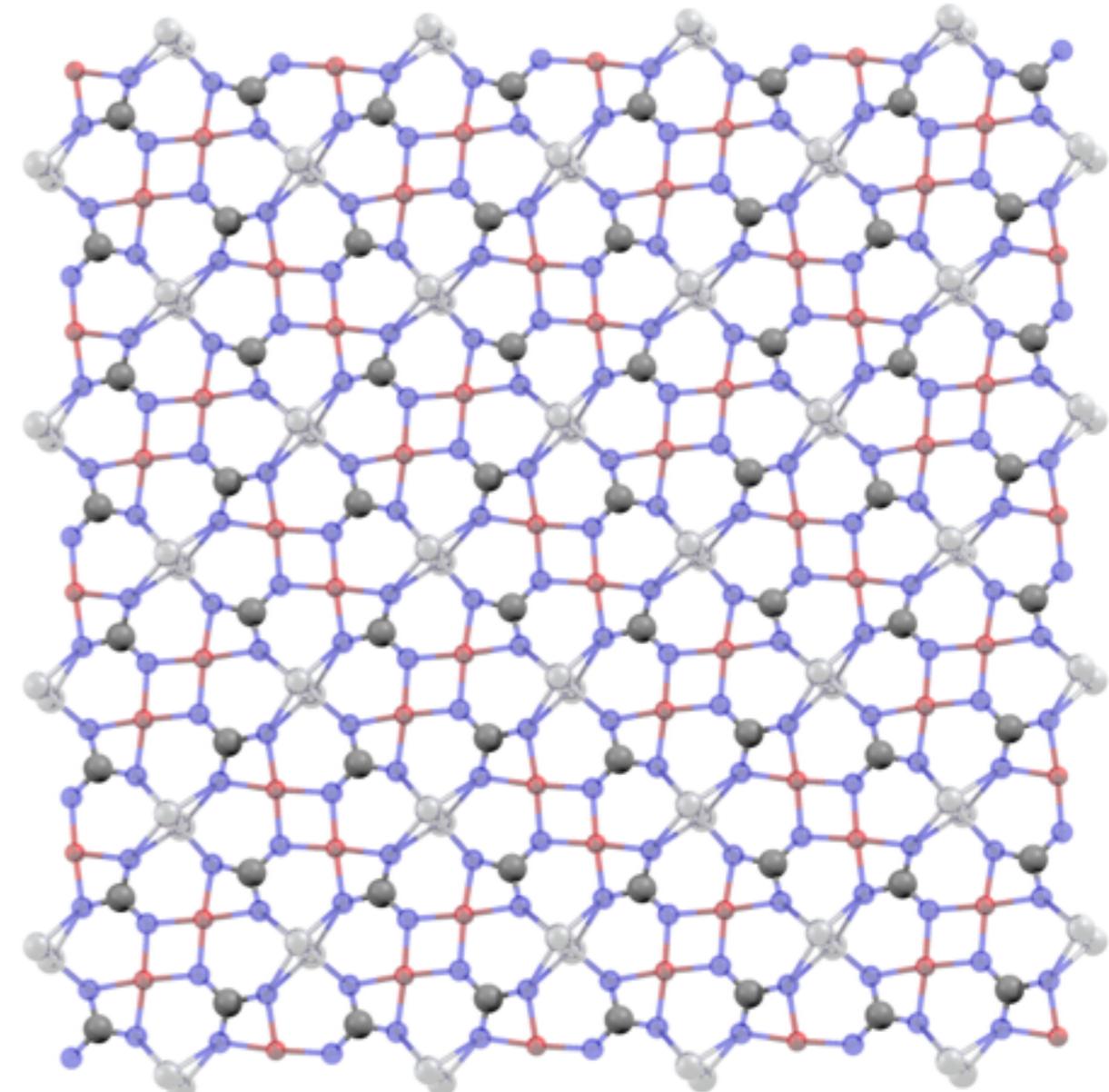


Fig. 1. The Lattice



Cu, O, B, Sr

$$\mathcal{H} = \sum_{\text{square lattice}} J' \vec{S}_i \cdot \vec{S}_j + \sum_{\text{dimers}} J \vec{S}_i \cdot \vec{S}_j$$

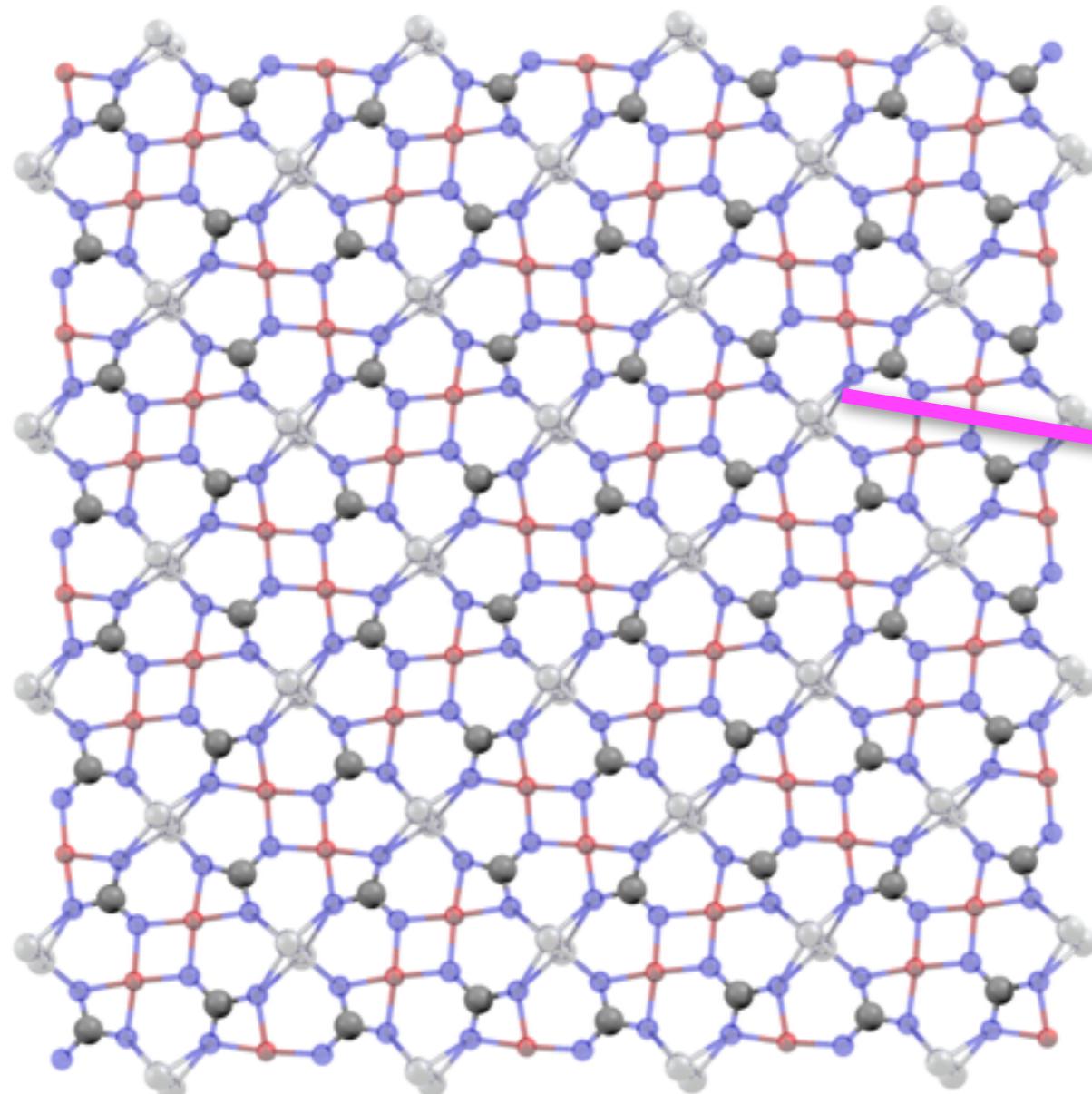
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UM MECHANICAL ANTFERROMAGNET

and Bill Sutherland

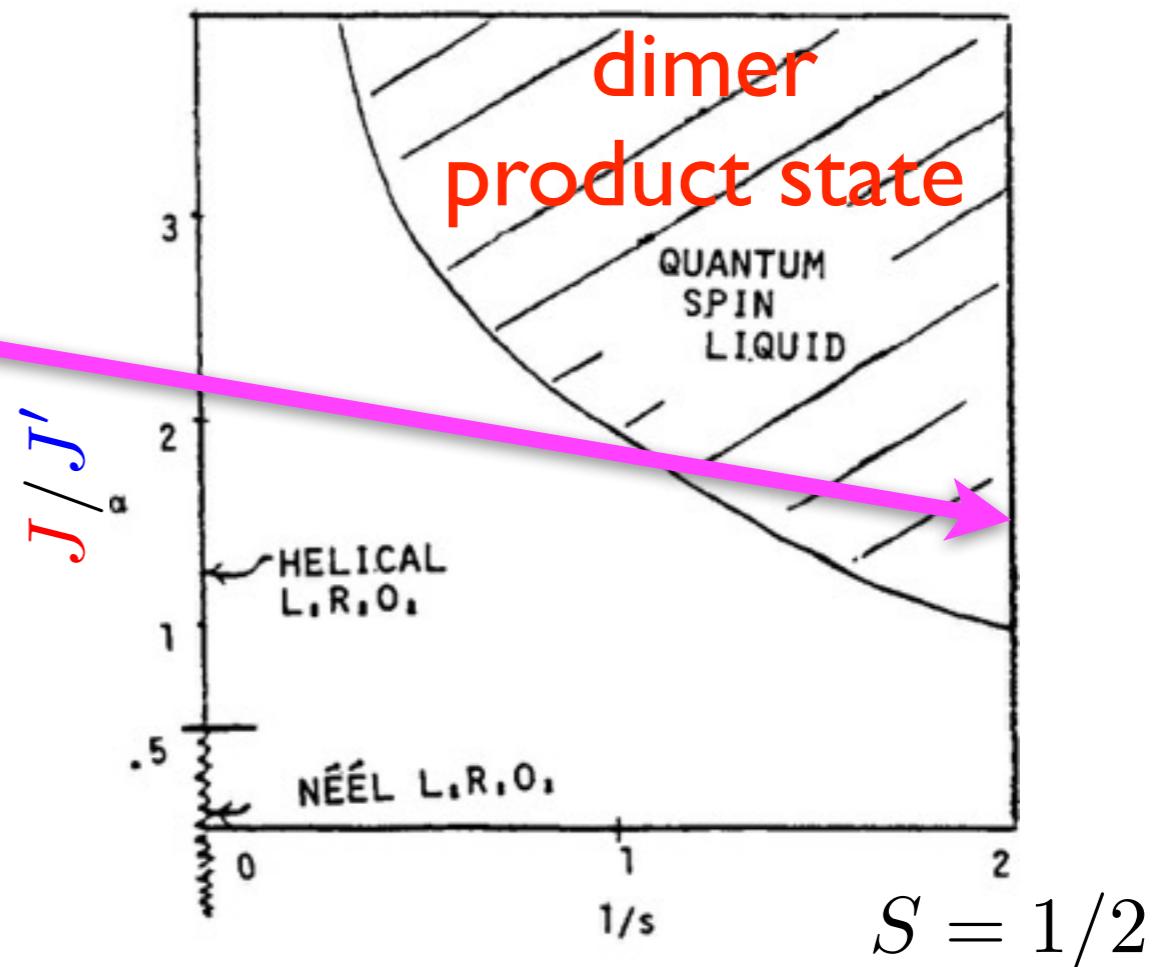
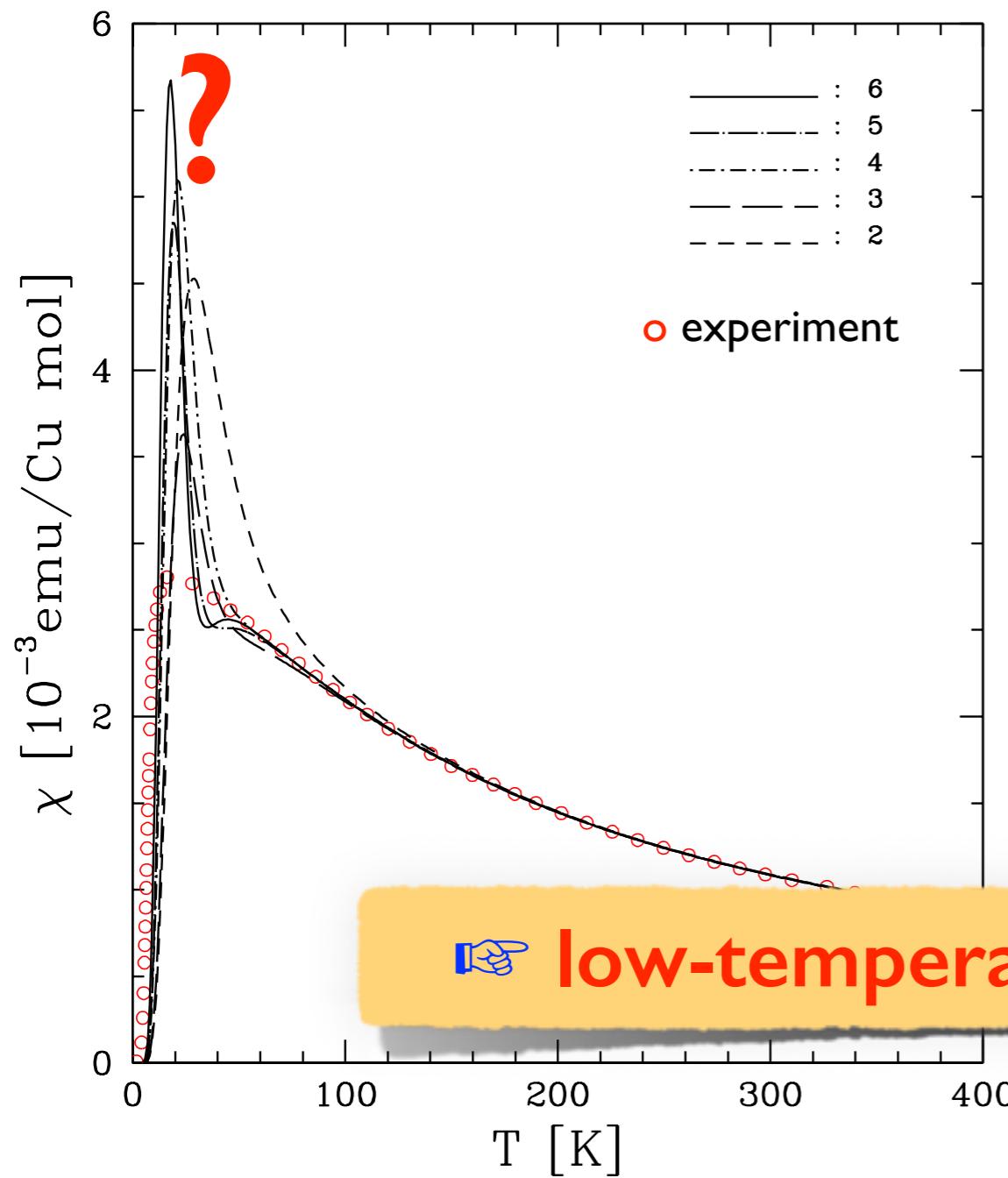


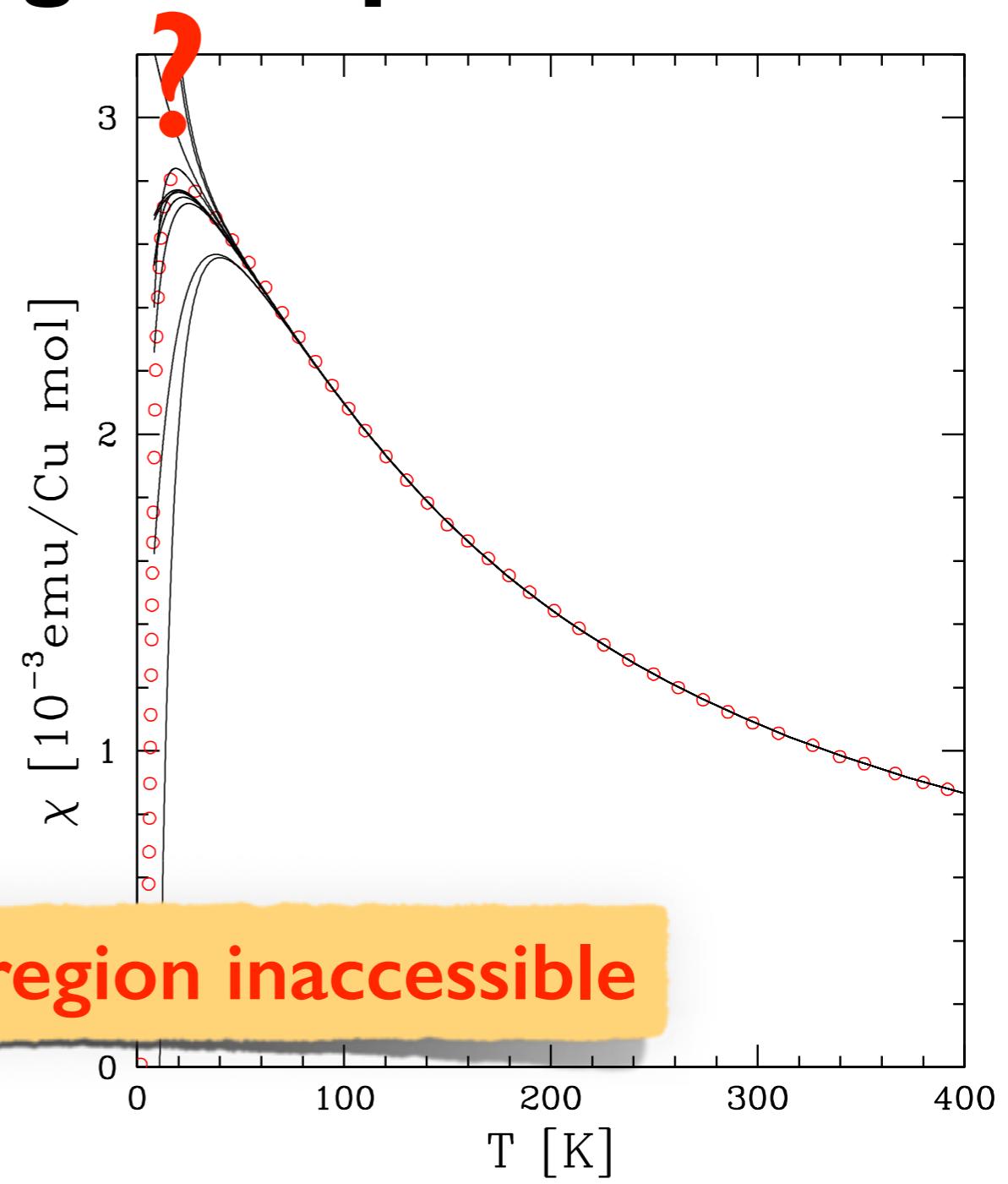
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# Magnetic susceptibility

## Dimer expansions

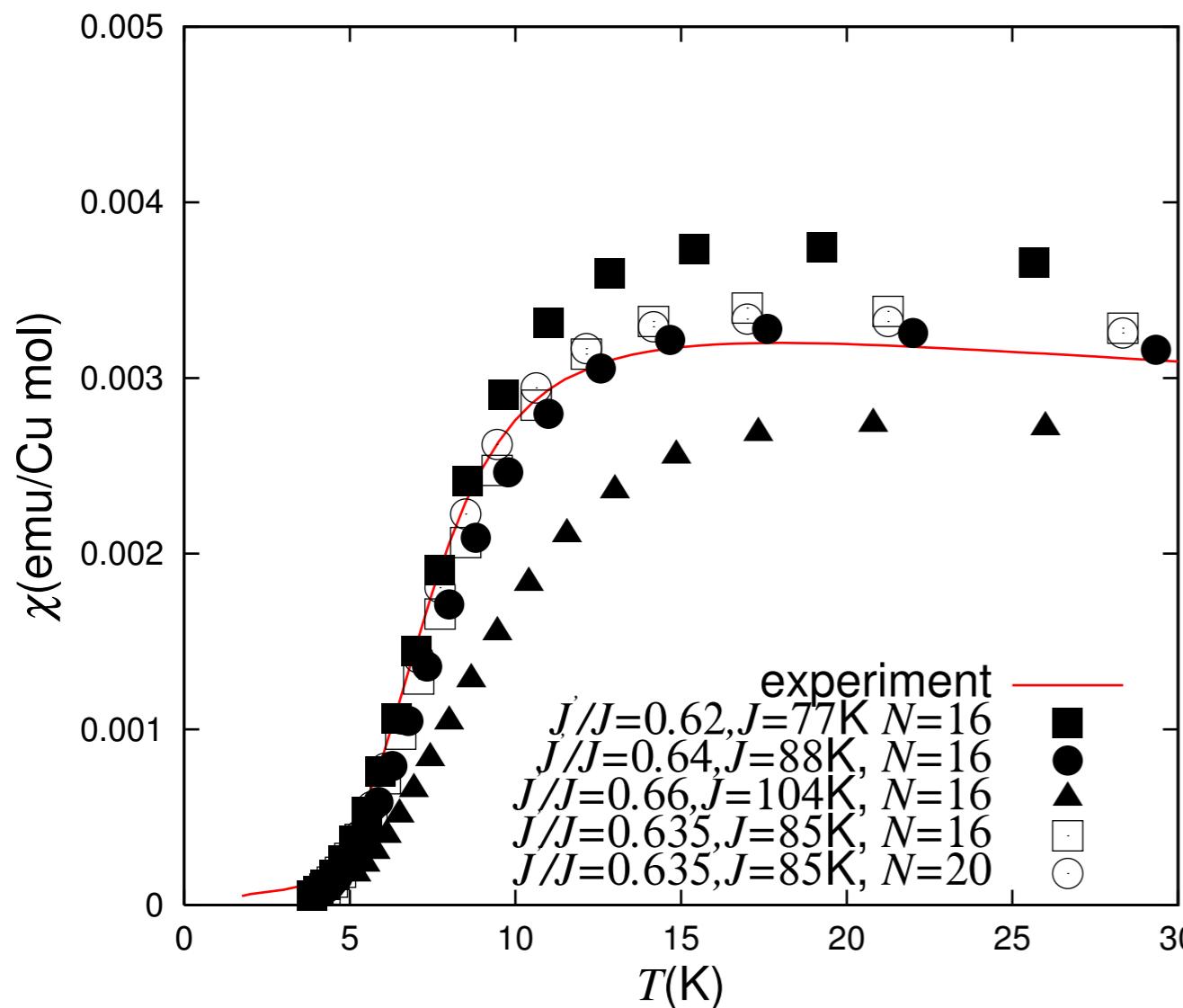


## High-temperature series

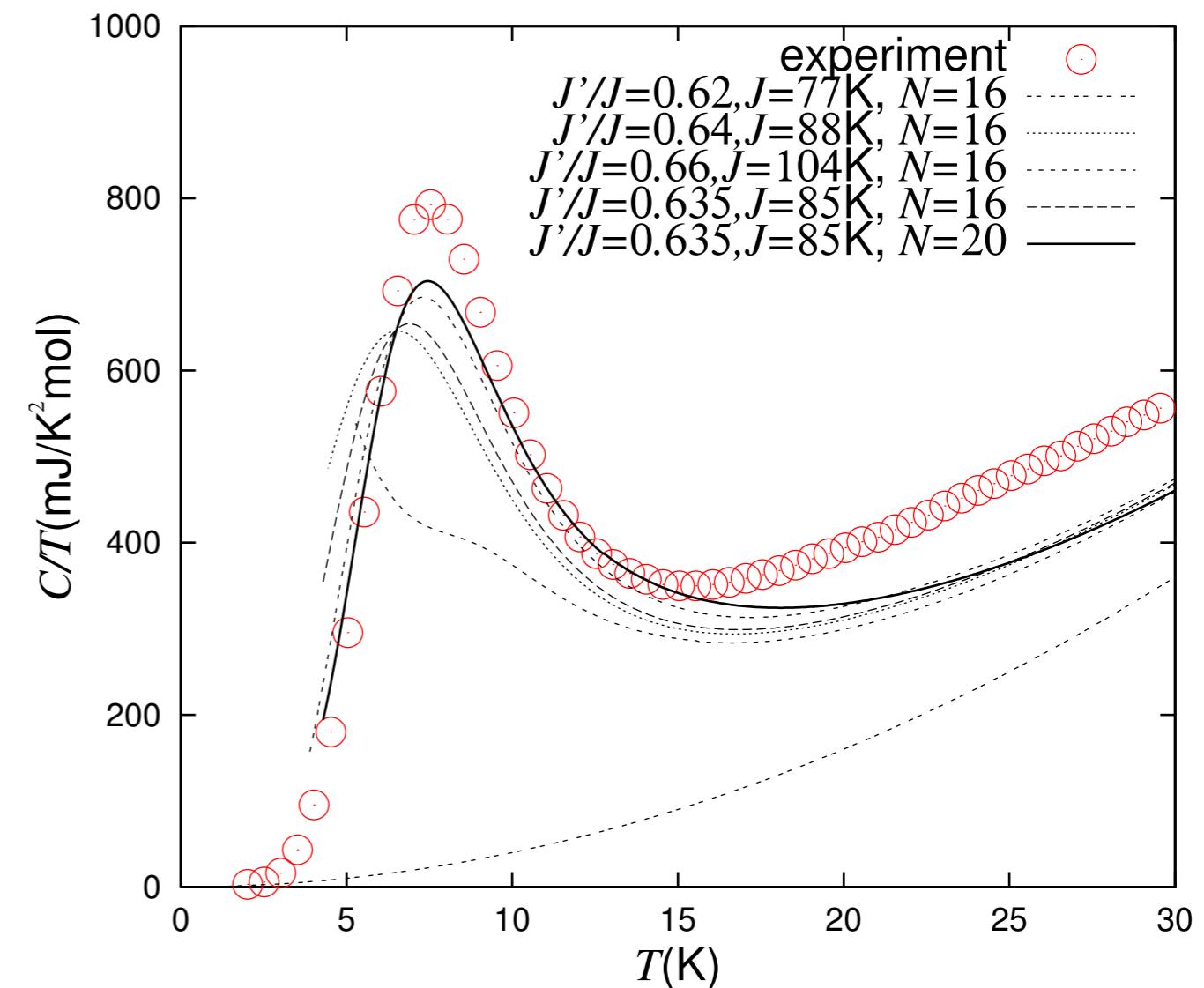


# Exact diagonalization

## Magnetic susceptibility



## Specific heat



S. Miyahara, K. Ueda, J. Phys. Soc. Jpn. Suppl. B **69**, 72 (2000)

👉 apparently good agreement for  $J'/J \approx 0.635$ ,  
but are  $N=16, \dots, 20$  spins really sufficient ?

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# Stochastic Series Expansion

A.W. Sandvik, J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991);

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**Hamiltonian:**

$$\mathcal{H} = \sum_{\text{bond } b} \mathcal{H}_b = \sum_{(b,t)} \mathcal{H}_{(b,t)}$$

**bond term**       $\mathcal{H}_b = \underbrace{\mathcal{H}_{(b,d)}}_{\text{diagonal}} + \underbrace{\mathcal{H}_{(b,o)}}_{\text{off-diagonal}}$

**Partition function:**

$$(\beta = 1/T)$$

$$Z = \text{Tr e}^{-\beta \mathcal{H}} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr} (-\mathcal{H})^n = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{|\alpha_n\rangle = |\alpha_1\rangle} \sum_{(b_n, t_n) \dots (b_1, t_1)} \prod_{i=1}^n \langle \alpha_{i+1} | -\mathcal{H}_{(b_i, t_i)} | \alpha_i \rangle$$

basis  $|\alpha_i\rangle$

**Sample (Monte Carlo)**

👉 **weights**  $\propto \langle \alpha_{i+1} | -\mathcal{H}_{(b_i, t_i)} | \alpha_i \rangle$

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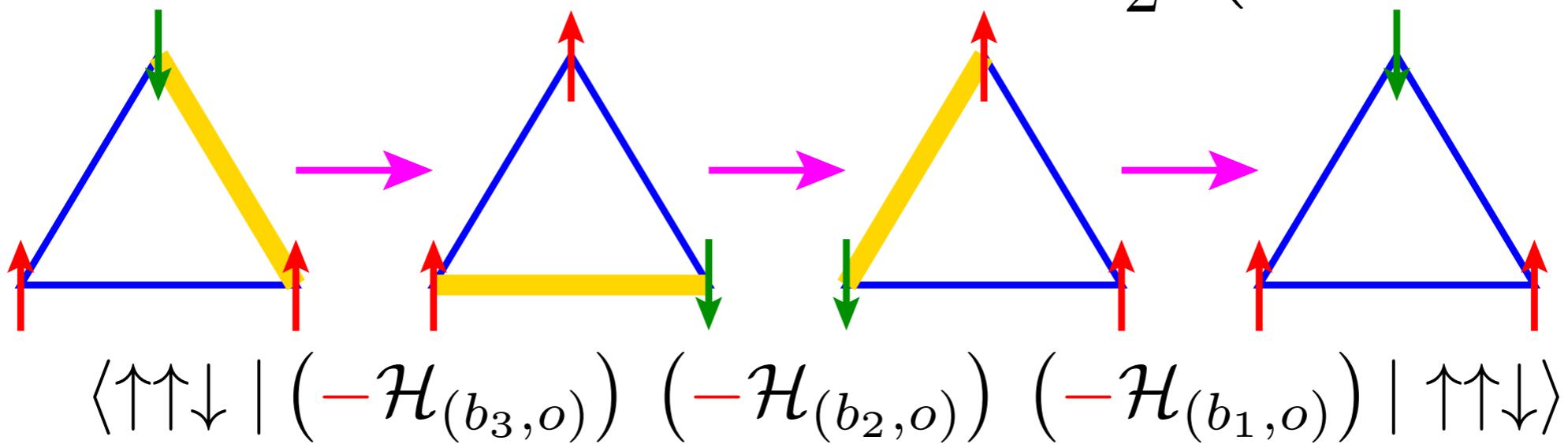
👉 **weights**  $\propto \langle \alpha_{i+1} | -\mathcal{H}_{(b_i, t_i)} | \alpha_i \rangle$     „**sign problem**“

# Sign problem

☞ off-diagonal terms may cause problems

☞ example: one triangle

$$\mathcal{H}_{(b,o)} = \frac{J}{2} \left( S_{b,1}^+ S_{b,2}^- + S_{b,1}^- S_{b,2}^+ \right)$$



☞ sample with absolute values of weights

$$\langle A \rangle = \frac{\langle A \text{ sign} \rangle_{||}}{\langle \text{sign} \rangle_{||}} = \frac{\sum_C |W(C)| A(C) \text{ sign}(C)}{\sum_C |W(C)| \text{ sign}(C)}$$

☞ average sign can get exponentially small

⇒ exponentially large error bars

☞ but this is basis-dependent ...

# Dimer basis

- 👉 eigenstates of a spin- $\frac{1}{2}$  dimer:  
 (well-defined magnetization)
 
$$|S\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$|0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|+\rangle = |\uparrow\uparrow\rangle \quad |-\rangle = |\downarrow\downarrow\rangle$$
- 👉 total spin  $\vec{T} = \vec{S}_1 + \vec{S}_2$  and spin-difference  $\vec{D} = \vec{S}_1 - \vec{S}_2$  operators

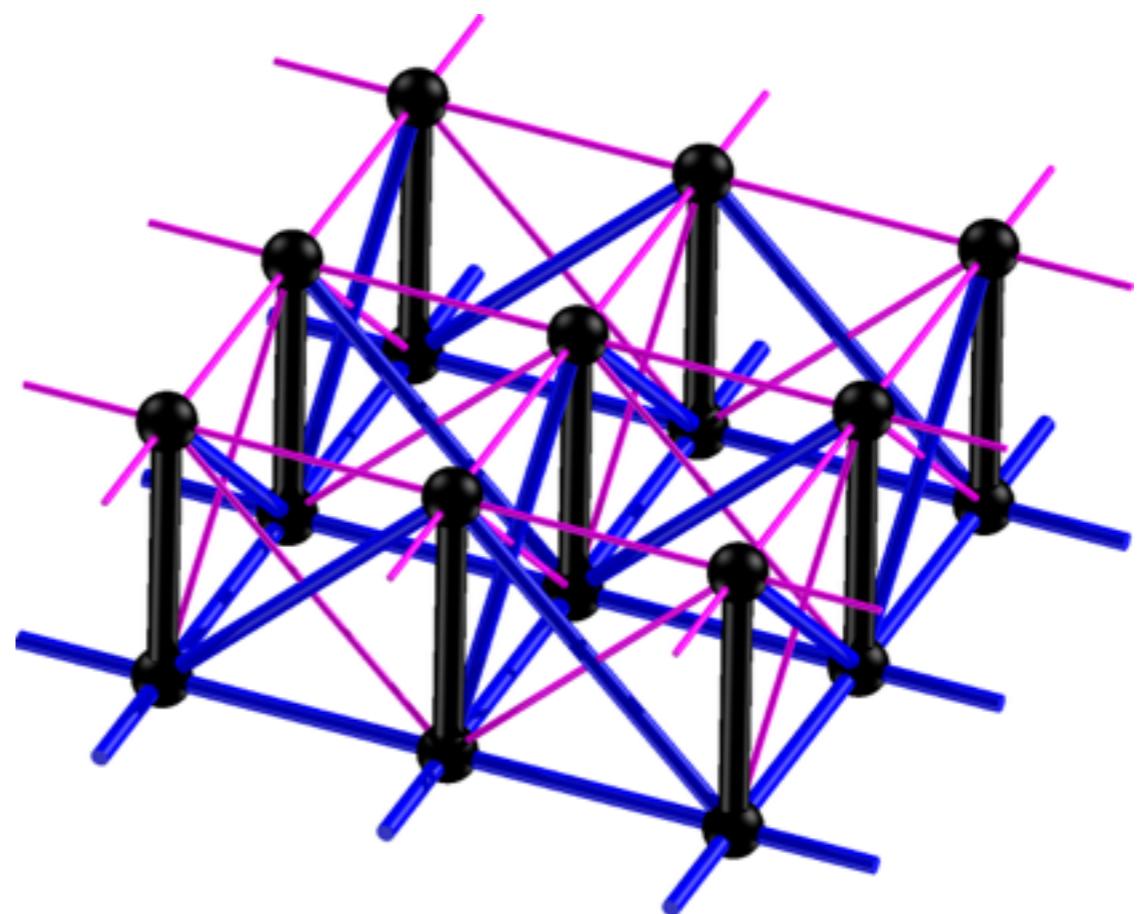
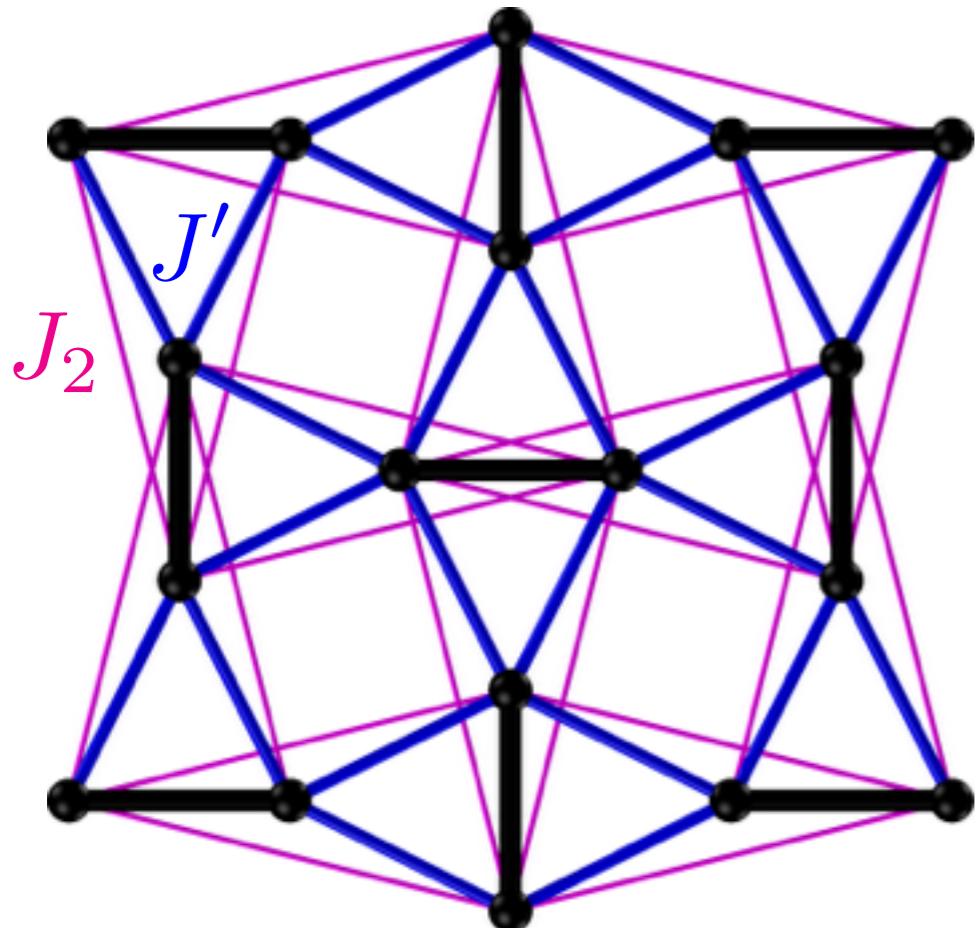
	$\vec{T}^2$	$T^z$	$T^+$	$T^-$	$D^z$	$D^+$	$D^-$
$ S\rangle$	0	0	0	0	$ 0\rangle$	$-\sqrt{2} +\rangle$	$\sqrt{2} -\rangle$
$ 0\rangle$	2	0	$\sqrt{2} +\rangle$	$\sqrt{2} -\rangle$	$ S\rangle$	0	0
$ +\rangle$	2	1	0	$\sqrt{2} 0\rangle$	0	0	$-\sqrt{2} S\rangle$
$ -\rangle$	2	-1	$\sqrt{2} 0\rangle$	0	0	$\sqrt{2} S\rangle$	0

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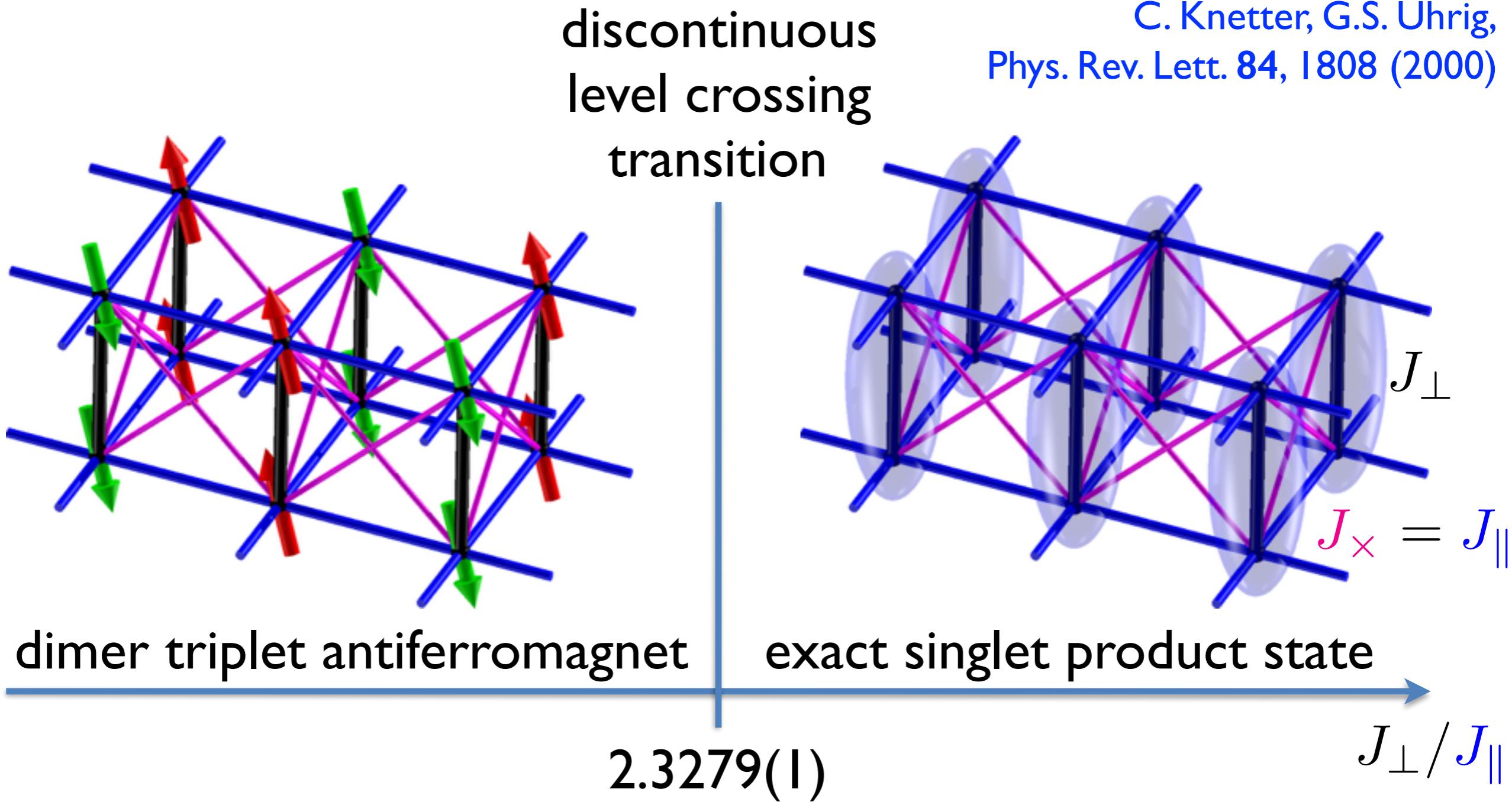
# From the Shastry-Sutherland model to the fully frustrated bilayer



- ➡ addition of  $J_2$  preserves the exact dimer ground state
- ➡  $J_2 = J'$ : **fully frustrated bilayer**  
(materials:  $\text{Ba}_2\text{CoSi}_2\text{O}_6\text{Cl}_2$  [H. Tanaka *et al.*, *J. Phys. Soc. Jpn.* **83**, 103701 (2014)])

# Ground-state phase diagram

E. Müller-Hartmann, R.R.P. Singh,  
C. Knetter, G.S. Uhrig,  
Phys. Rev. Lett. 84, 1808 (2000)



What are the thermodynamic properties ?

# Hamiltonian in dimer basis

in terms of dimer  $d$ : total

$$\vec{T}_d = \vec{S}_{d,1} + \vec{S}_{d,2}$$

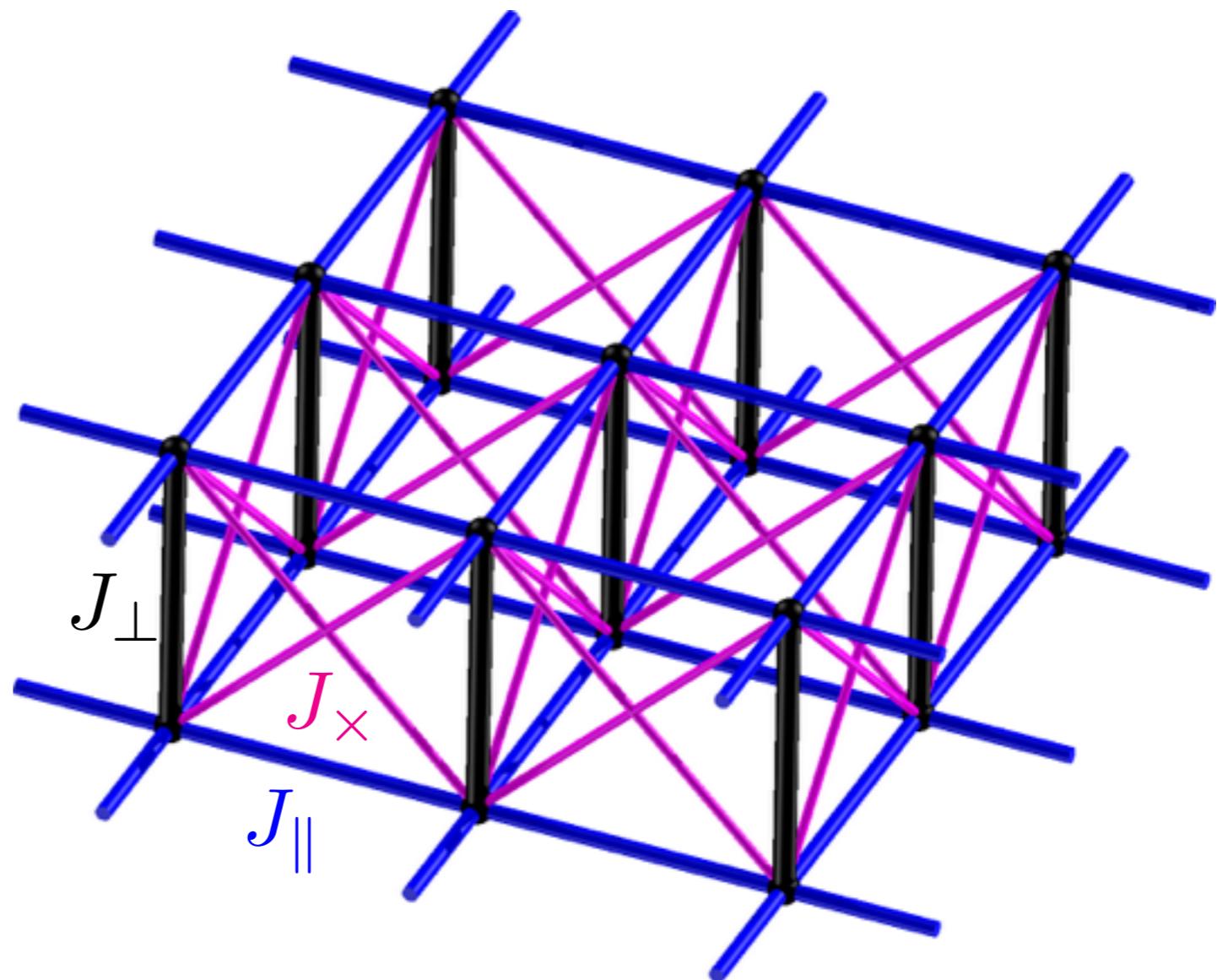
and difference spin operators

$$\vec{D}_d = \vec{S}_{d,1} - \vec{S}_{d,2}$$

⇒

$$H = \frac{J_{\perp}}{2} \sum_d \left( \vec{T}_d^2 - \frac{3}{2} \right)$$

$$+ \sum_{\langle d,d' \rangle} \left( \frac{J_{\parallel} + J_{\times}}{2} \vec{T}_d \cdot \vec{T}_{d'} + \frac{J_{\parallel} - J_{\times}}{2} \vec{D}_d \cdot \vec{D}_{d'} \right)$$



sign problem disappears for  $J_{\times} = J_{\parallel}$

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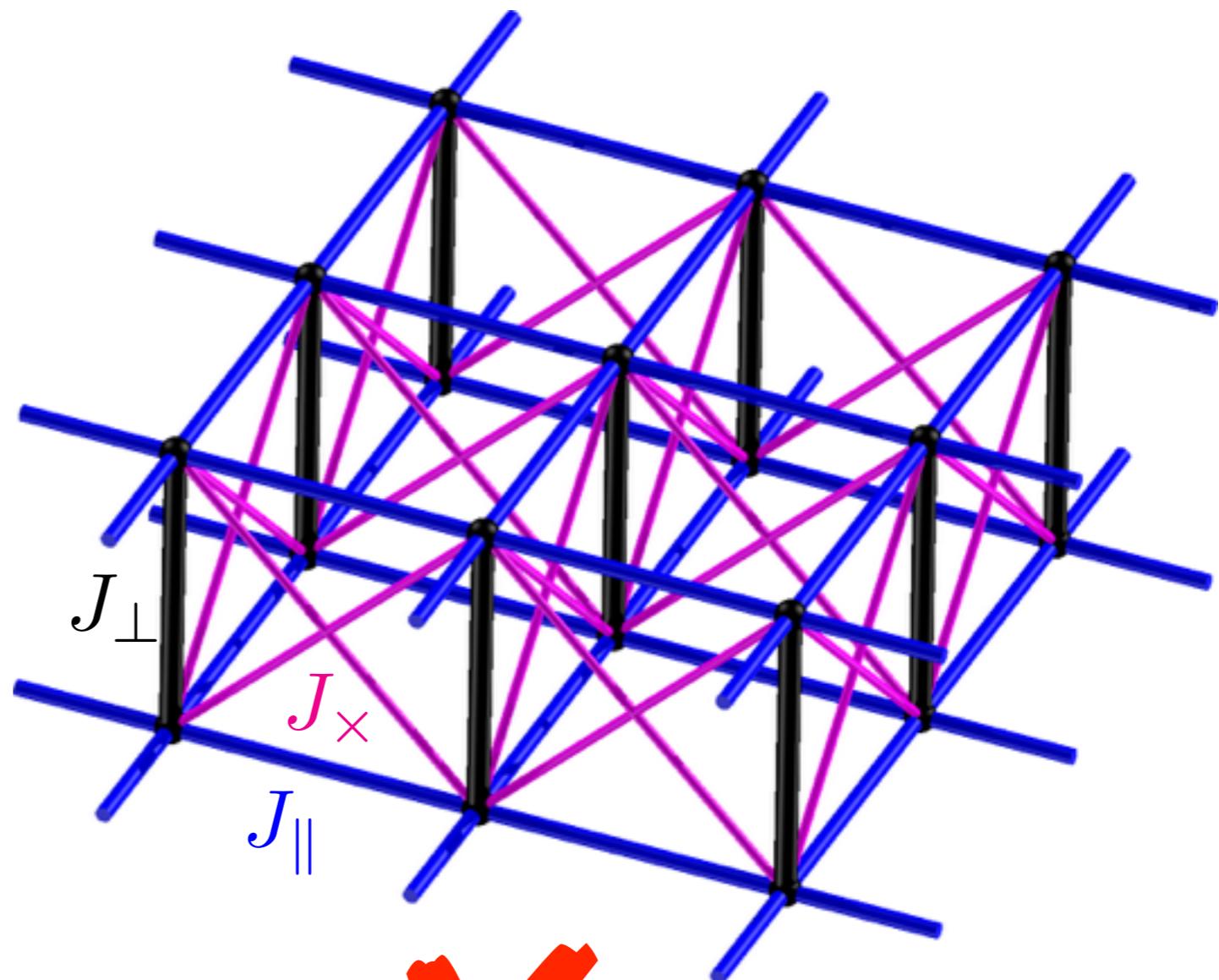
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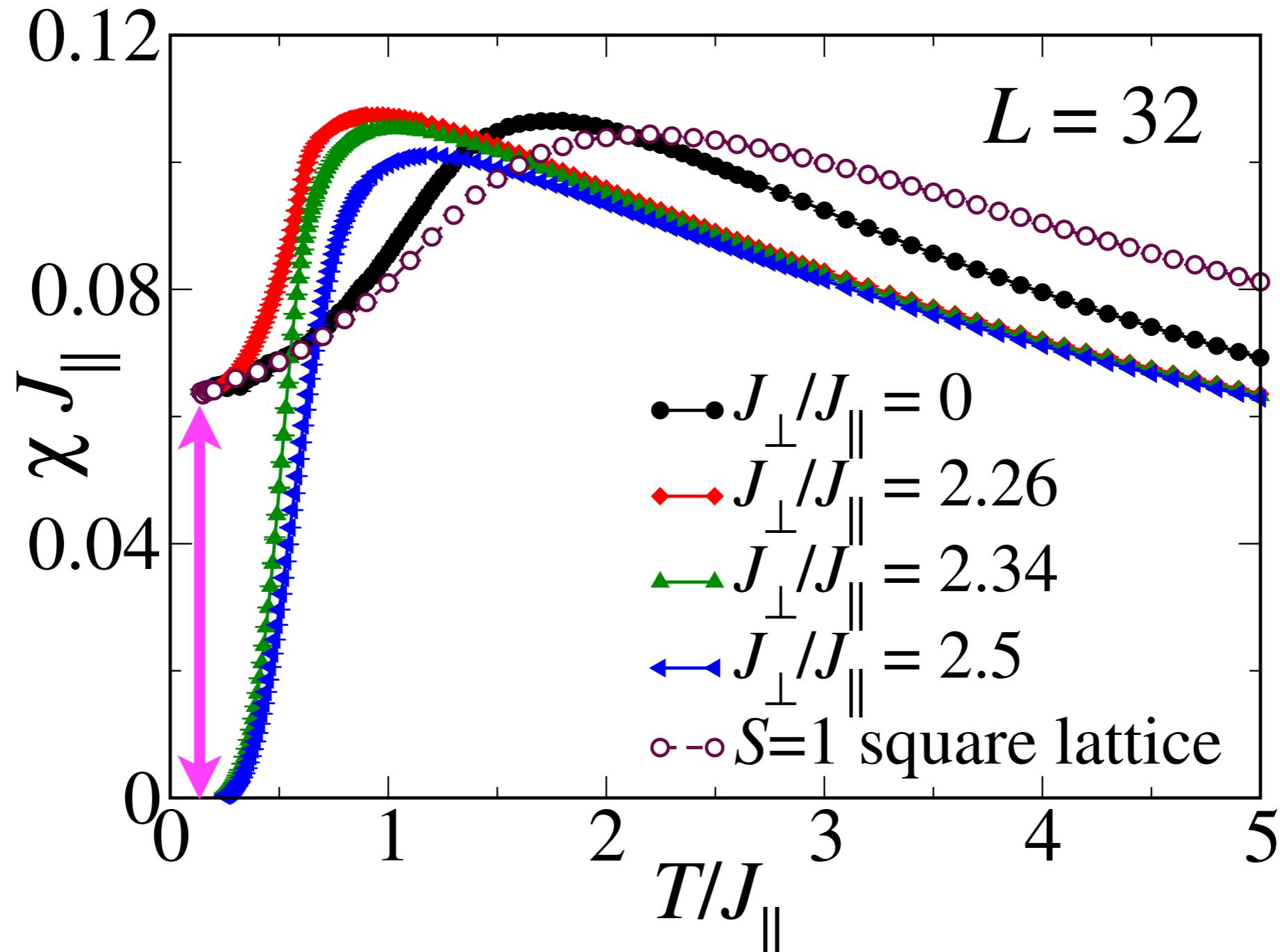
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# Magnetic susceptibility

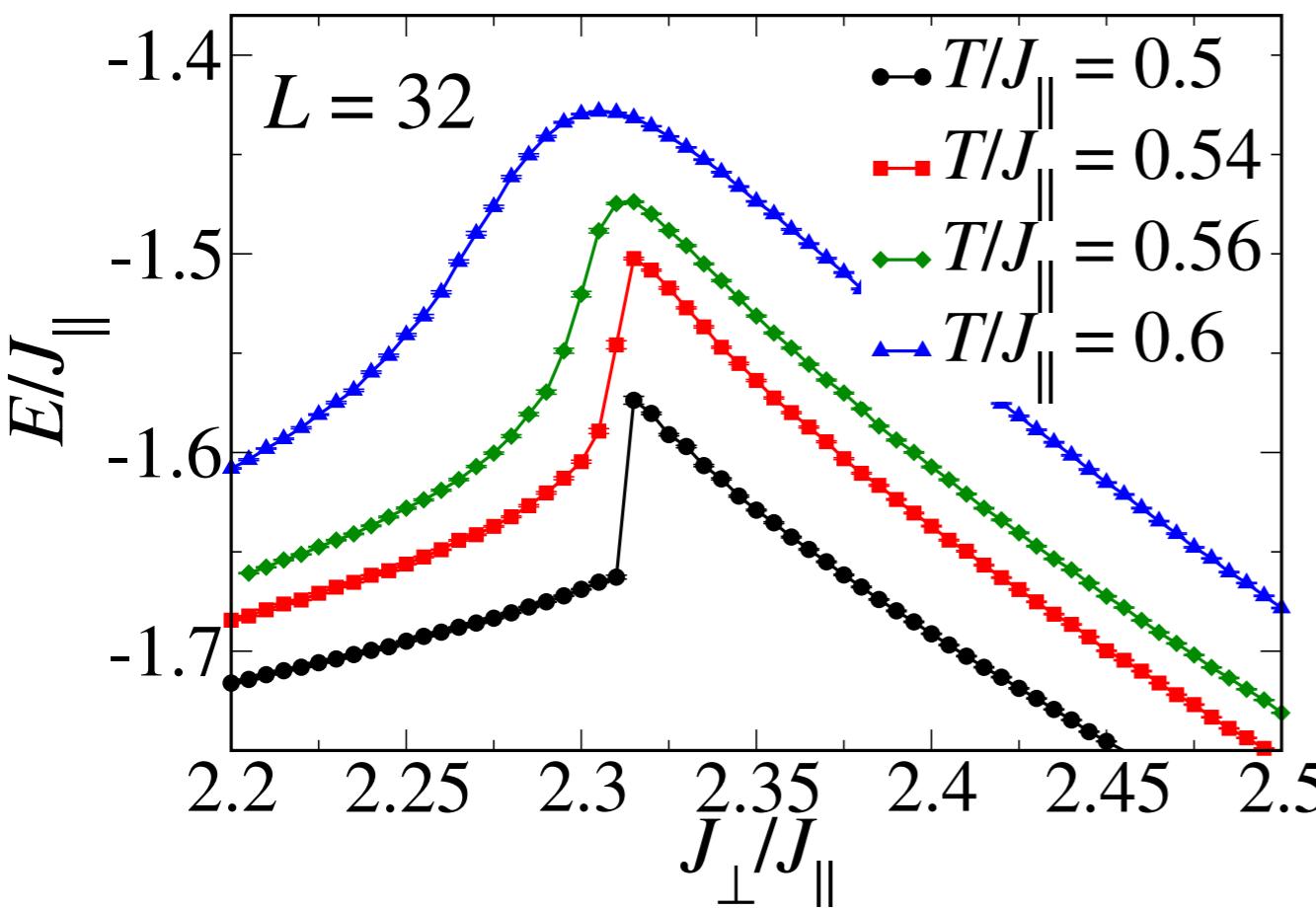


👉 transition from gapped to ordered  $S = 1$  state between  $J_\perp/J_\parallel = 2.26$  and  $2.34$

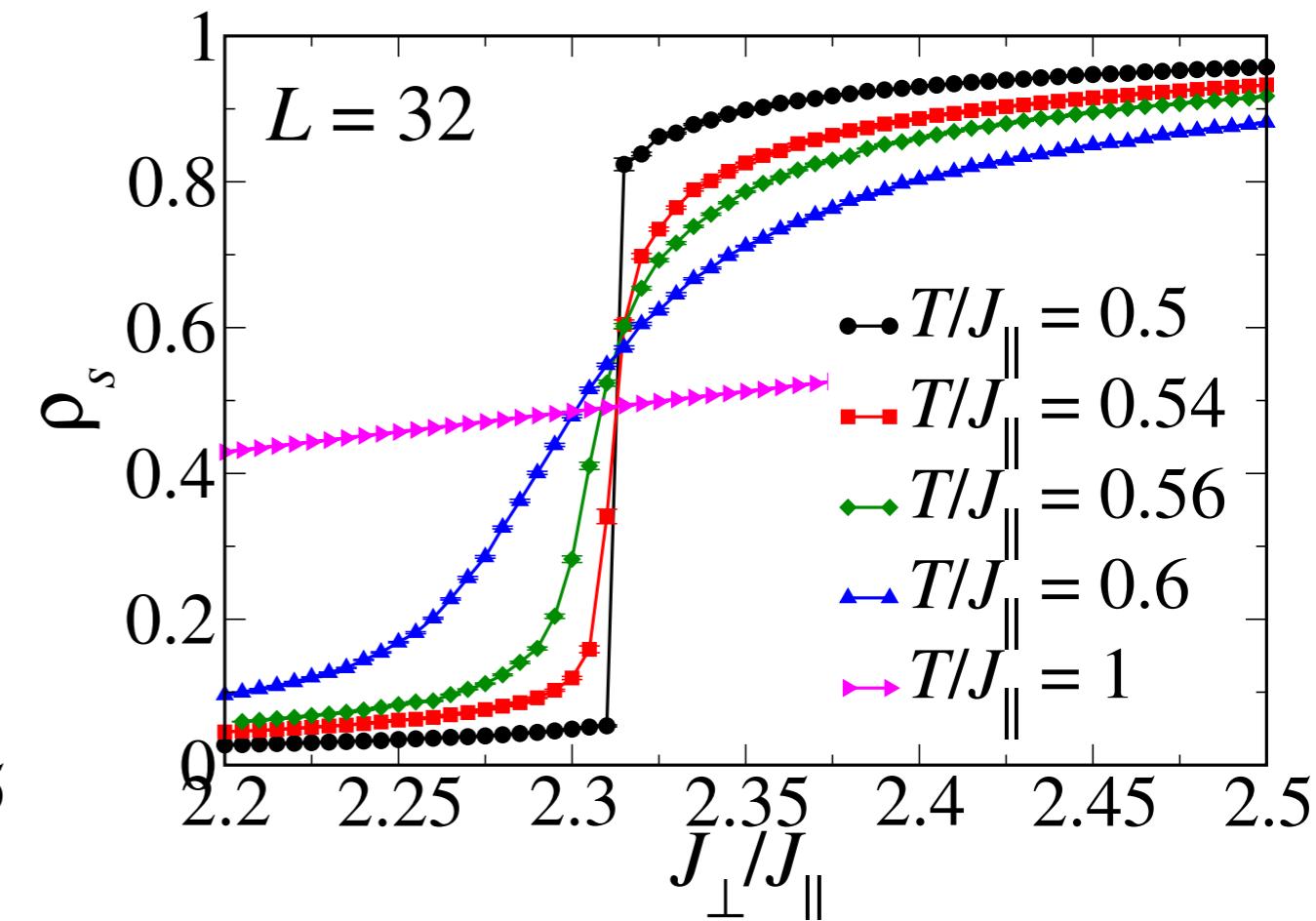
$$J_x = J_\parallel$$

# Scanning the transition region

## Internal energy



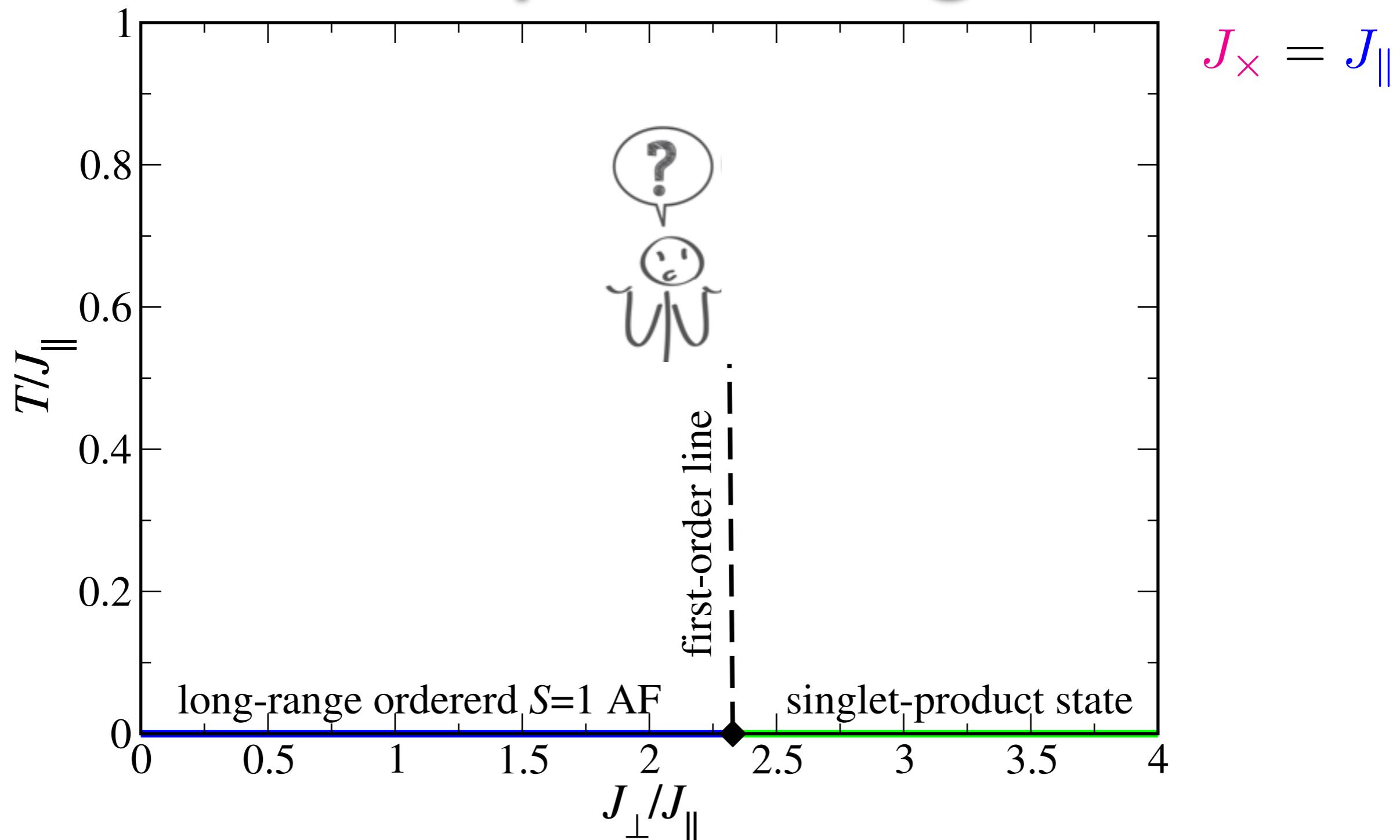
## Singlet density



- 👉 discontinuous behavior extends up to  $T \approx 0.54J$
- 👉 continuous crossover at higher  $T$
- 👉 enhanced singlet-triplet fluctuations upon approaching the first-order transition line

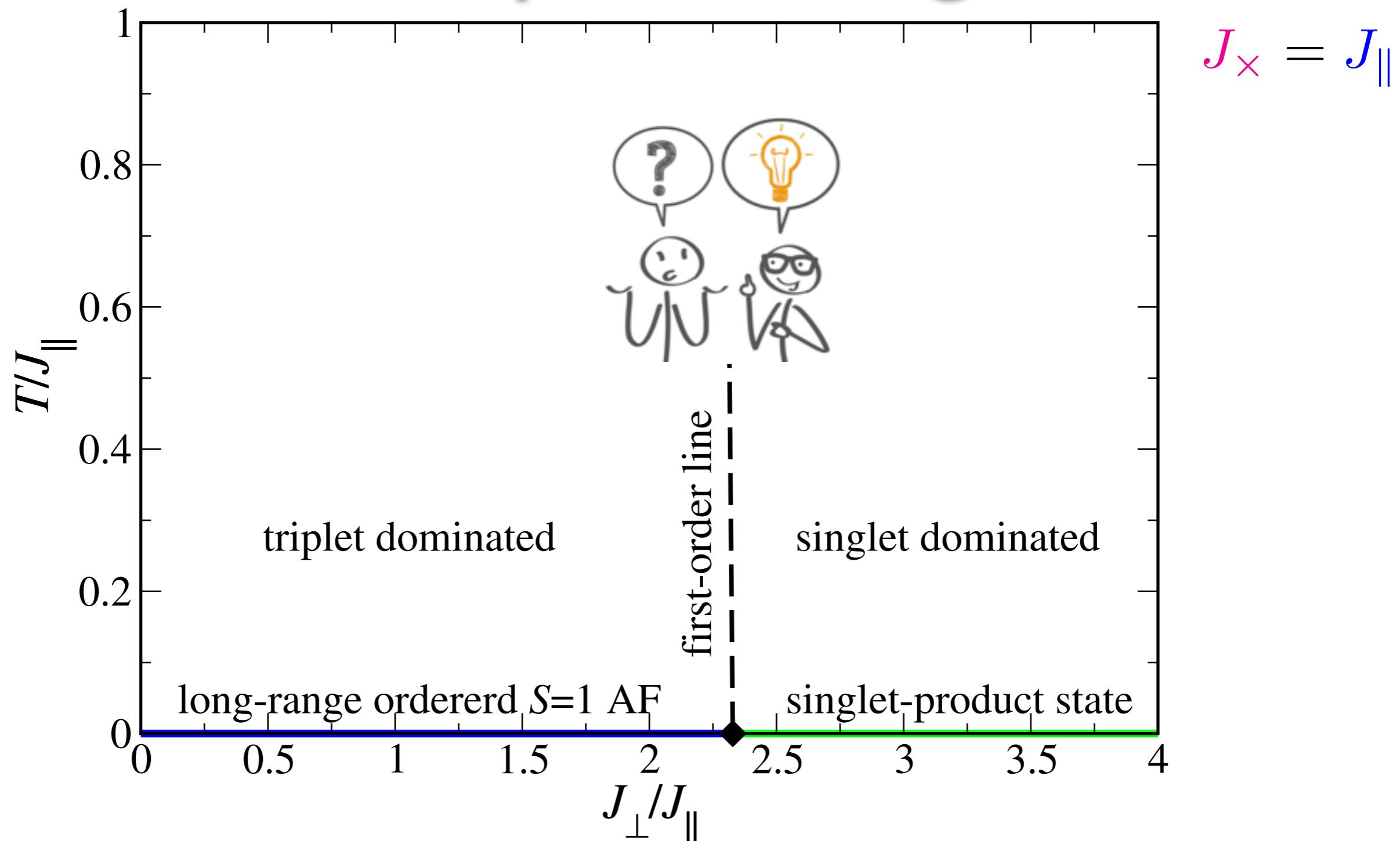
$$J_{\times} = J_{\parallel}$$

# Finite- $T$ phase diagram



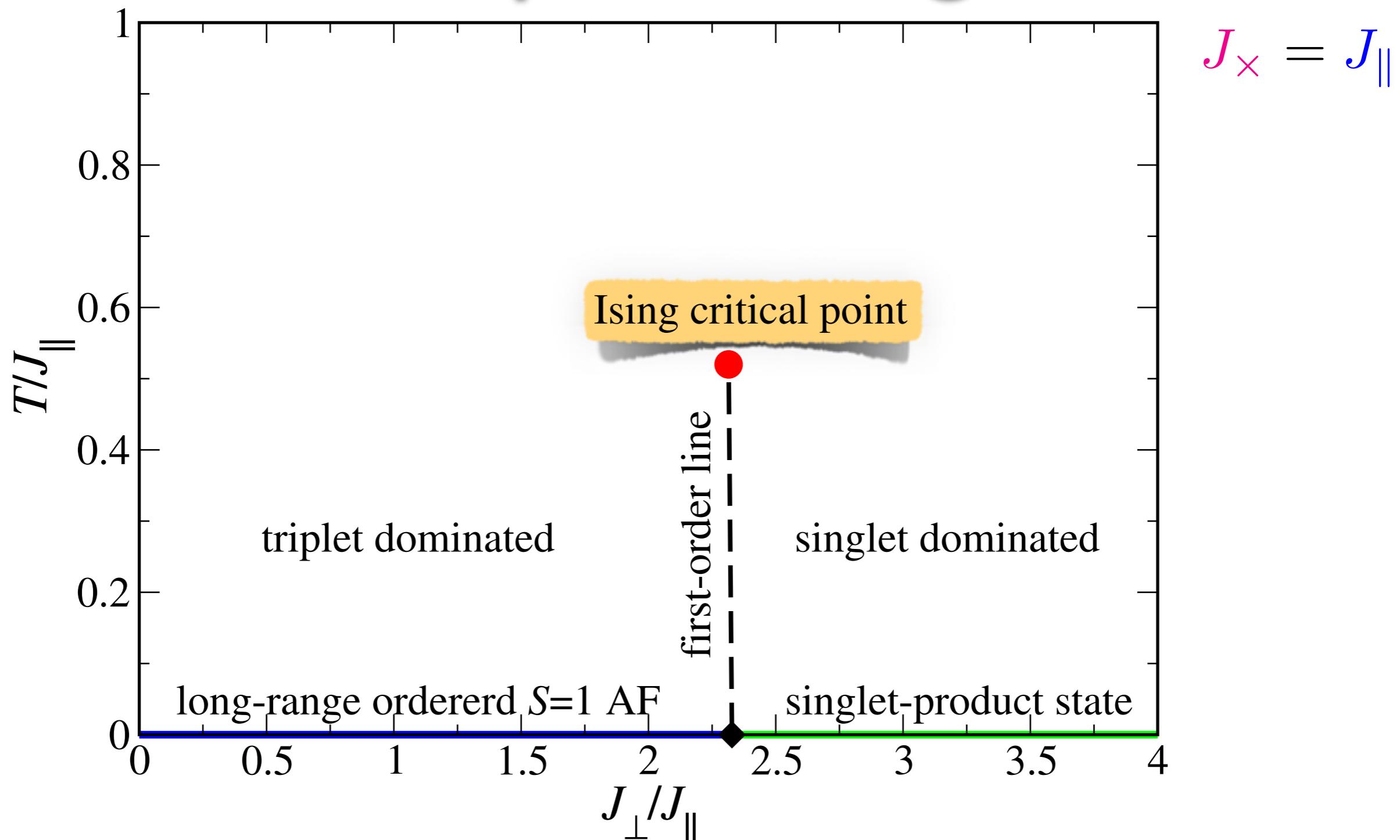
- 👉  $SU(2)$  symmetry  $\Rightarrow$  Mermin-Wagner theorem forbids finite-temperature ordering transition

# Finite- $T$ phase diagram



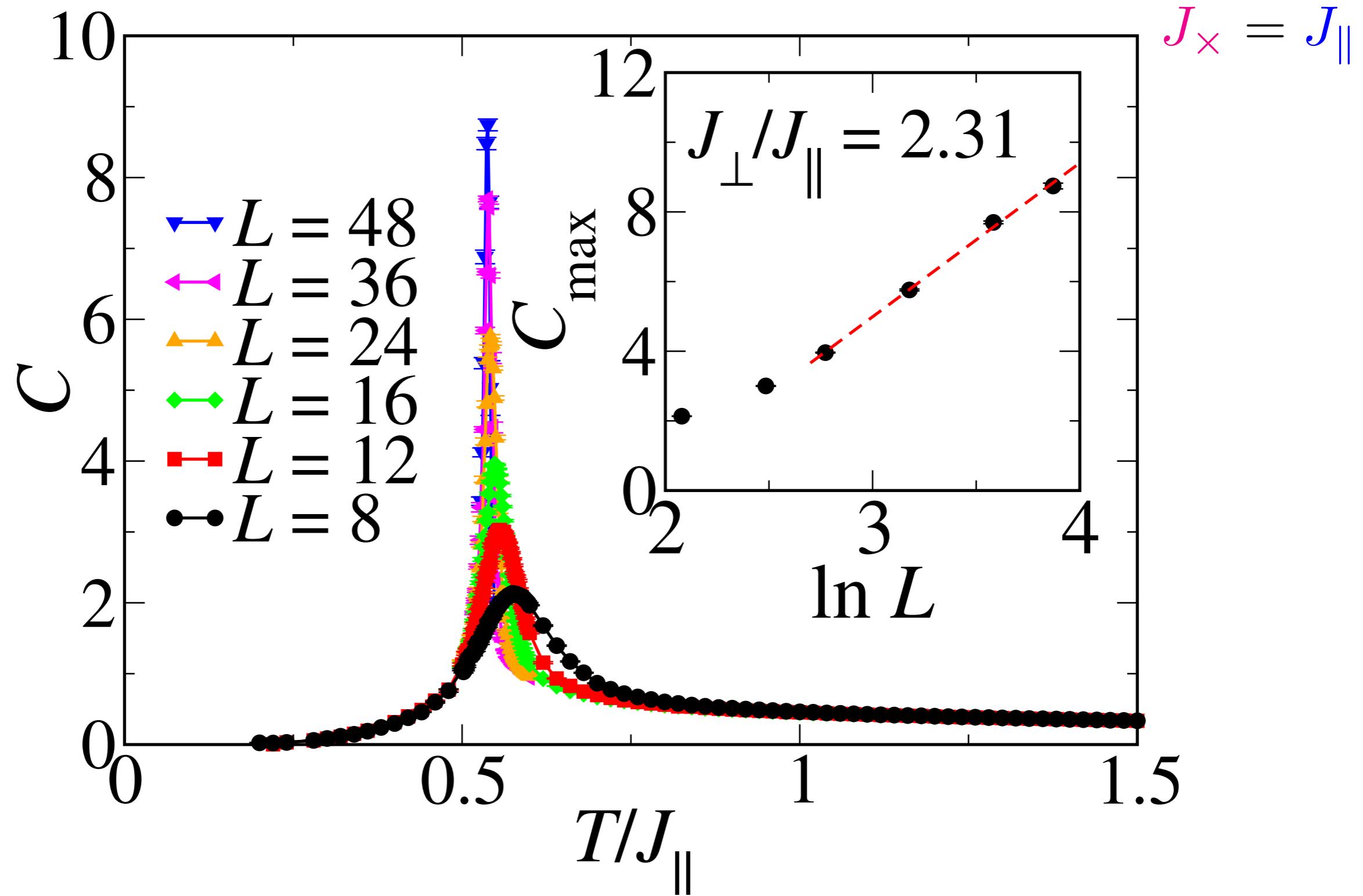
- 👉 binary variable on each dimer: singlet versus triplet ( $SU(2)$  symmetry  $\Rightarrow$  equivalence of 3 components)

# Finite- $T$ phase diagram



- 👉 binary variable on each dimer: singlet versus triplet ( $SU(2)$  symmetry  $\Rightarrow$  equivalence of 3 components)  
 $\Rightarrow$  Ising critical point

# Logarithmic specific heat scaling



👉 compatible with 2D Ising universality class

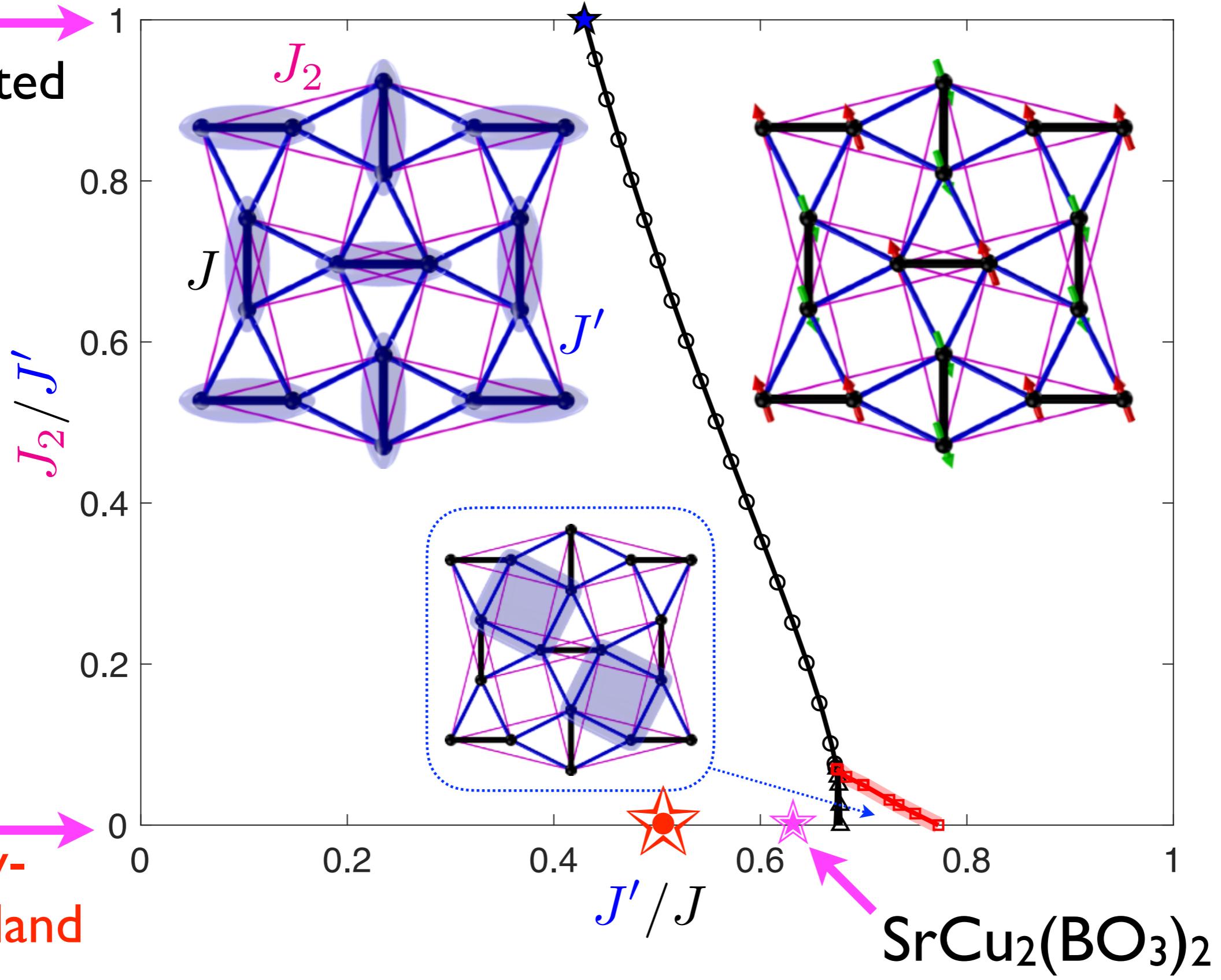
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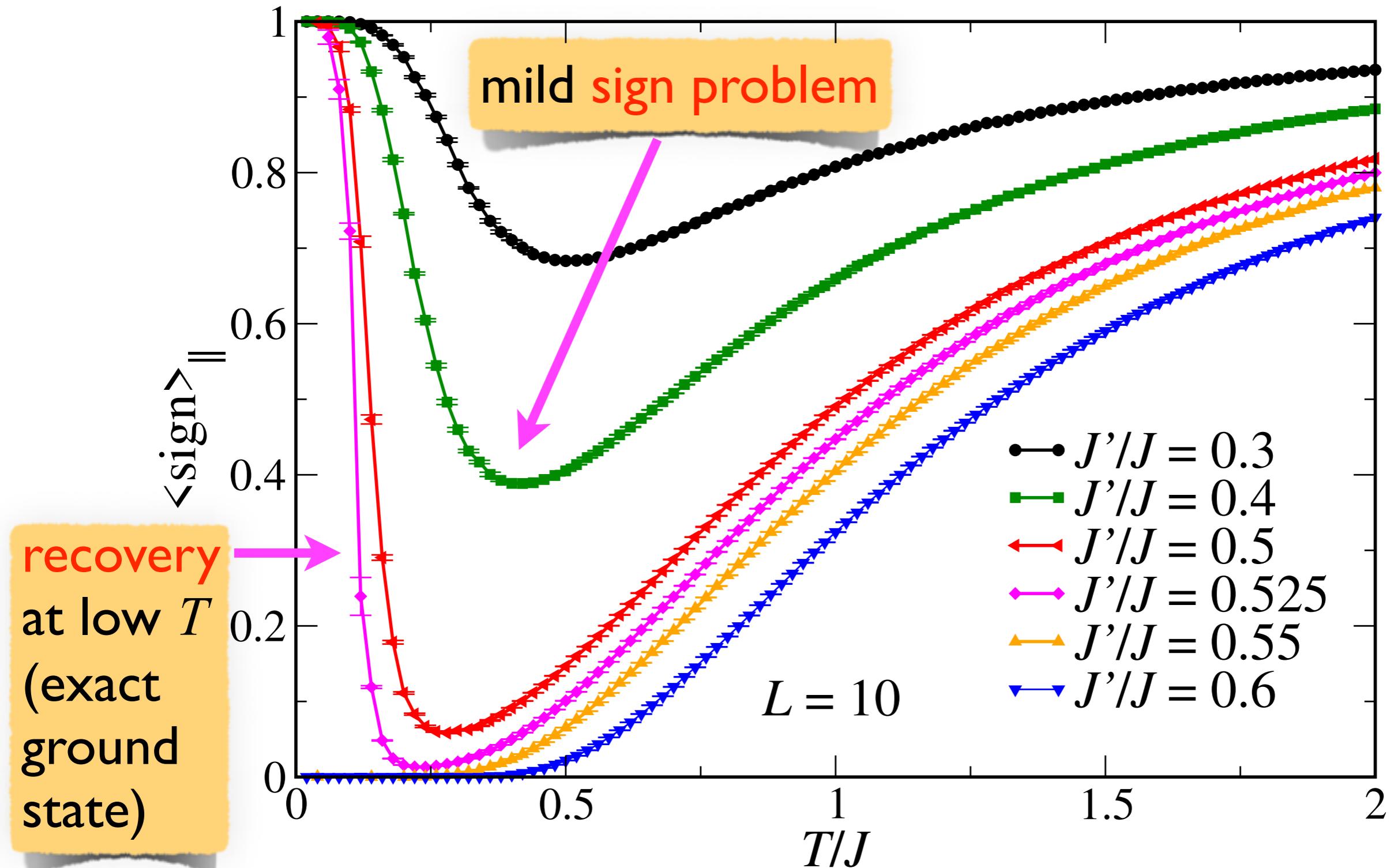
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fully  
frustrated  
bilayer



# Average sign

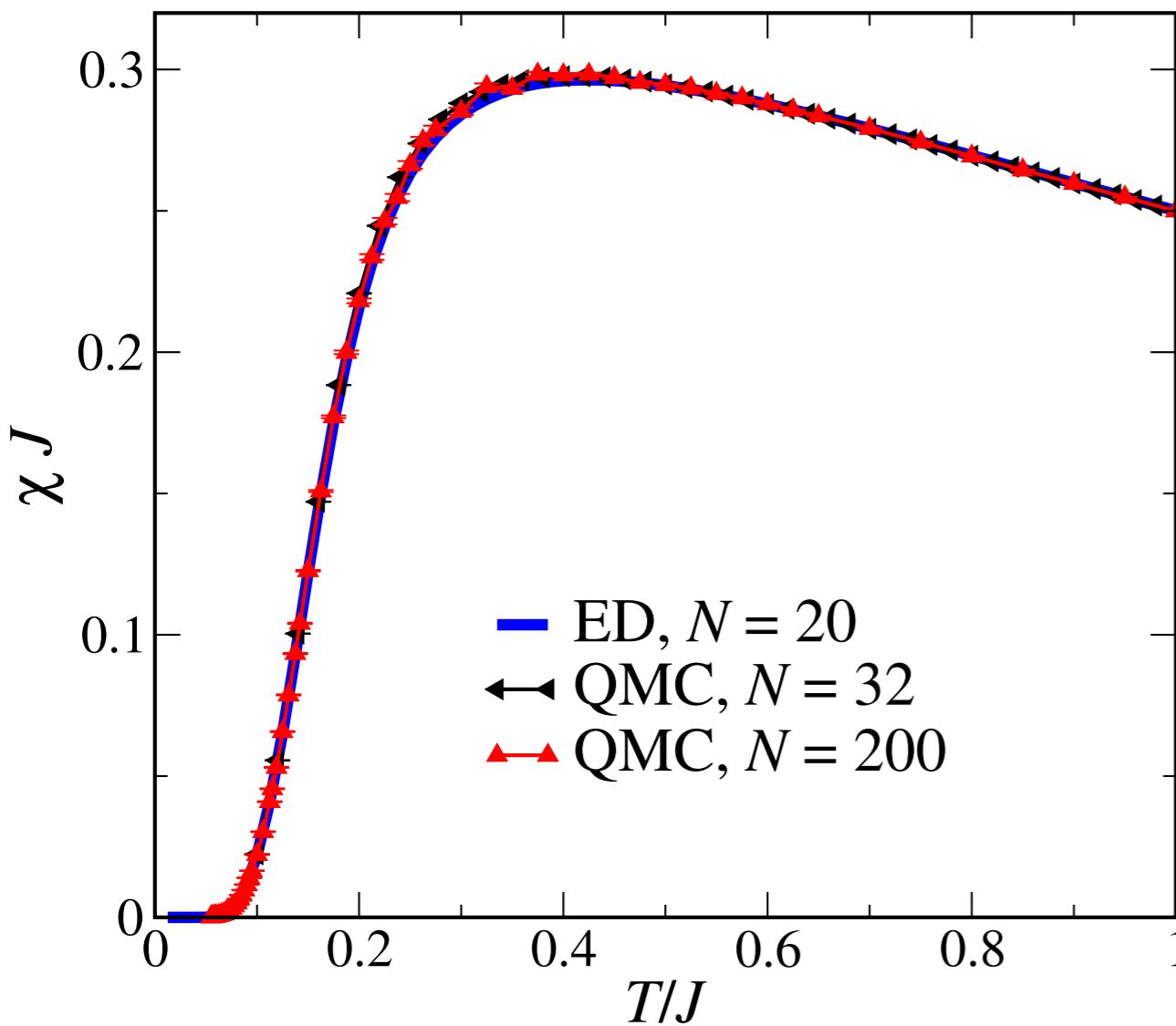
$J_2 = 0$



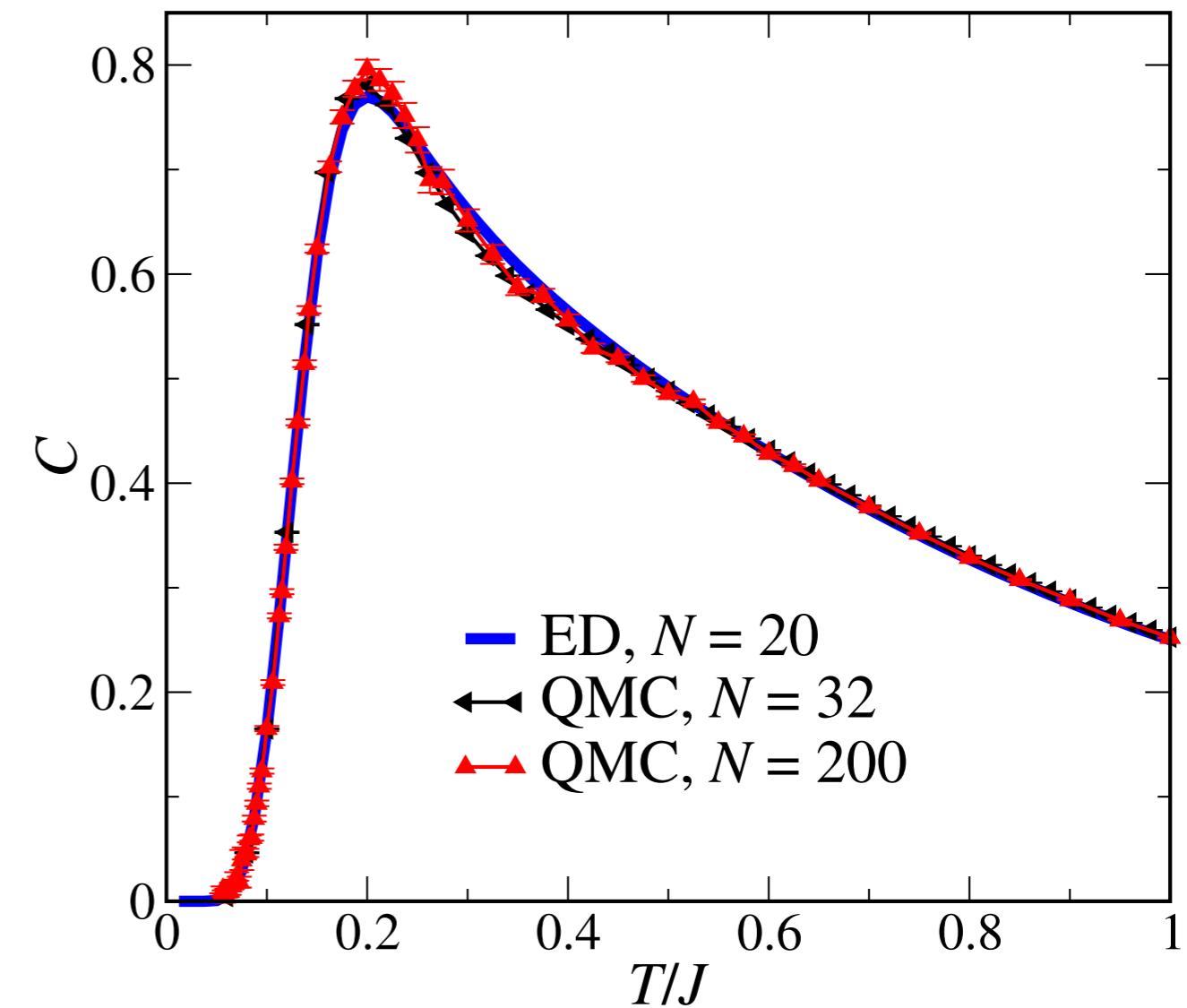
# Example: $J'/J = 0.5$

$J_2 = 0$

## Magnetic susceptibility



## Specific heat



- 👉 Quantum Monte Carlo (QMC) with  $N=200$  spins ✓
- 👉 Exact diagonalization (ED) for  $N=20$  correct, except for persistent finite-size effects close to the maximum of  $C$

# Summary

## 2D Shastry-Sutherland Model:

- progress with QMC, but  $\text{SrCu}_2(\text{BO}_3)_2$  remains open

## fully frustrated square lattice:

- detailed analysis of finite- $T$  properties possible:  
first-order transition terminating in Ising critical point

## other possible applications:

- 3D bicubic dimer model
- planar pyrochlore (checkerboard)
- kagome, pyrochlore, ...

J. Stapmanns, P. Corboz, F. Mila,  
A.H., B. Normand, S. Wessel,  
[arXiv:1805.11017](https://arxiv.org/abs/1805.11017)



## Thanks:



*Efficient Quantum Monte-Carlo simulations can be performed for certain highly frustrated quantum magnets using a suitable computational basis.*