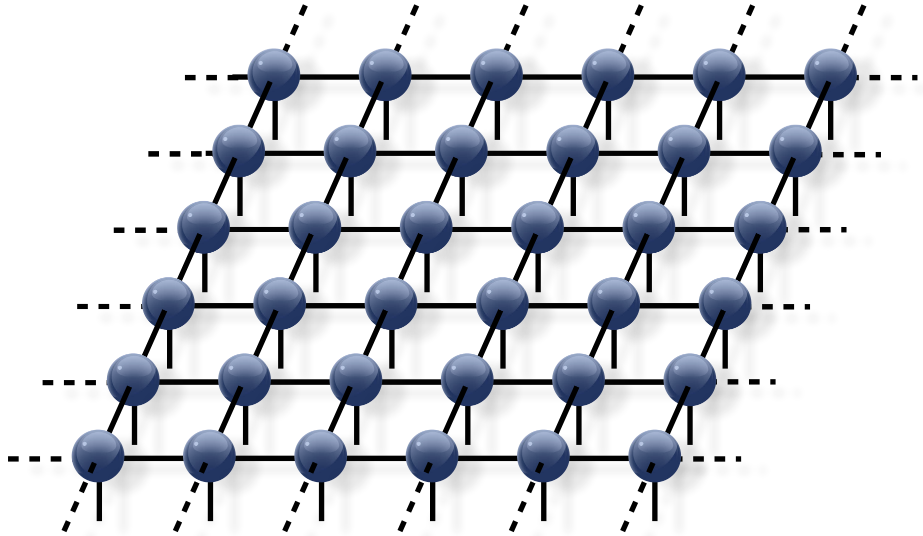
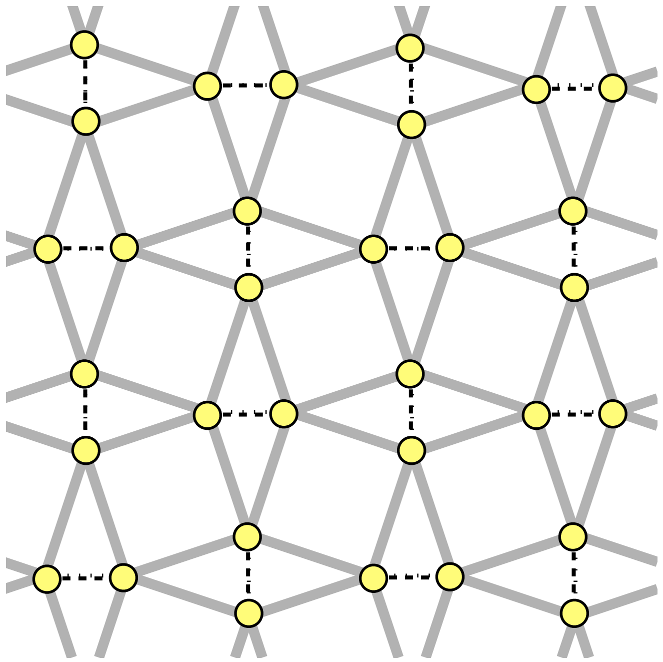
Tensor network studies of the Shastry-Sutherland model ($SrCu_2(BO_3)_2$)

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



iPEPS
2D tensor network ansatz



The Shastry-Sutherland model (*$SrCu_2(BO_3)_2$*)

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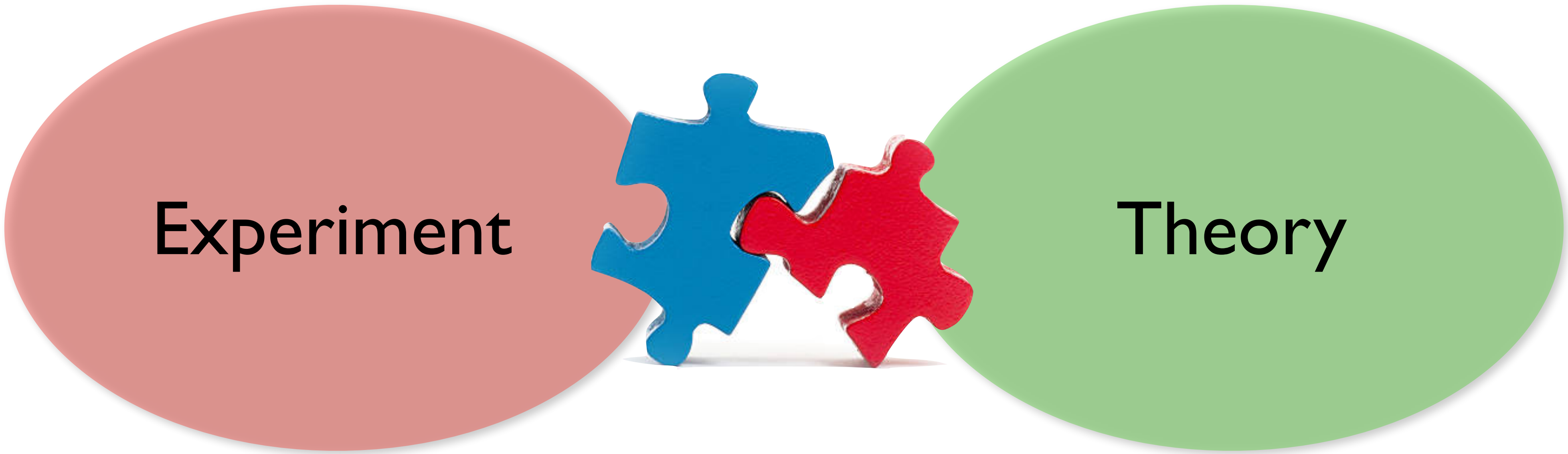

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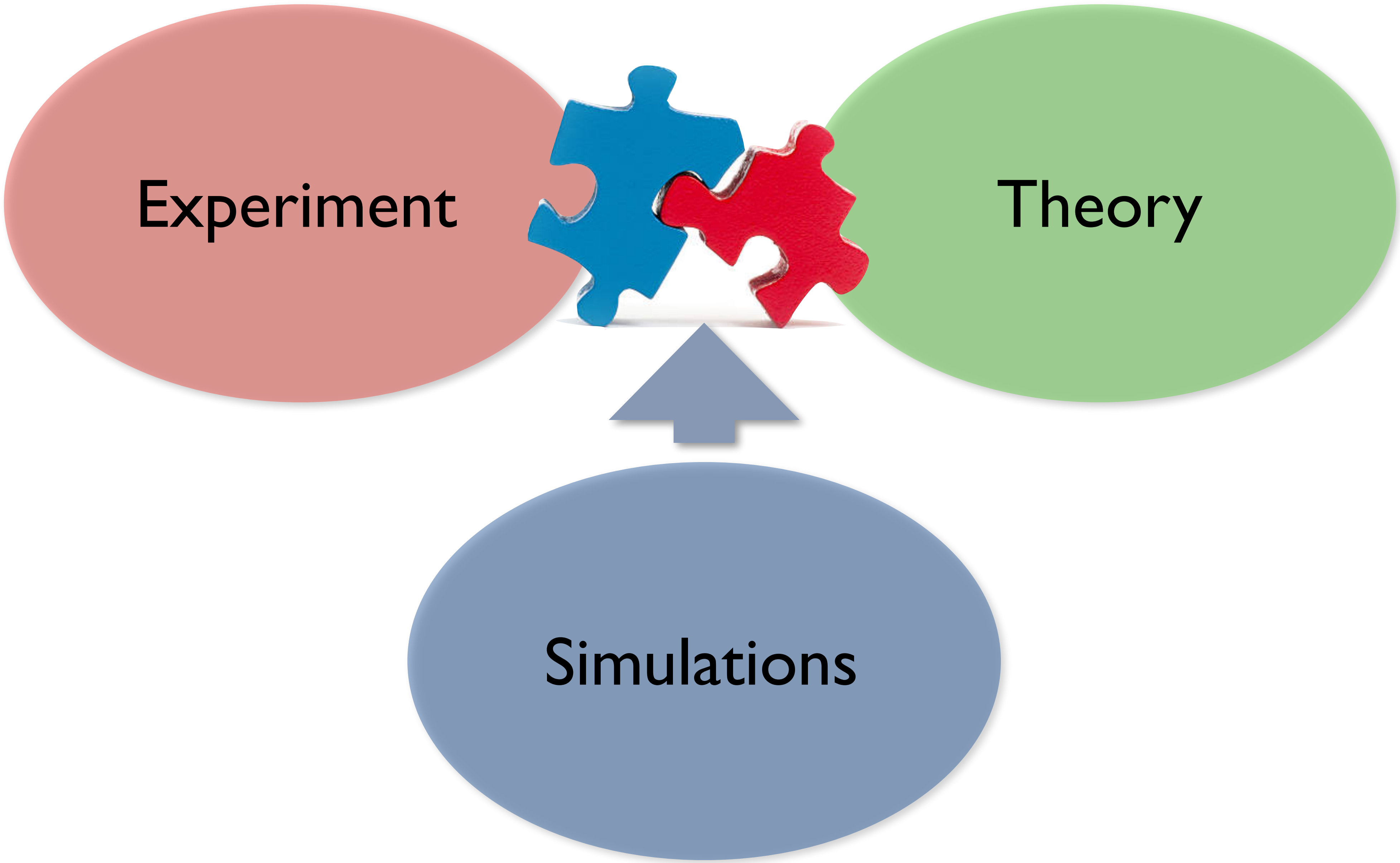

- *Unbiased numerical simulations* $\longrightarrow$ ***SURPRISE***
  - ✦ New understanding of the magnetization process in $SrCu_2(BO_3)_2$

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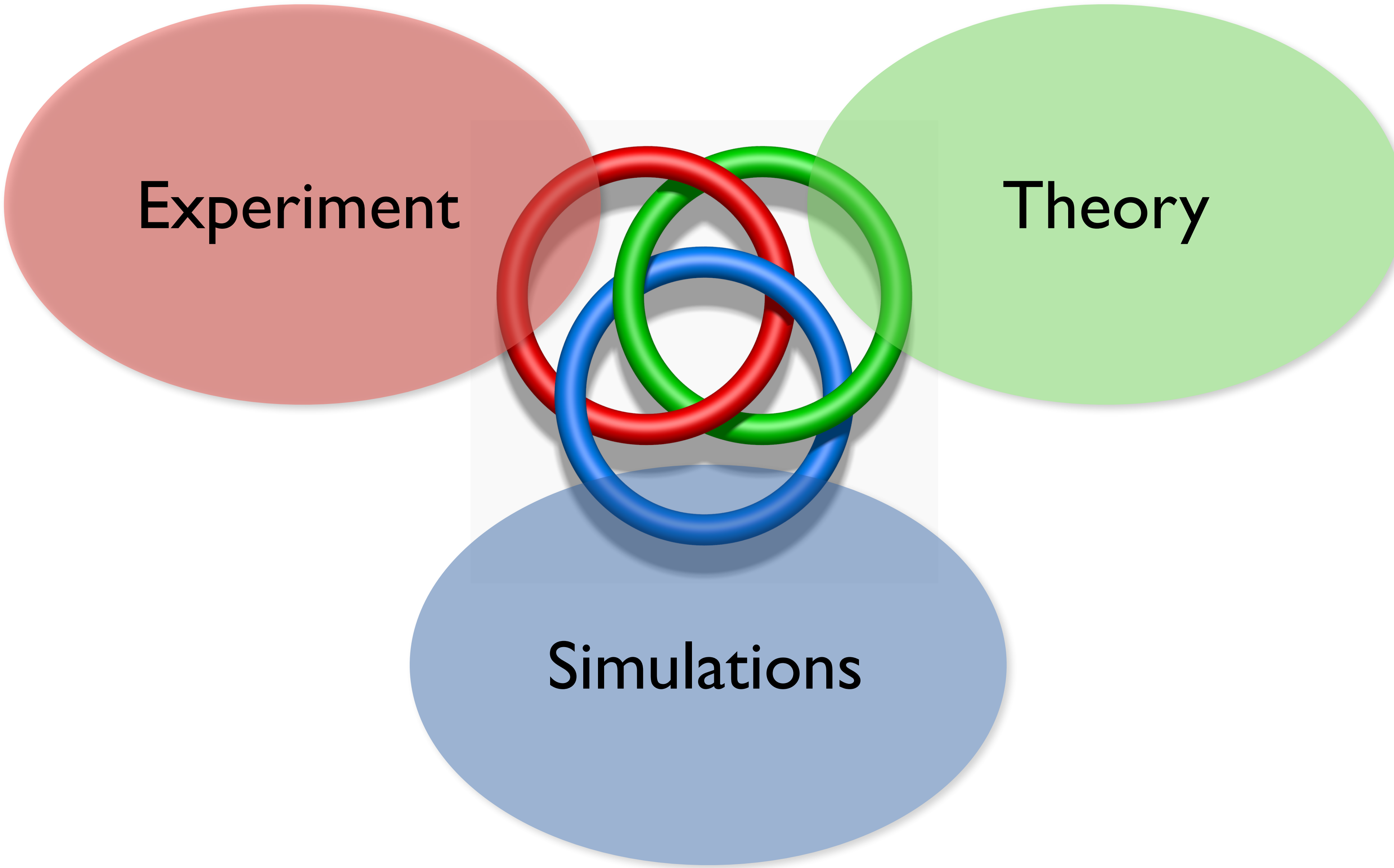

- *Unbiased numerical simulations* $\longrightarrow$ ***SURPRISE***
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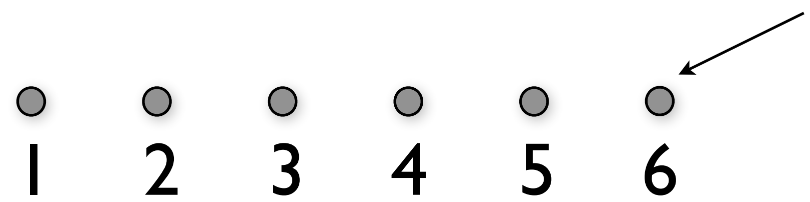
Outline

- Introduction to iPEPS (2D tensor network ansatz)
- The Shastry-Sutherland model (SSM) in a magnetic field
  - ✦ *Magnetization plateaus = crystals made of Sz=2 bound states (not triplets!)*
  - ✦ *Supersolid phases at high magnetic fields*
- The chemically doped Shastry-Sutherland system ($SrCu_{2-x}Mg_x(BO_3)_2$)
  - ✦ *New anomalies in the magnetization process*
- $SrCu_2(BO_3)_2$ under pressure: extended SSM
  - ✦ *Competition between full plaquette phase vs empty plaquette phase*
- Outlook & summary

Tensor network ansatz for a wave function

Lattice:



2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

Tensor network ansatz for a wave function

Lattice: 1 2 3 4 5 6

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2^6 basis states

2^6 coefficients

State: $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4 i_5 i_6} \boxed{\Psi_{i_1 i_2 i_3 i_4 i_5 i_6}} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$

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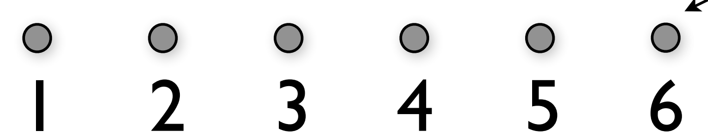

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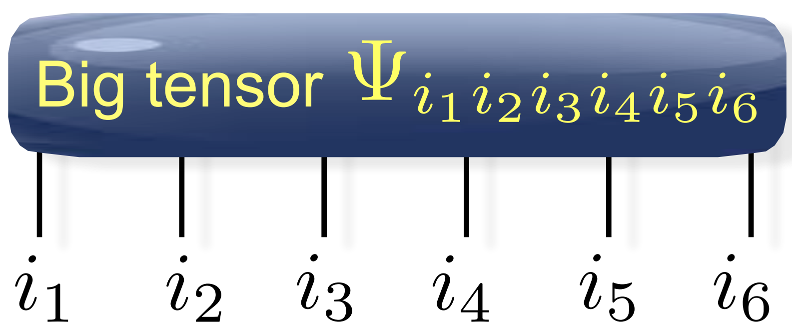
Tensor/multidimensional array



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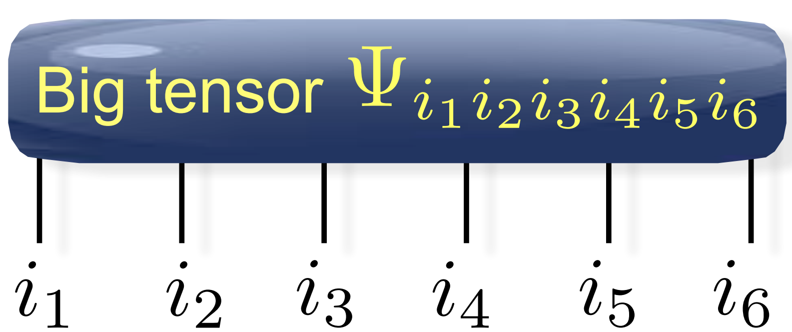
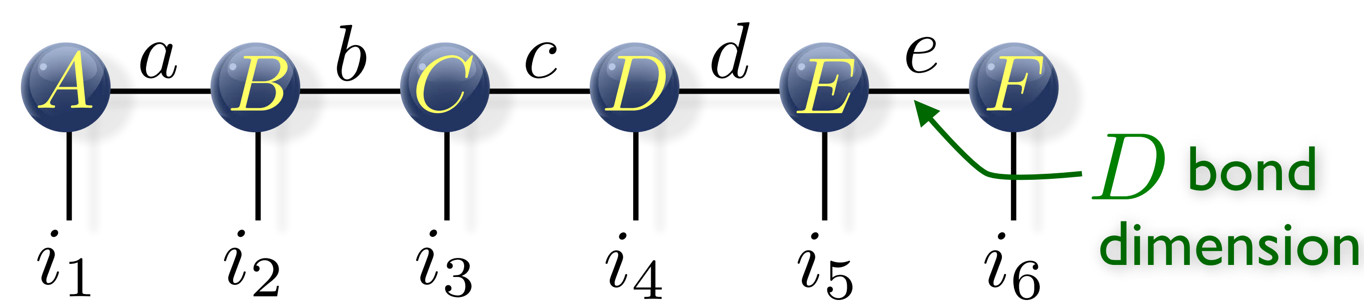


Tensor network: matrix product state (**MPS**)



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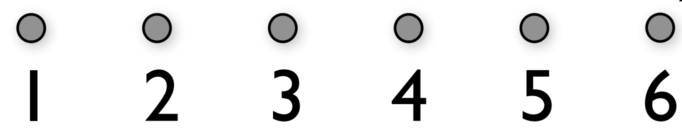

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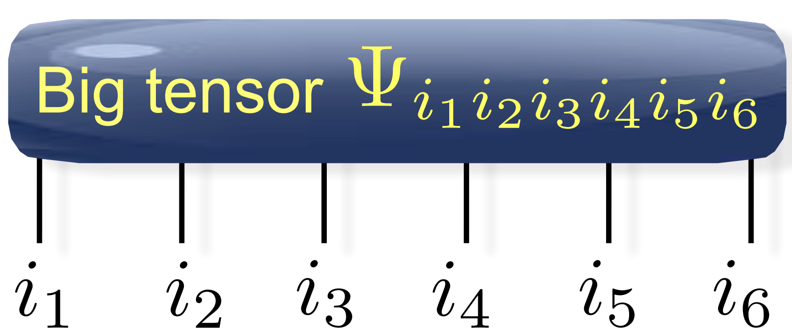

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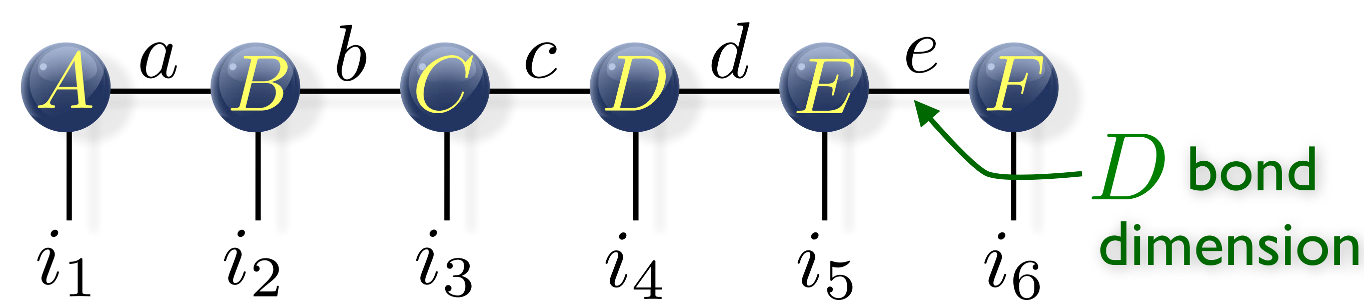

$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

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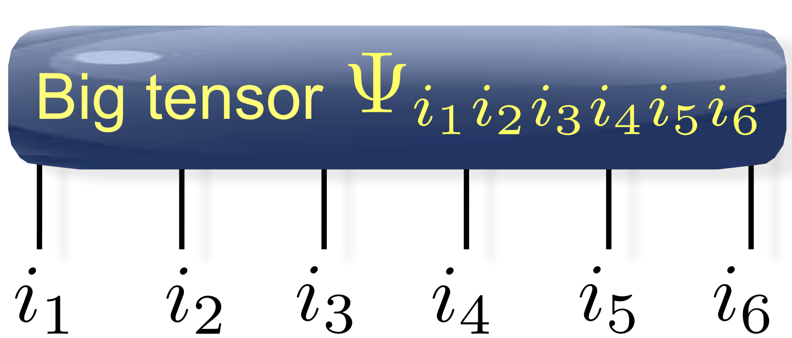

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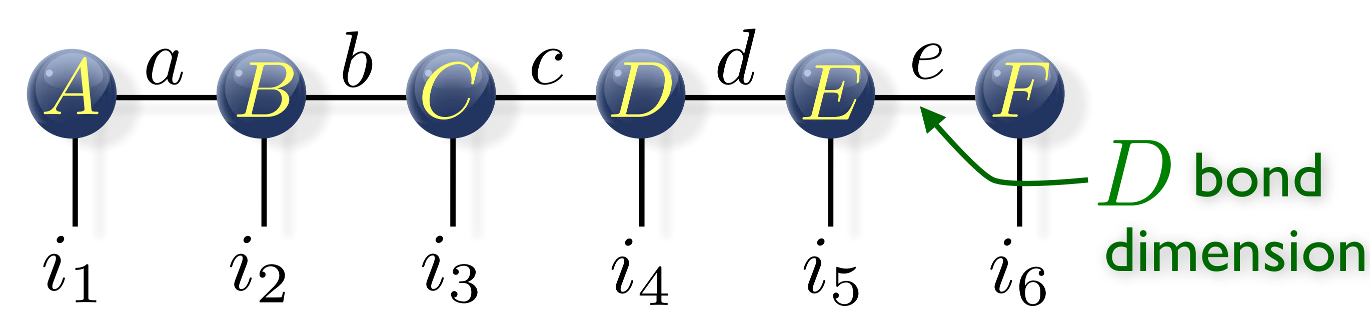

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exp(N) many numbers **vs** poly(D,N) numbers

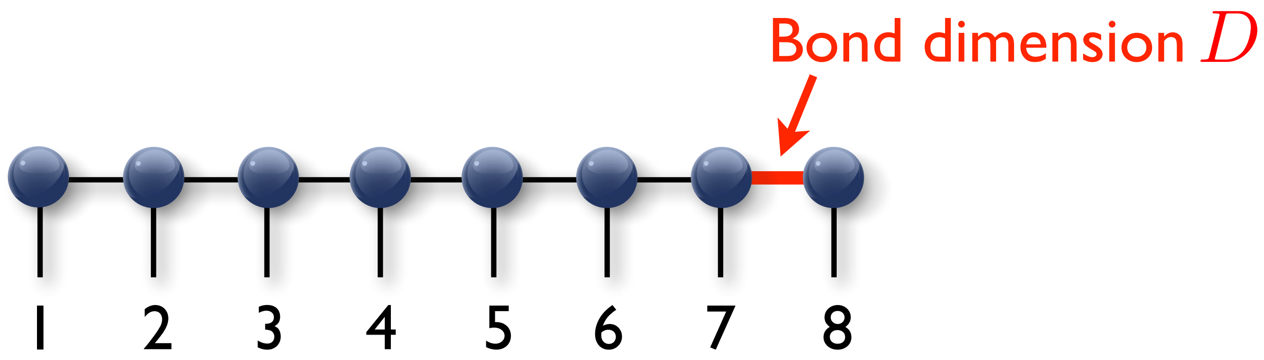
Efficient representation!

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

S. R. White, PRL 69, 2863 (1992)

Fannes et al., CMP 144, 443 (1992)

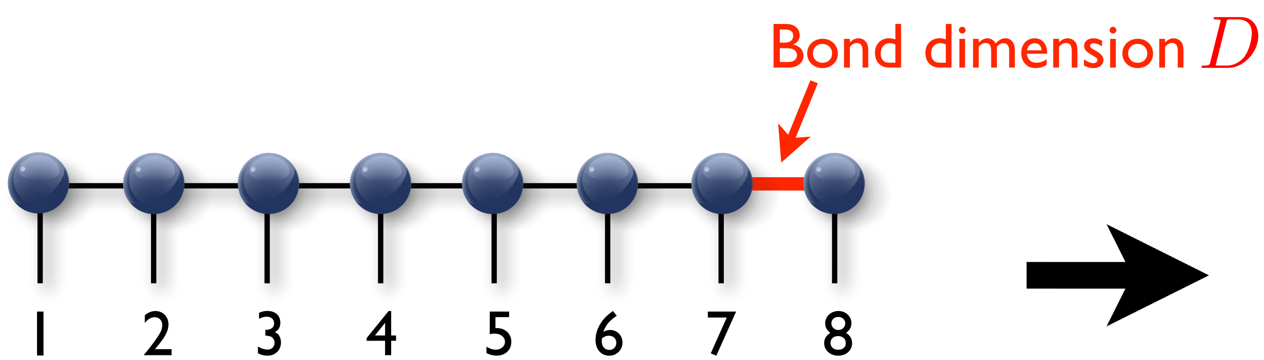
Östlund, Rommer, PRL 75, 3537 (1995)

MPS & PEPS

1D

MPS

Matrix-product state



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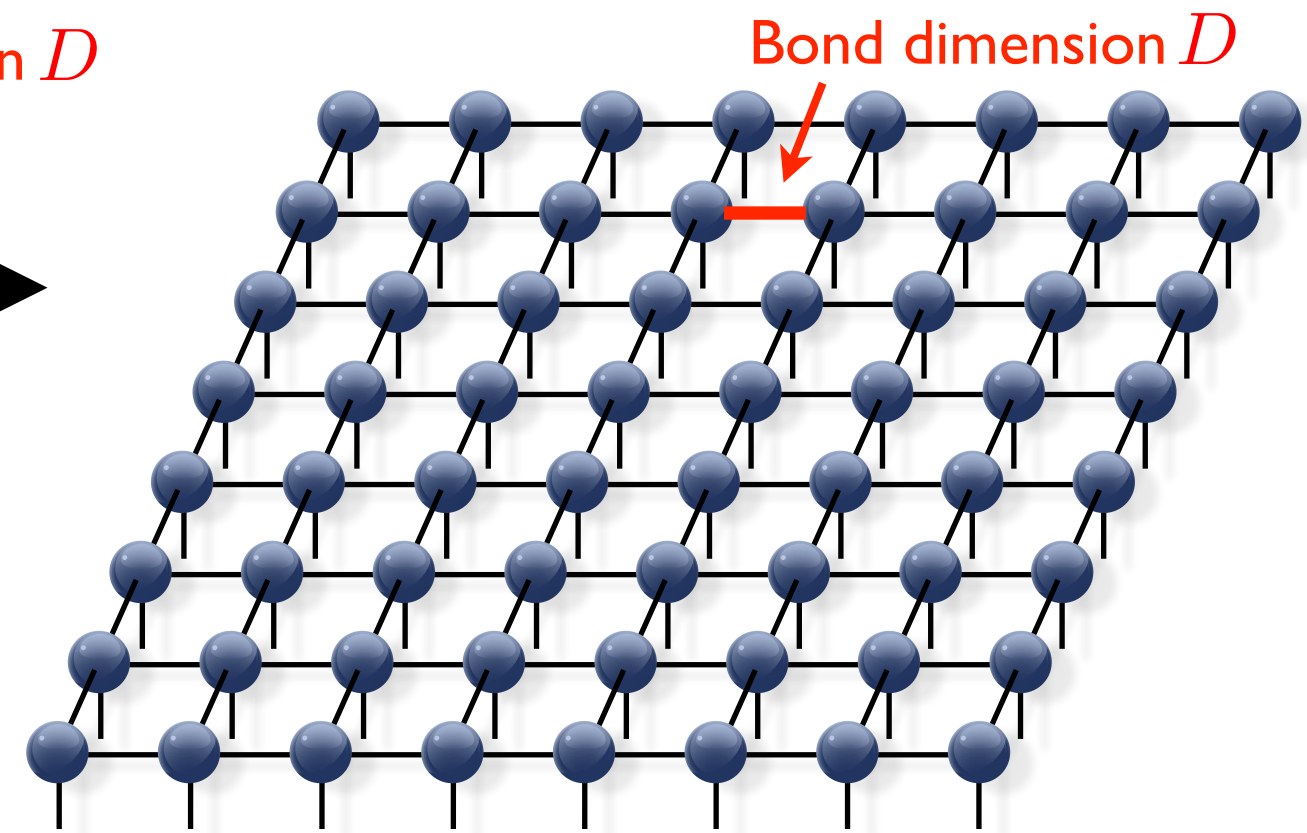
2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



F. Verstraete, J. I. Cirac, cond-mat/0407066

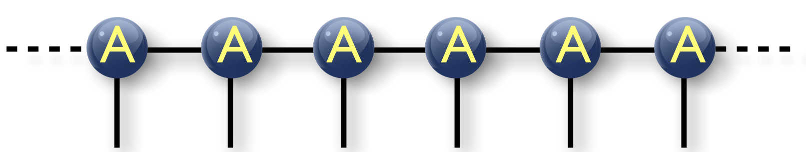
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

Infinite PEPS (iPEPS)

1D

iMPS

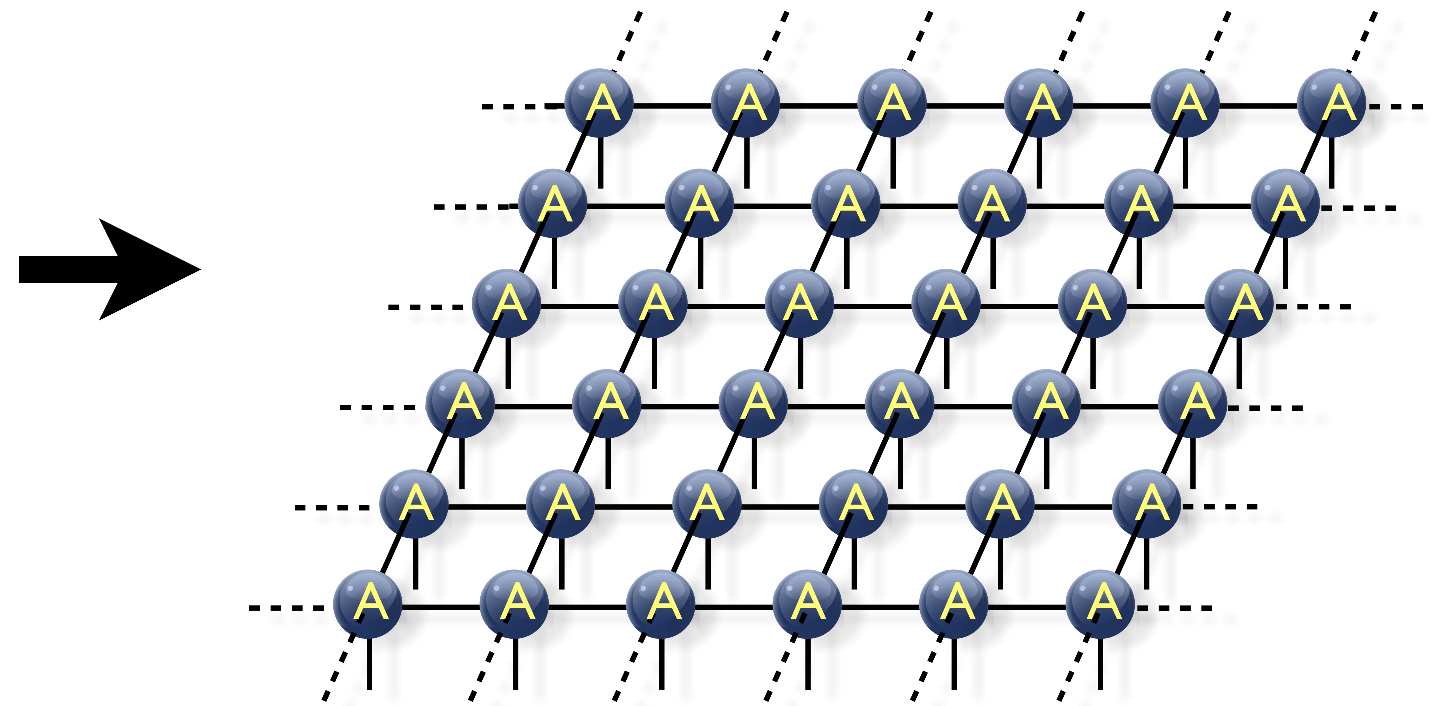
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

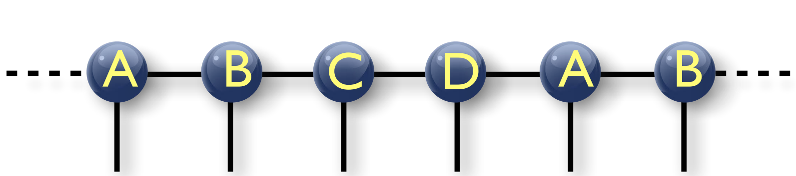
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

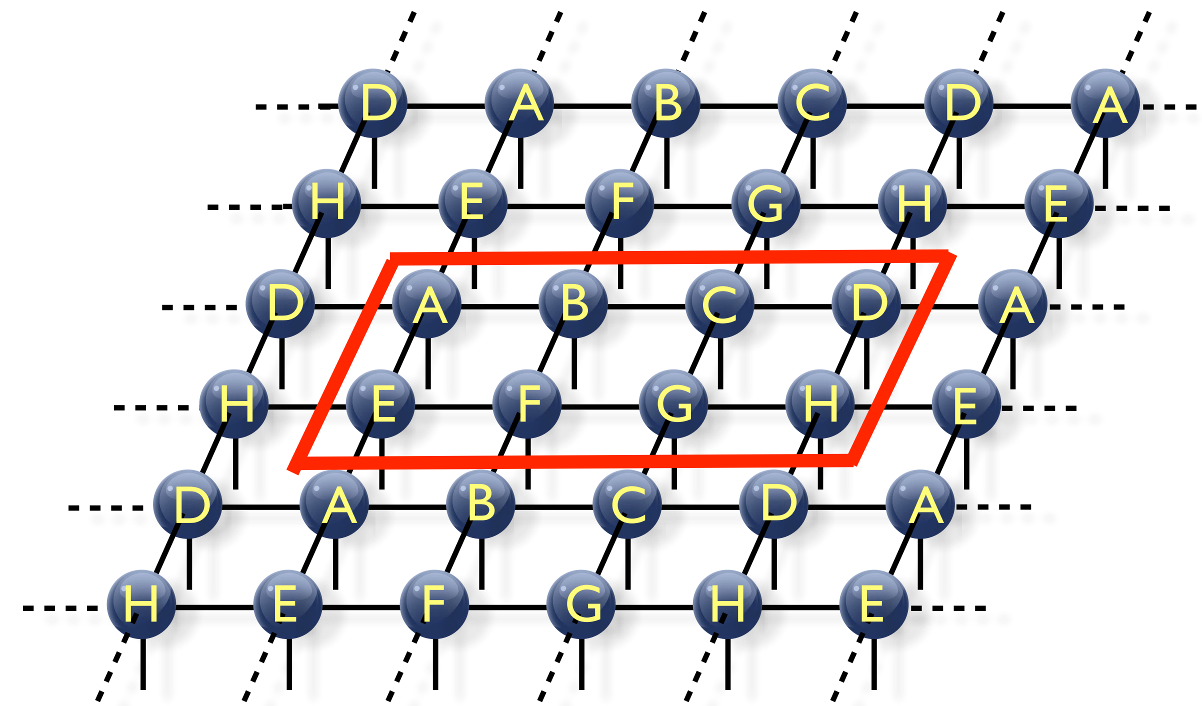
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



here: 4x2 unit cell

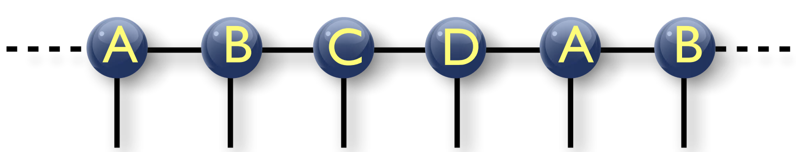
PC, White, Vidal, Troyer, PRB **84** (2011)

iPEPS with arbitrary unit cells

1D

iMPS

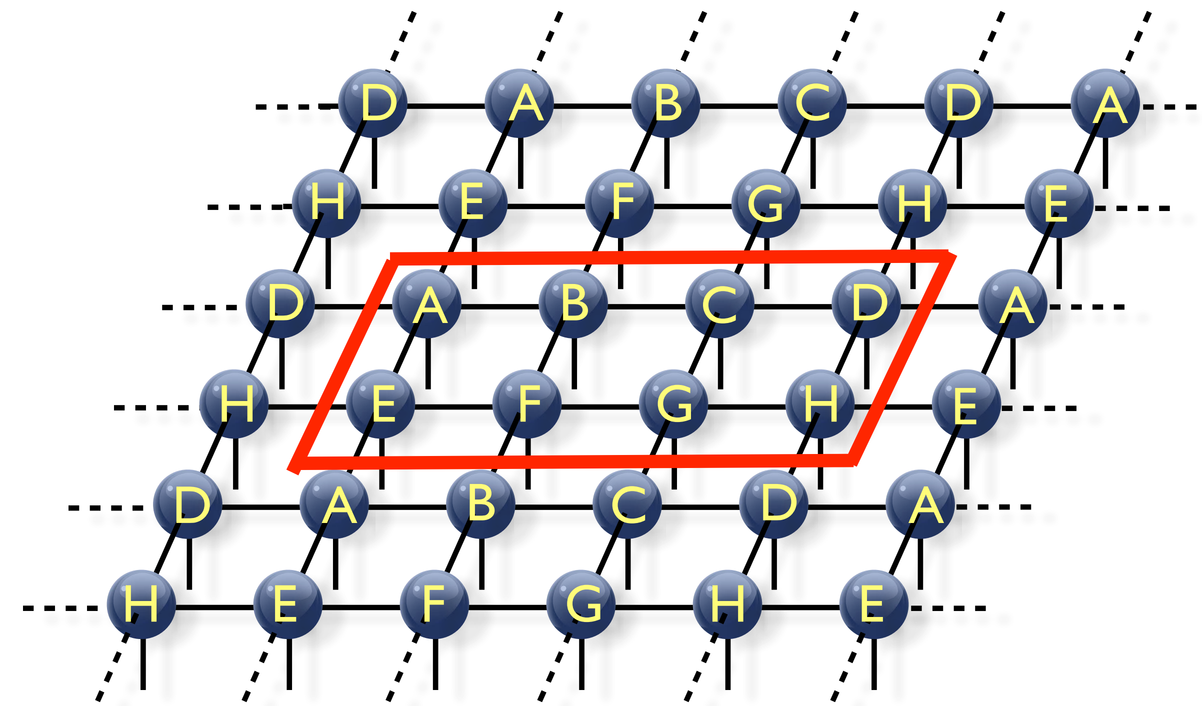
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



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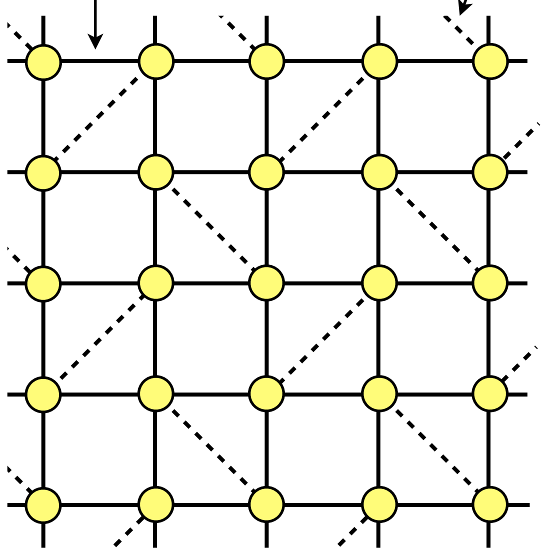
★ Run simulations with different unit cell sizes and compare variational energies

The Shastry-Sutherland model

$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$



Shastry & Sutherland, Physica B+C **108** (1981).

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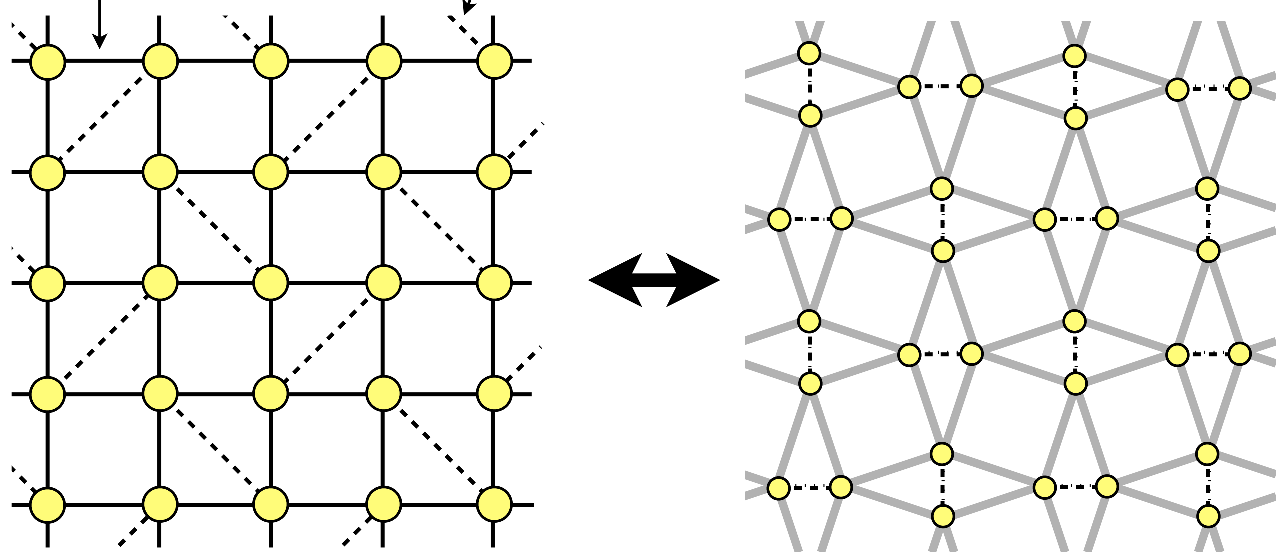

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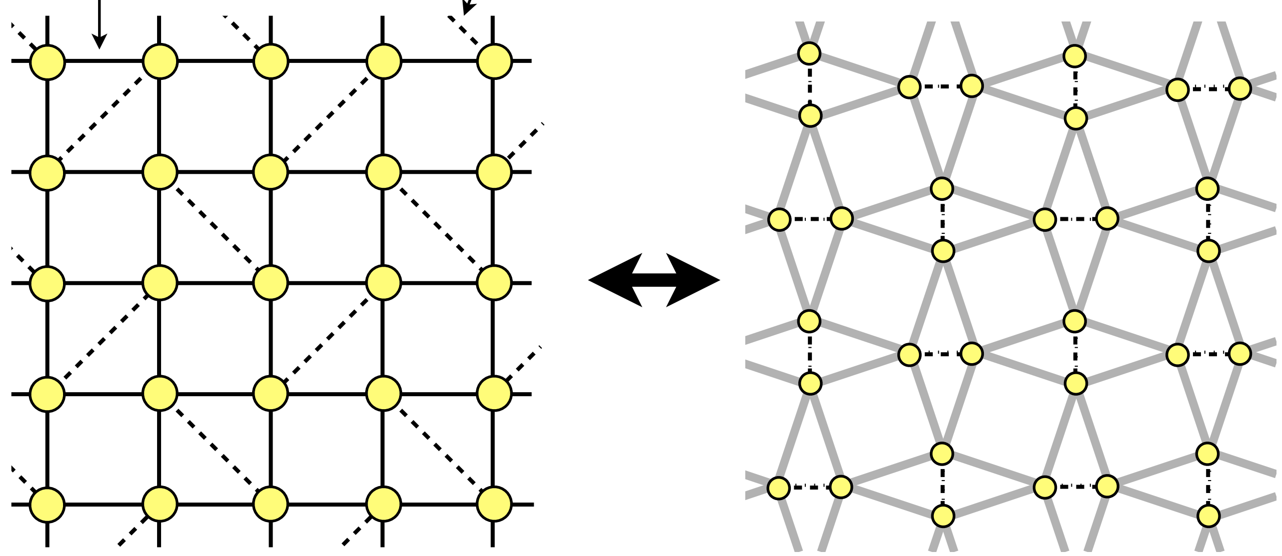

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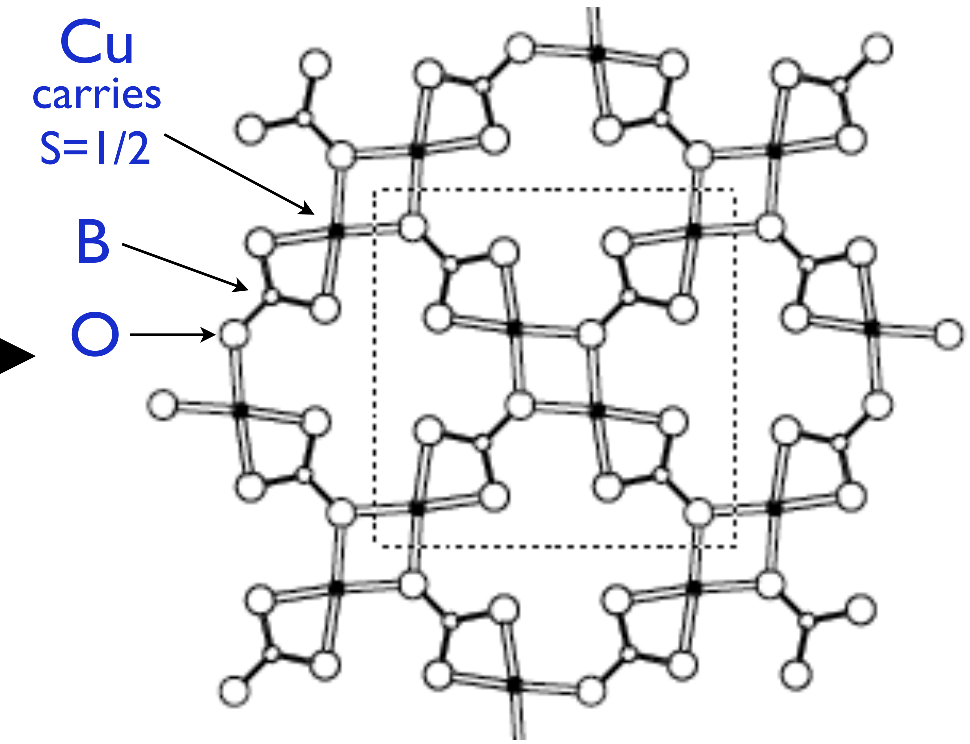
$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



Kageyama et al. PRL **82** (1999)

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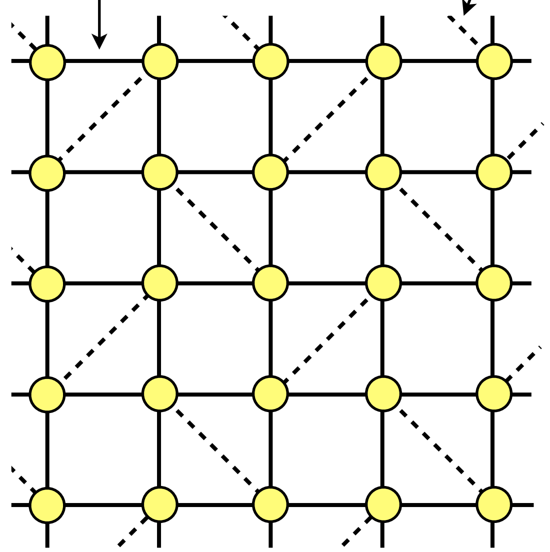

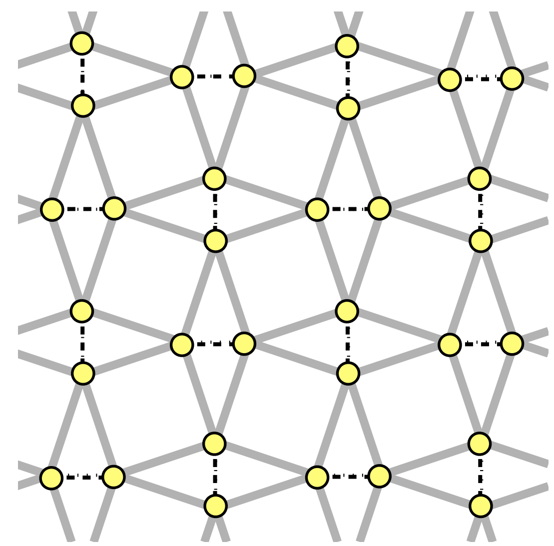

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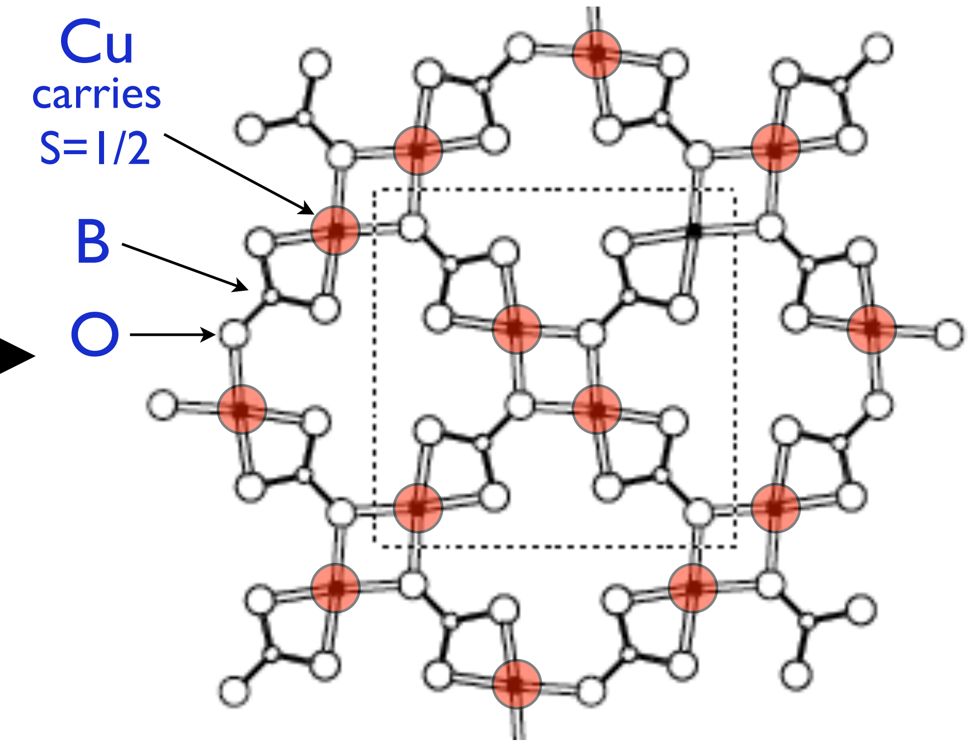

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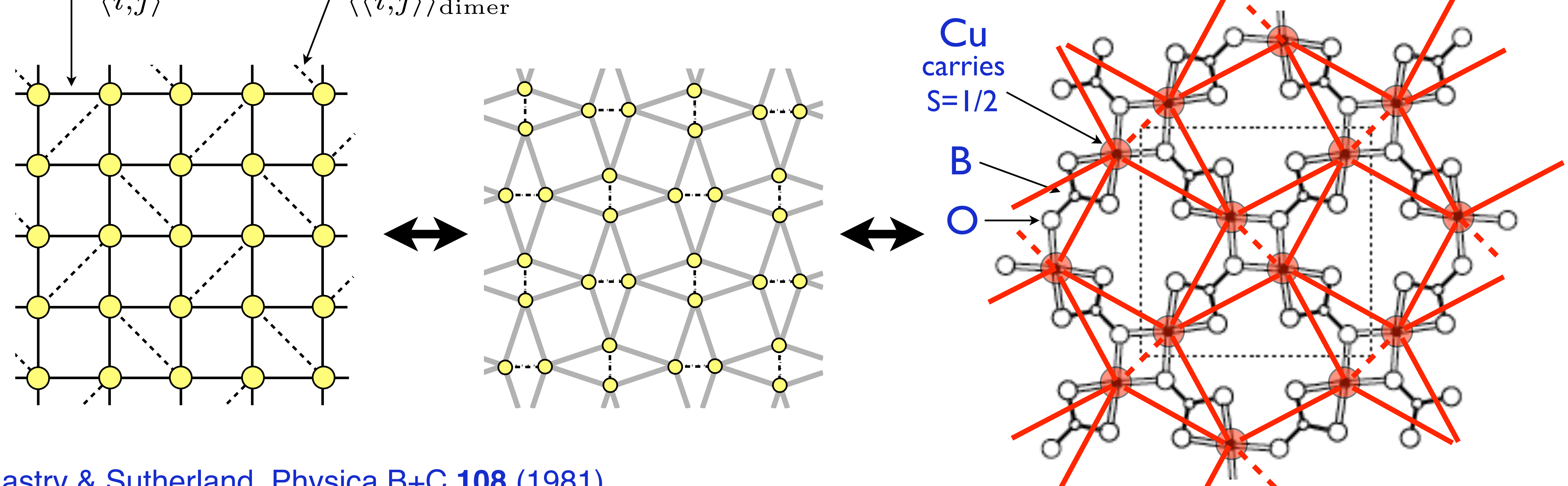

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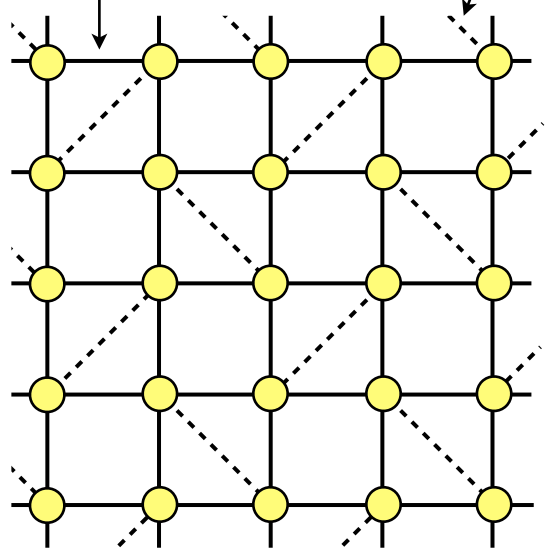
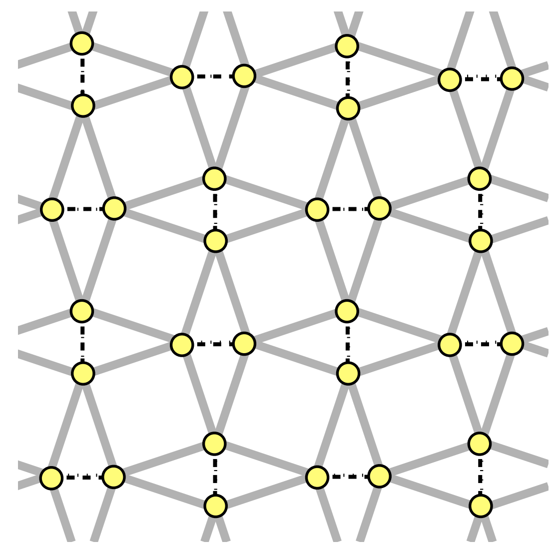


$\leftrightarrow$



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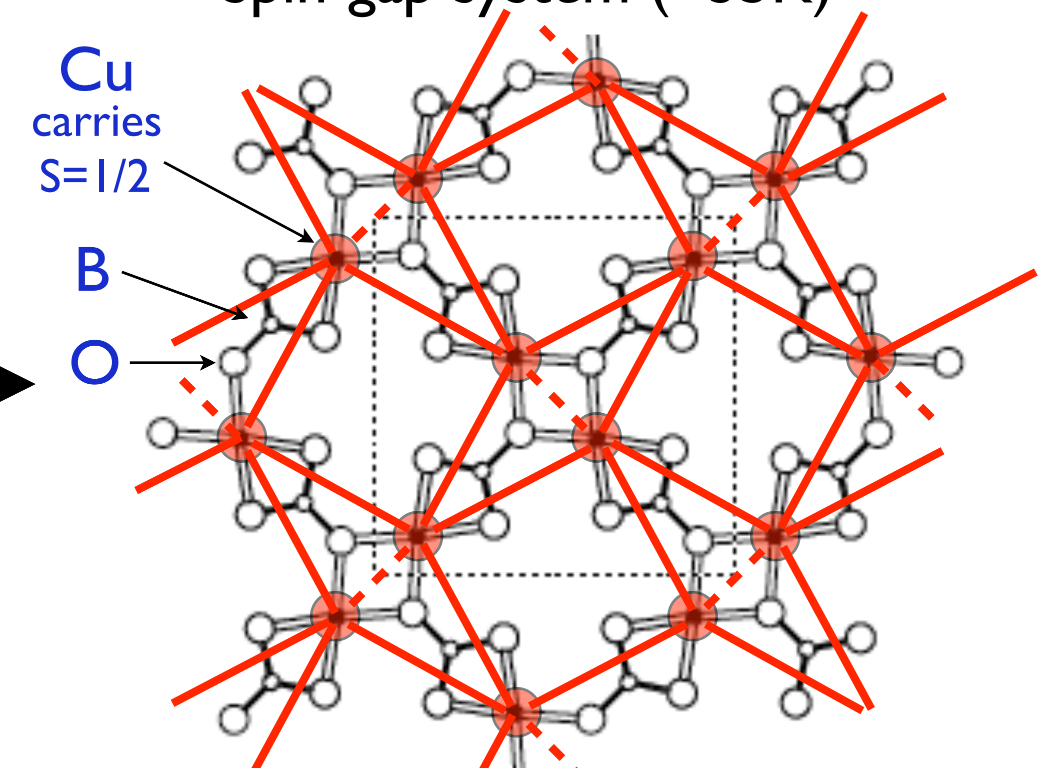

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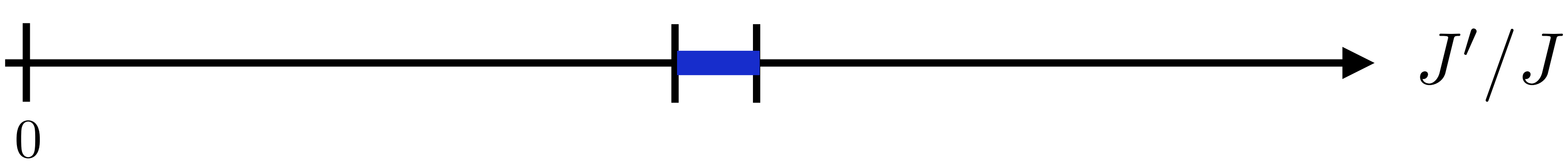

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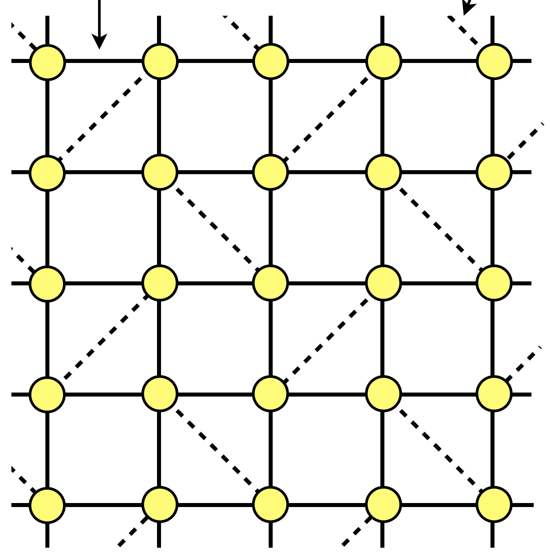

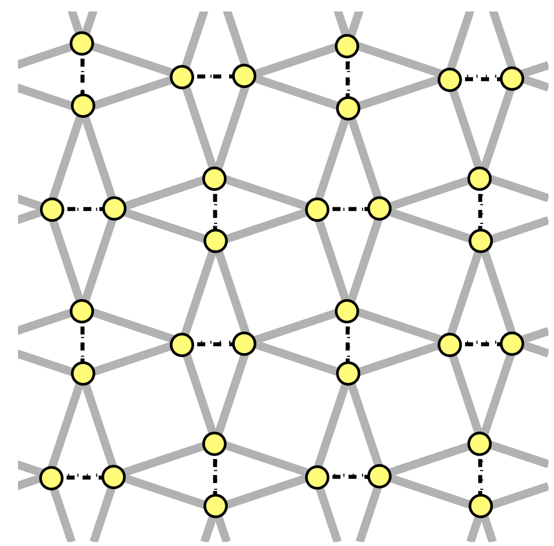

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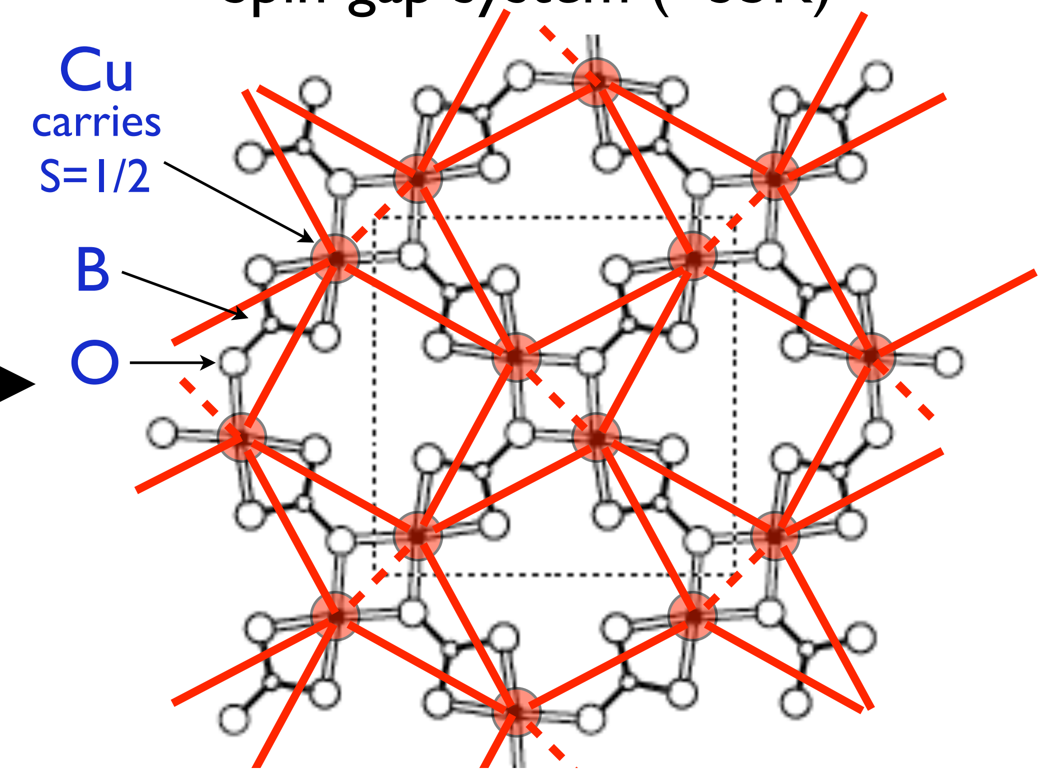
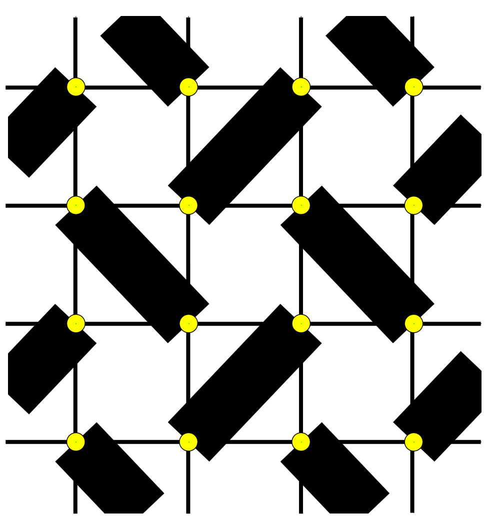
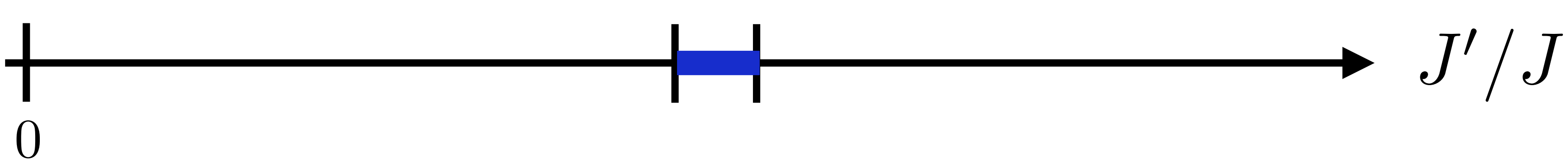


Kageyama et al. PRL **82** (1999)

Dimer phase





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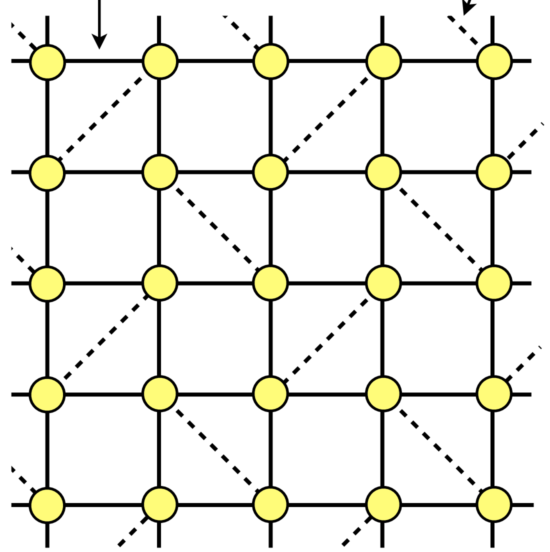

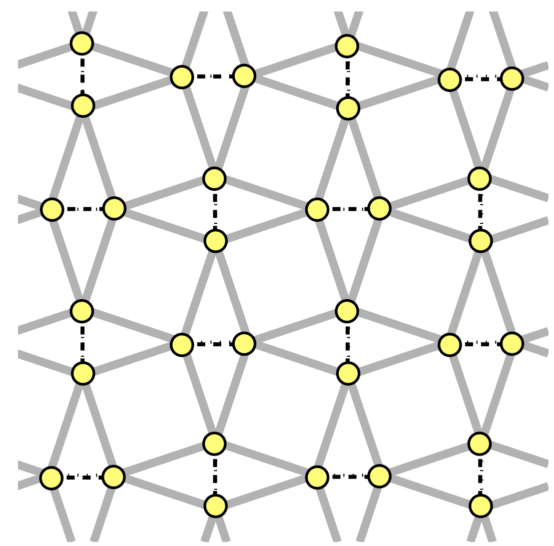

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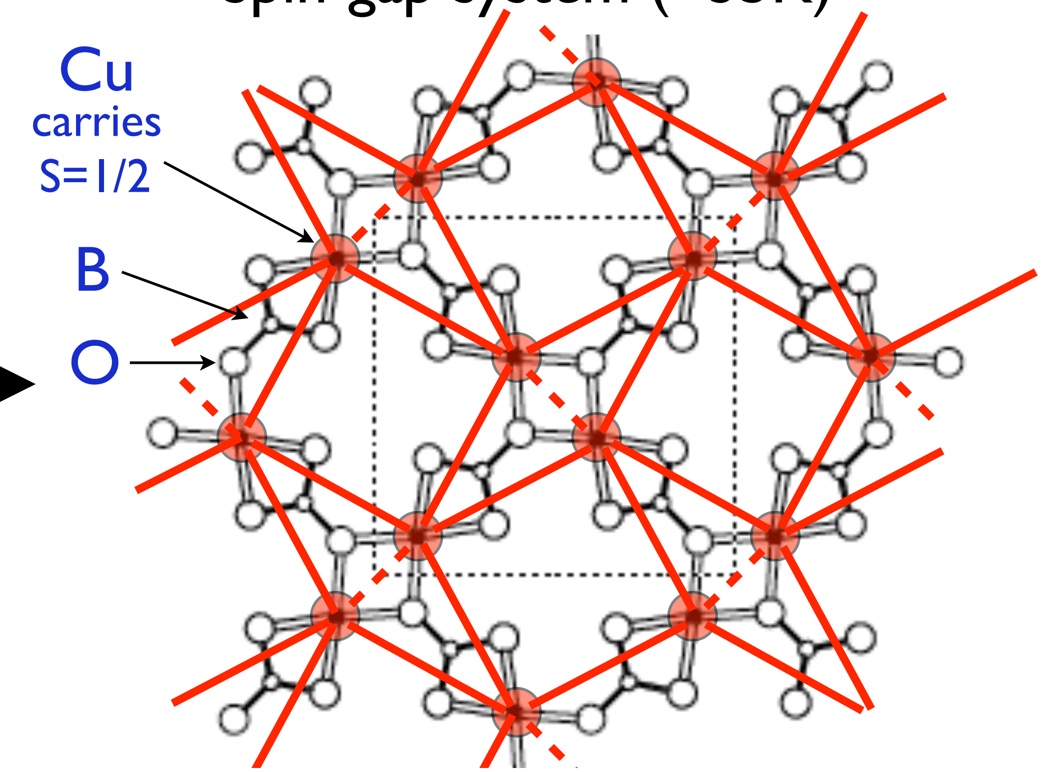

Kageyama et al. PRL **82** (1999)

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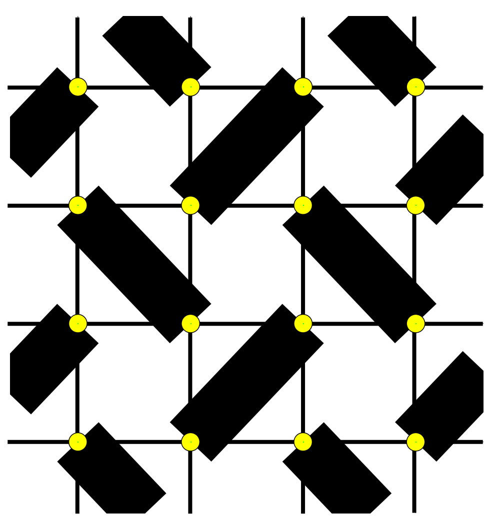
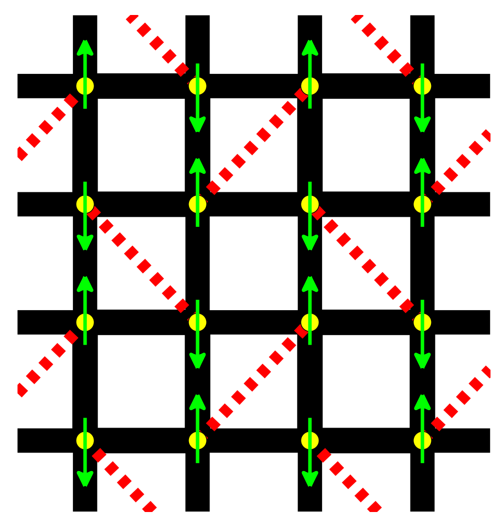
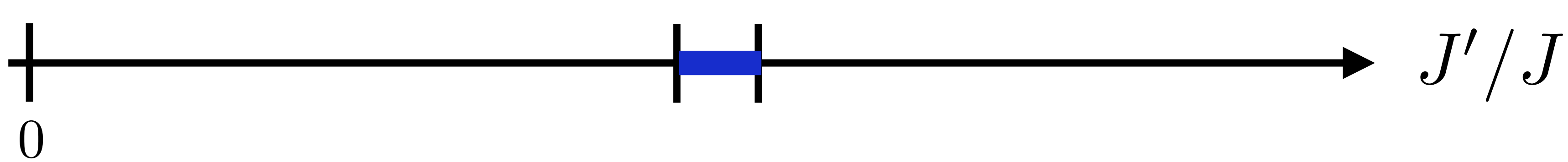


Néel phase





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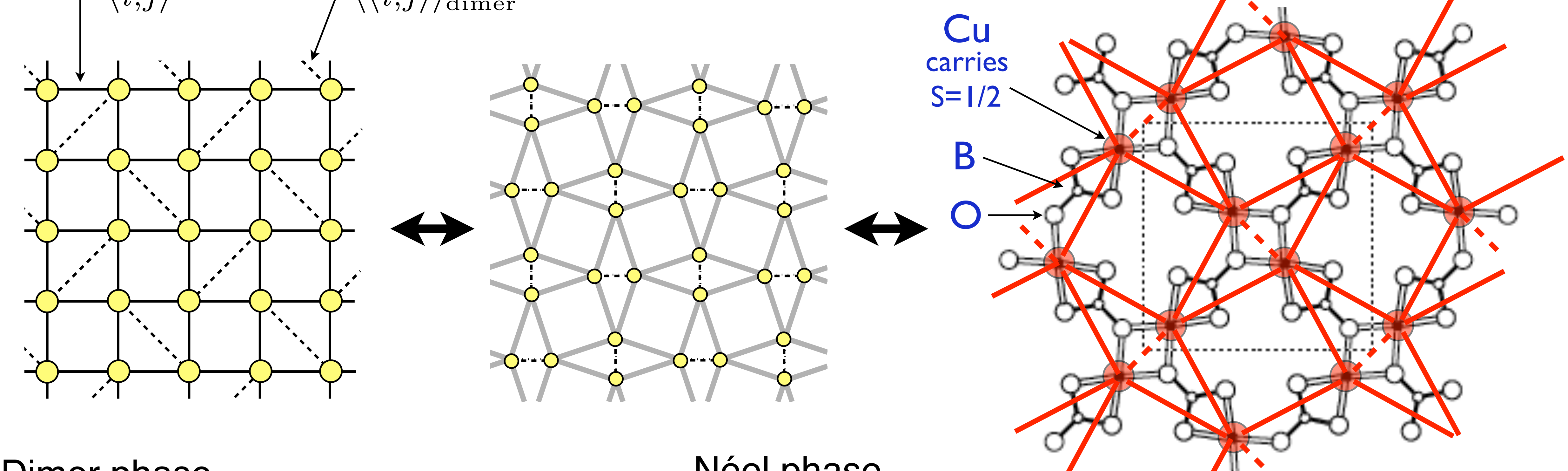

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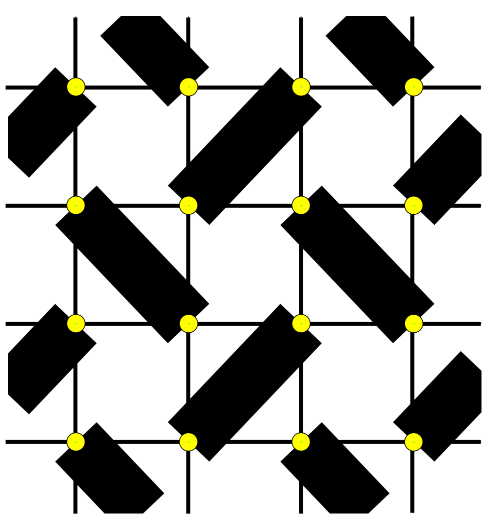
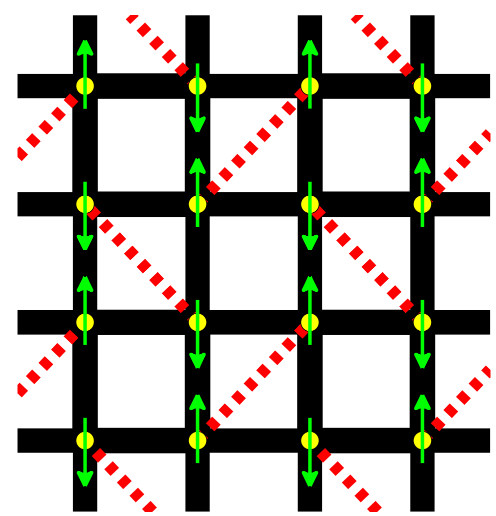
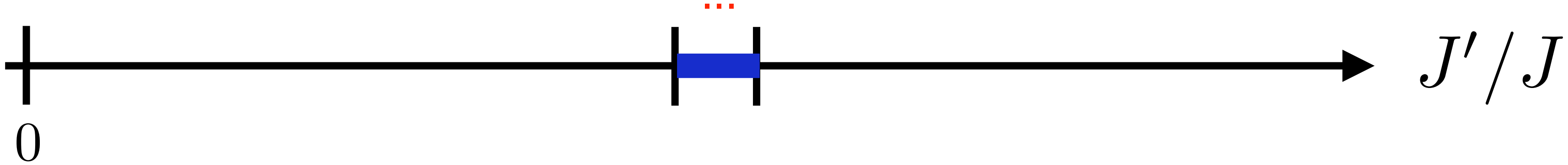


?

helical?
columnar-dimer?
plaquette?
spin-liquid?
...

Néel phase





The Shastry-Sutherland model

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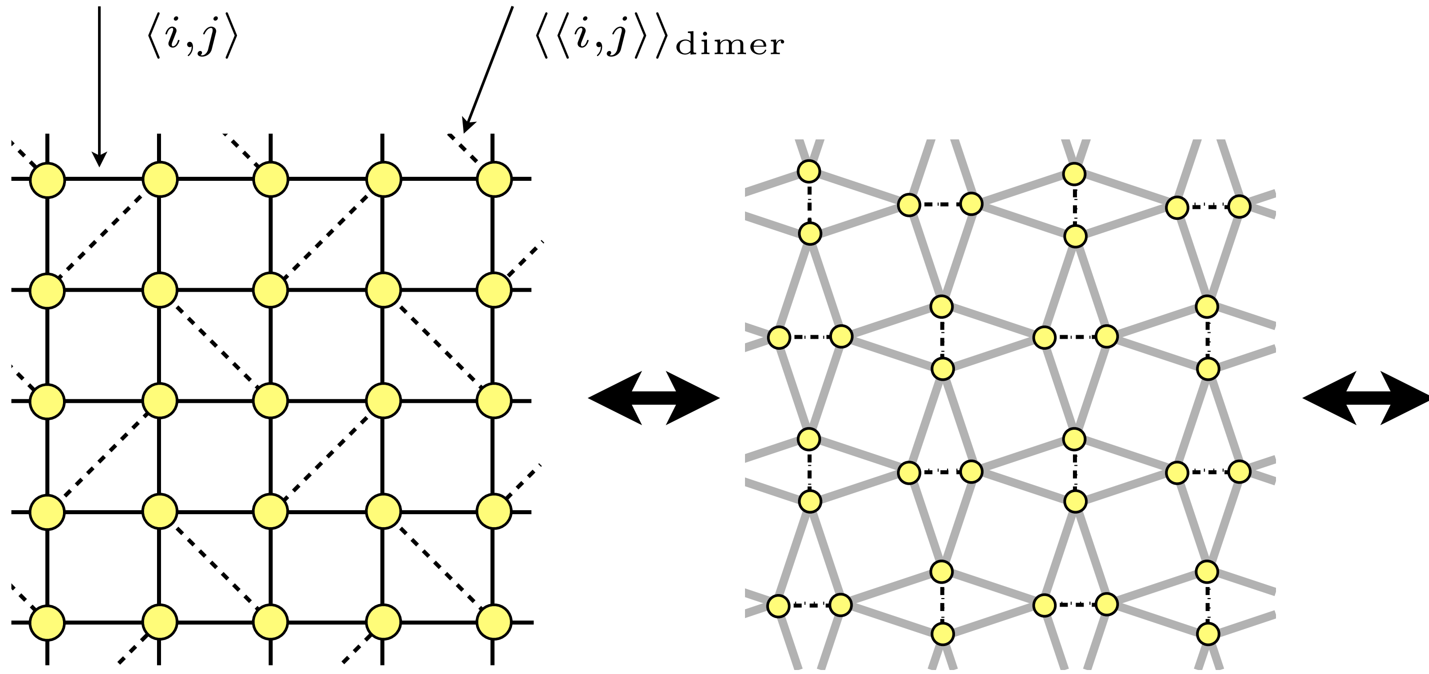
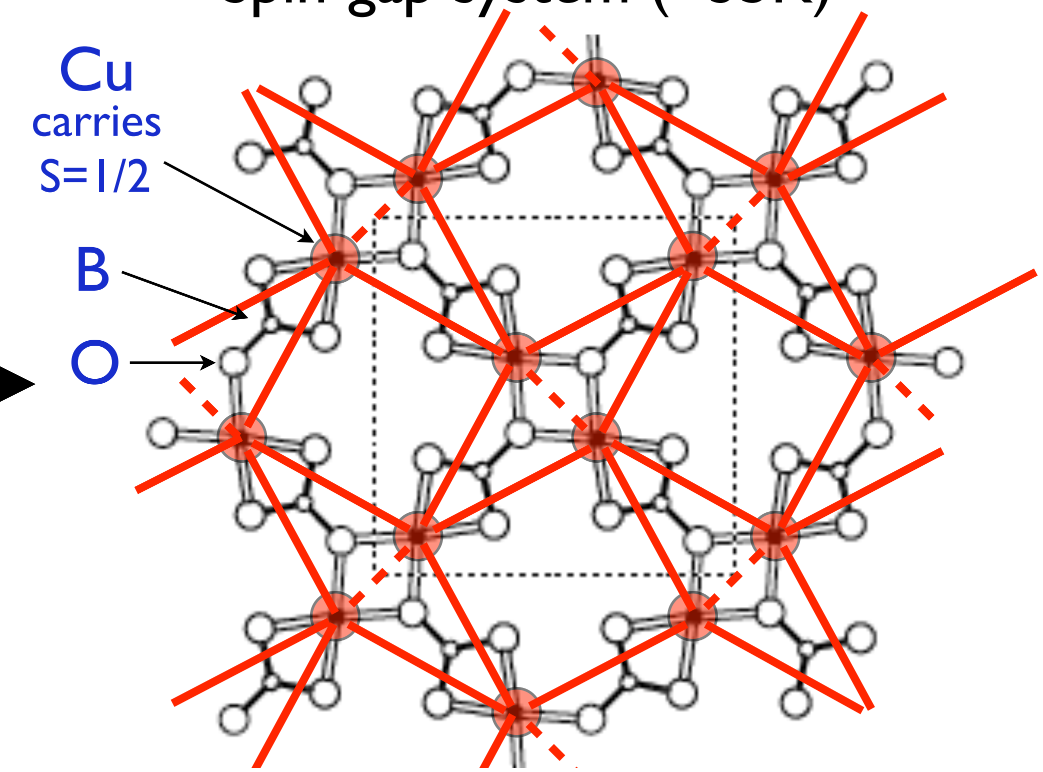
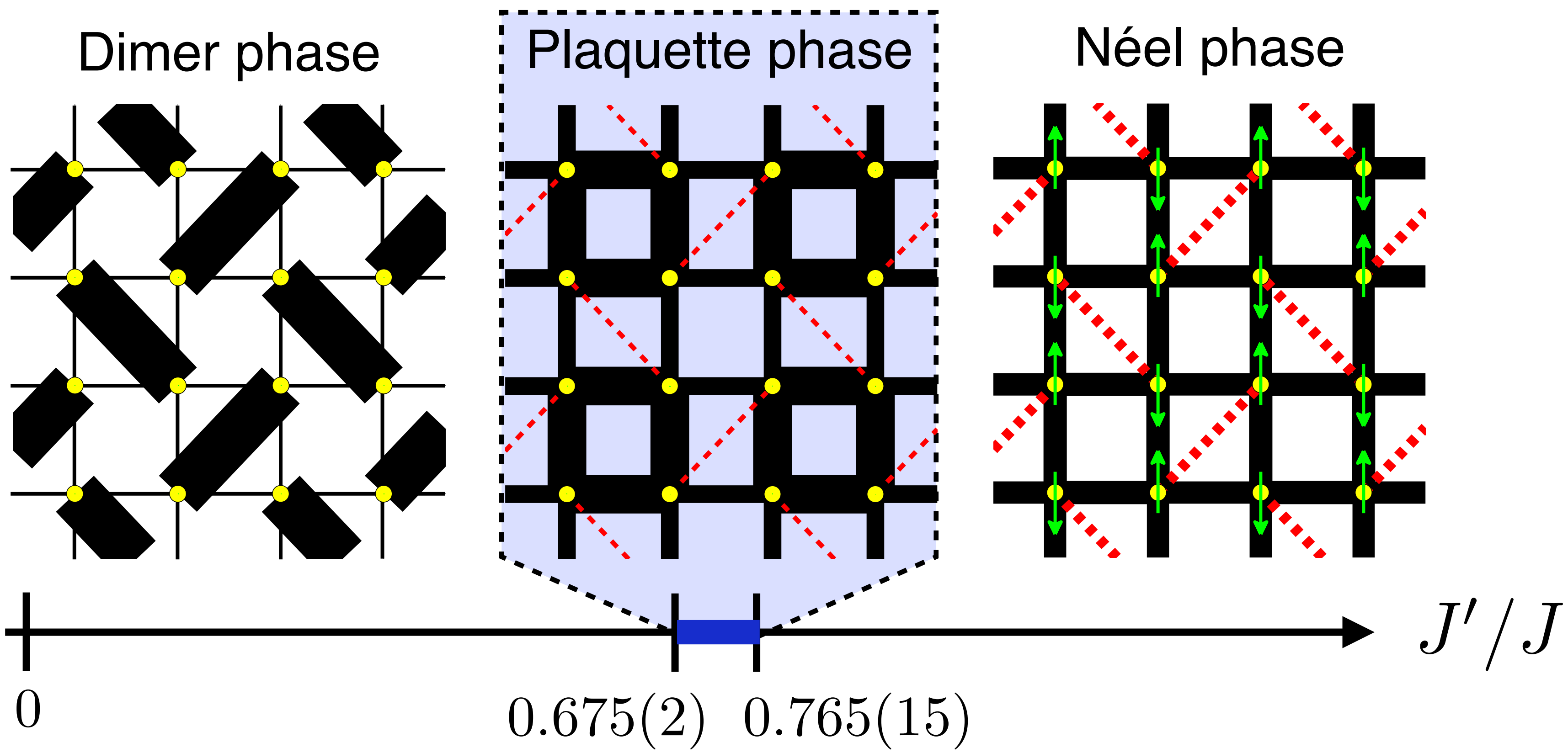


$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



Kageyama et al. PRL **82** (1999)



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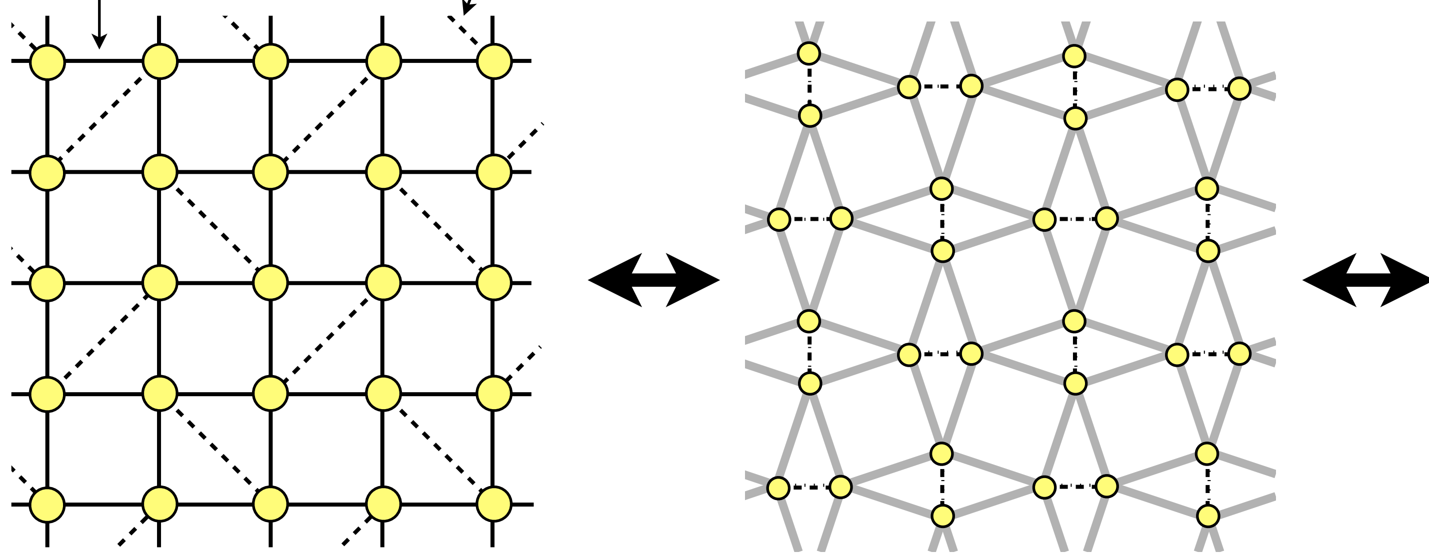

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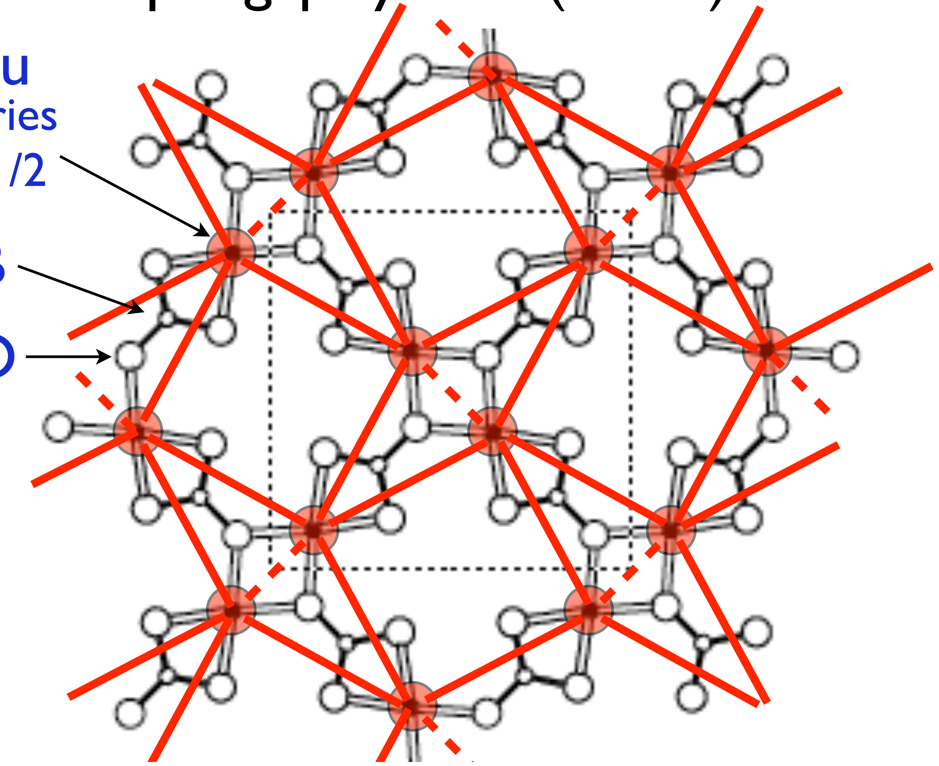

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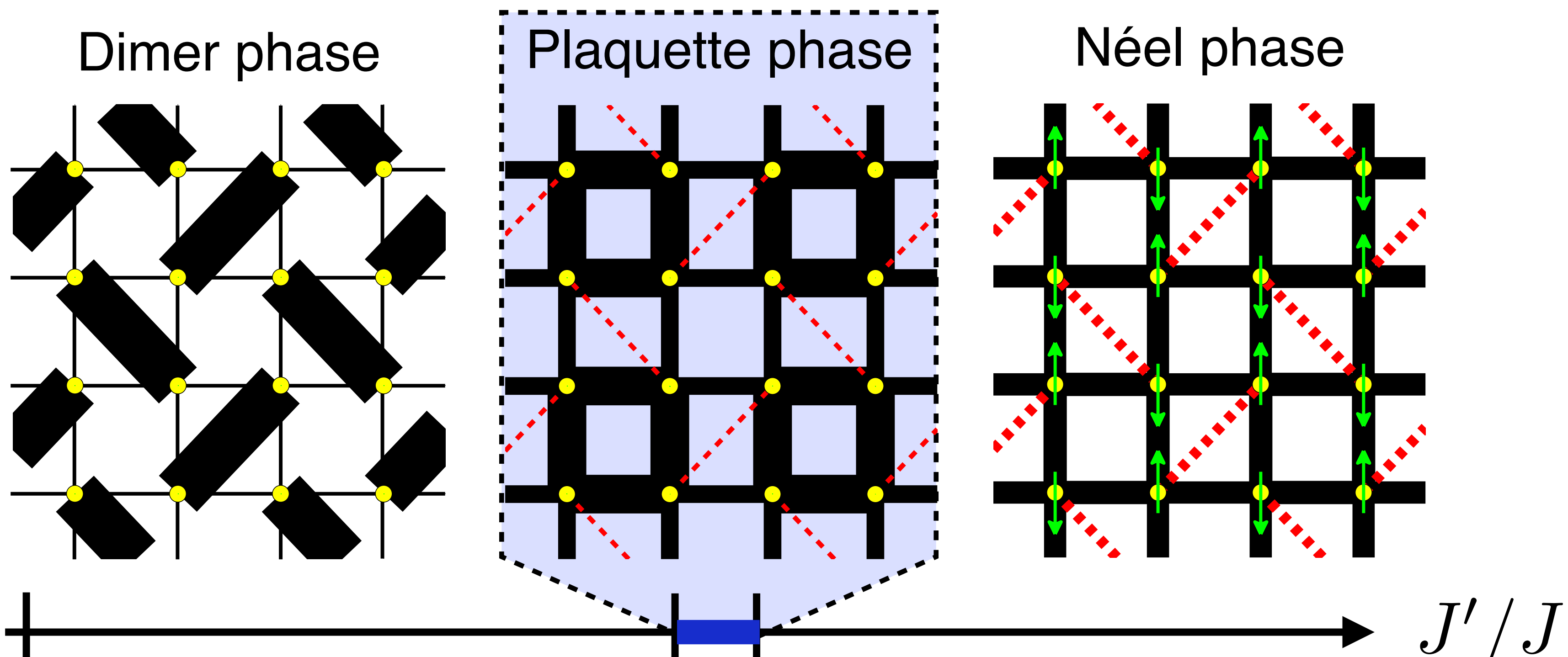

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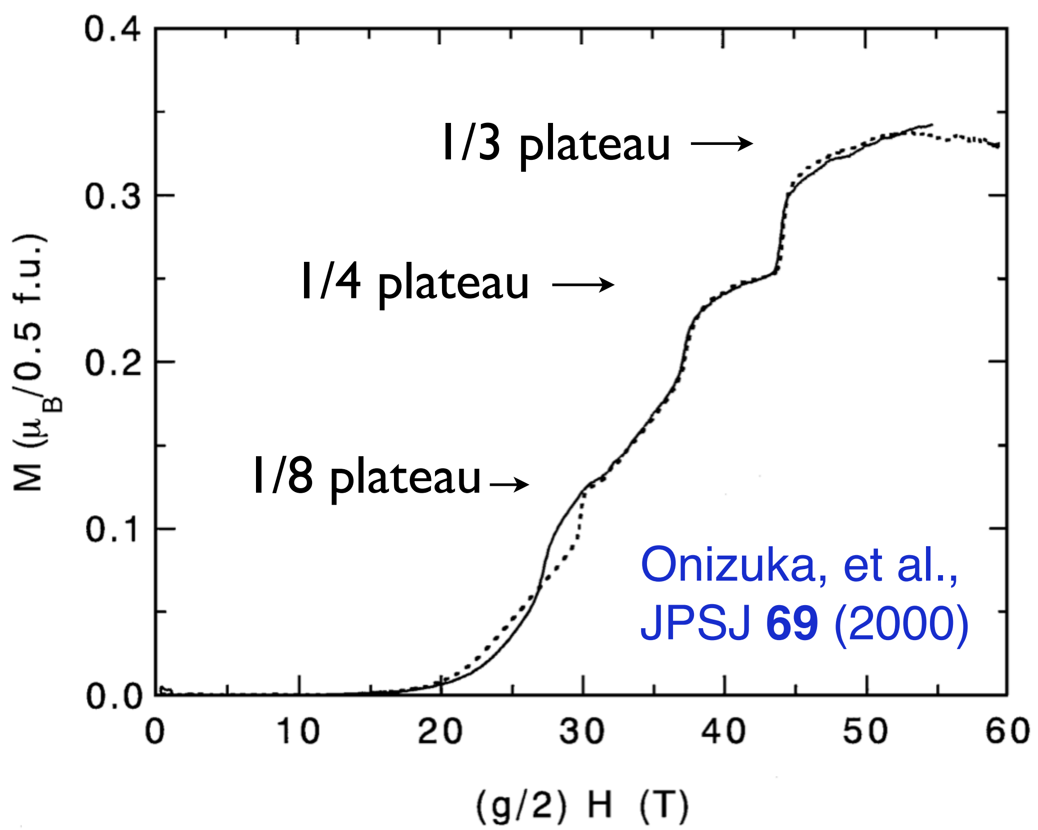
Magnetization plateaus

$SrCu_2(BO_3)_2$ in a magnetic field exhibits several magnetization plateaus



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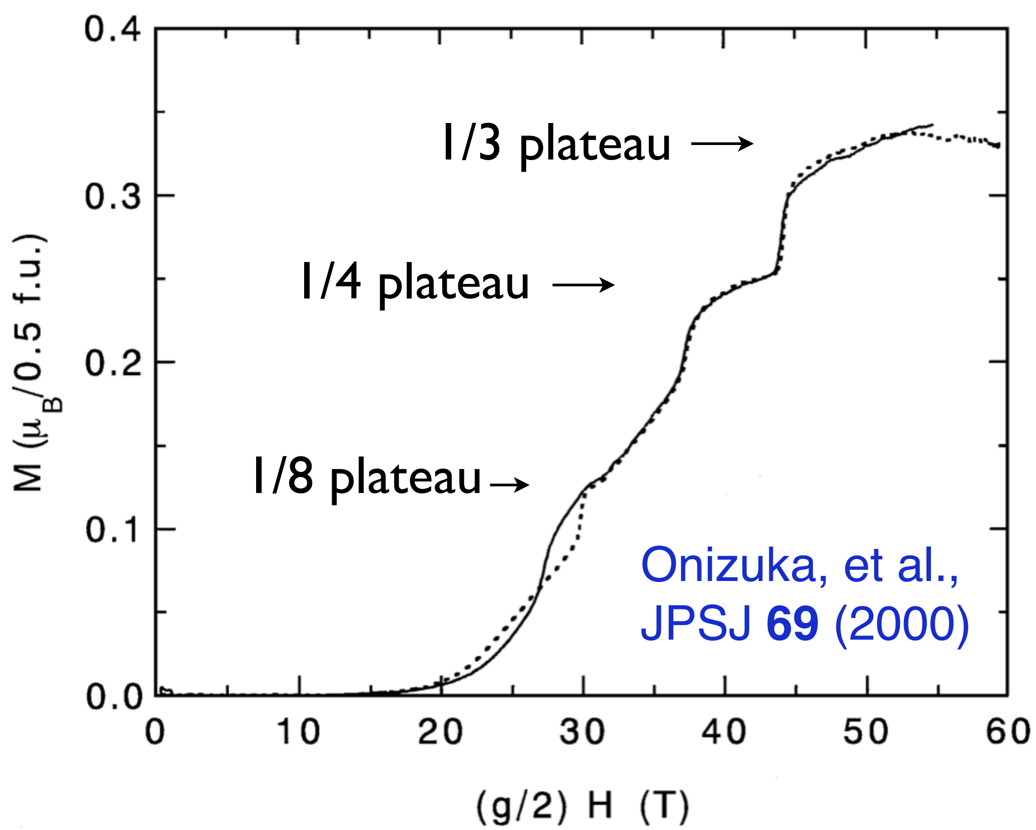

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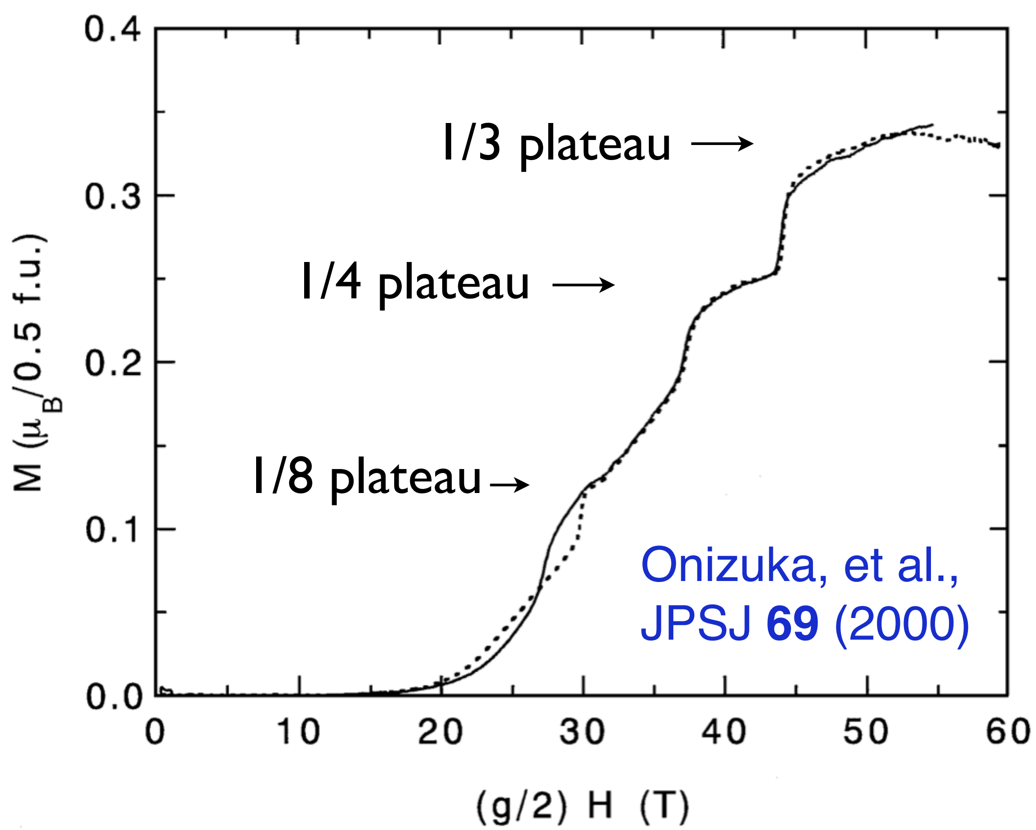

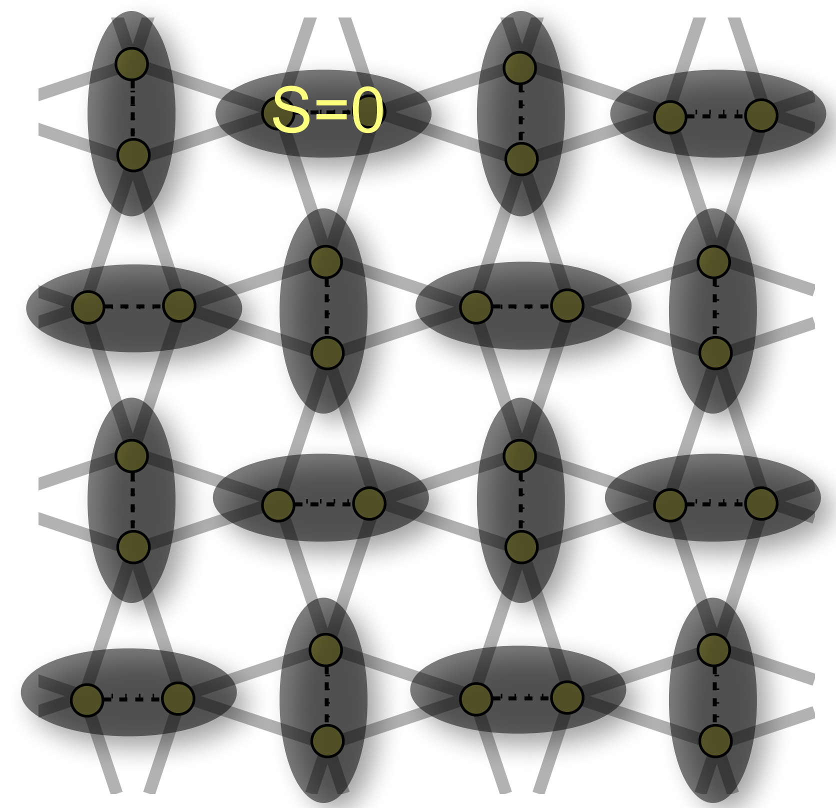

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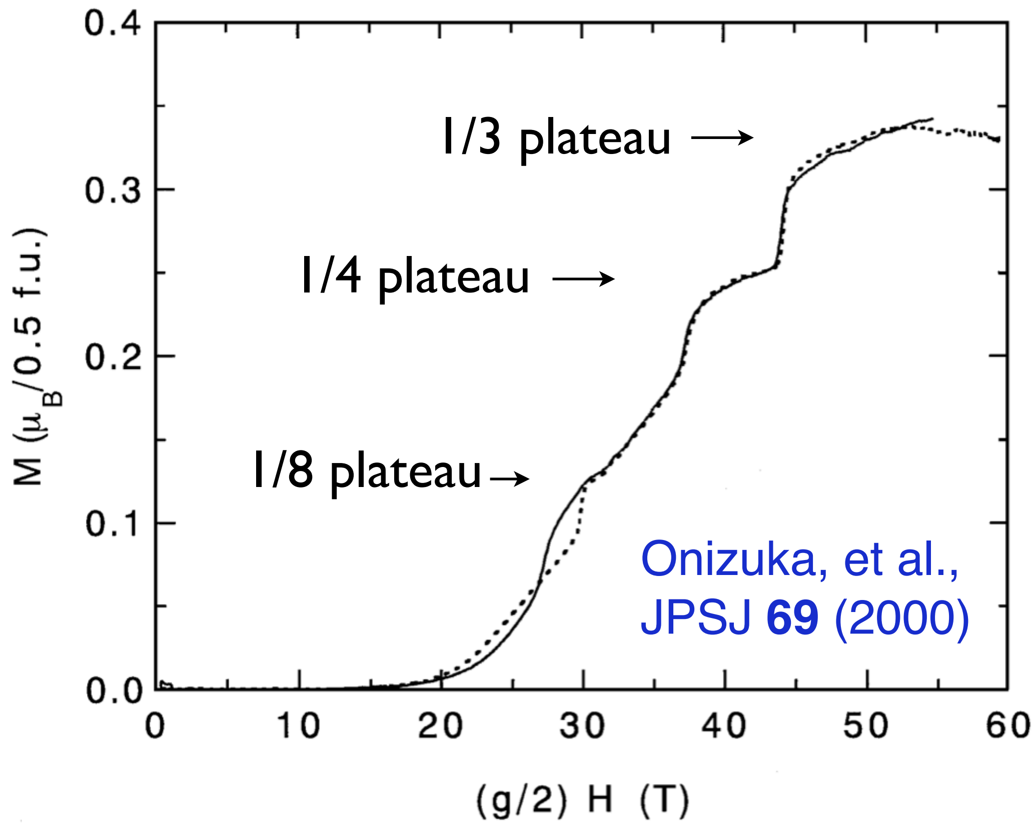

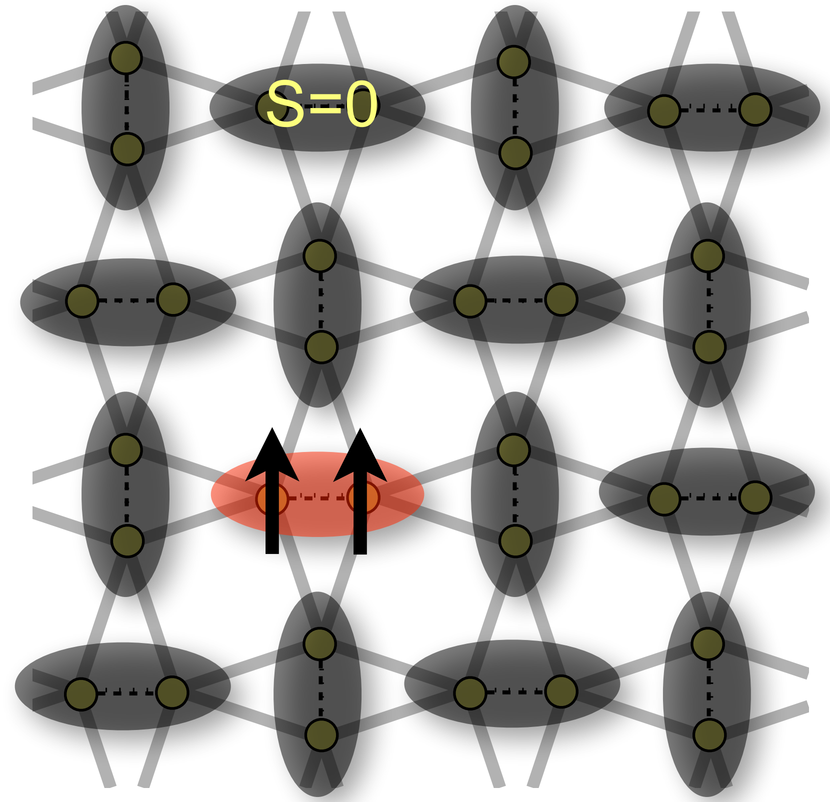

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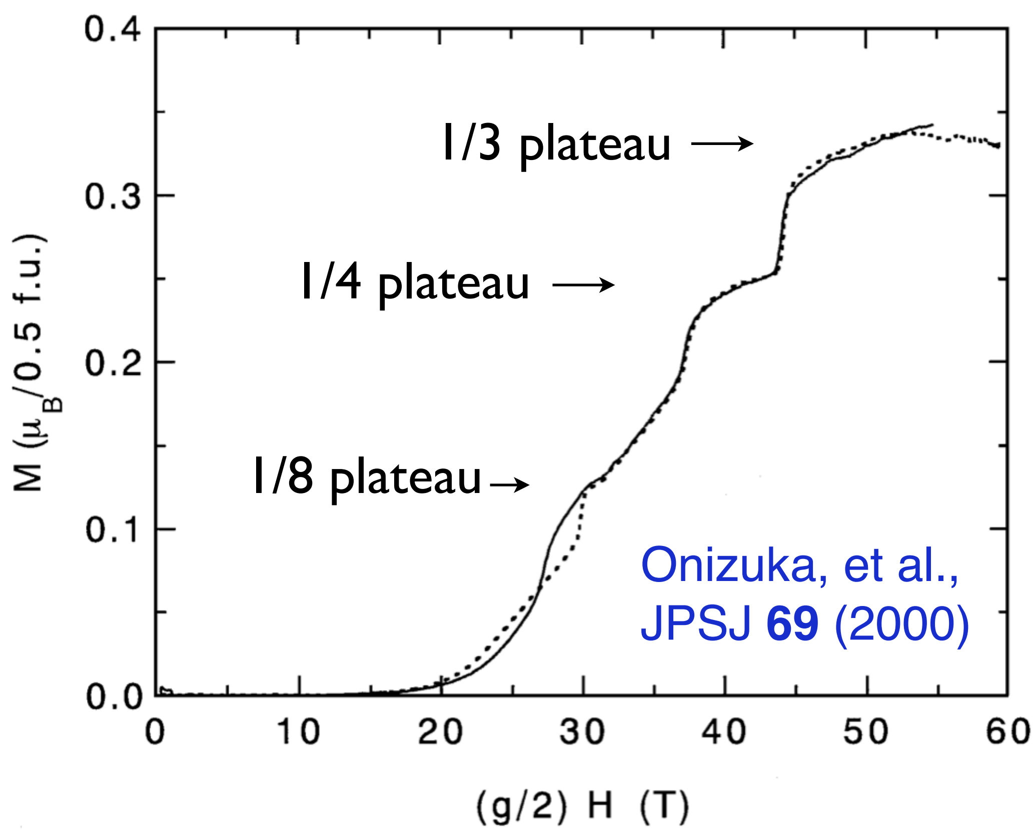

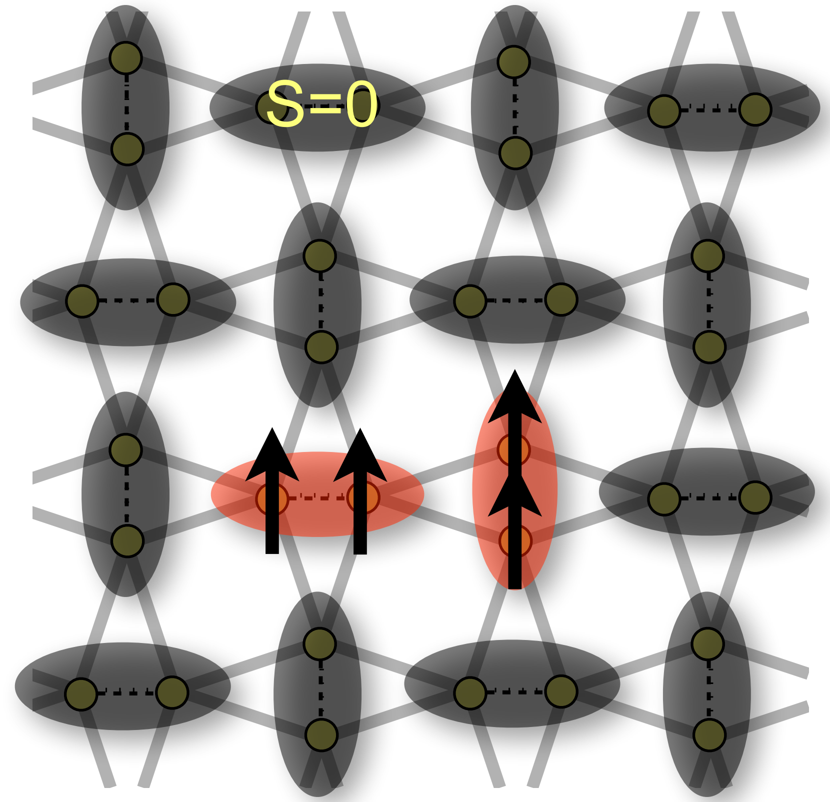

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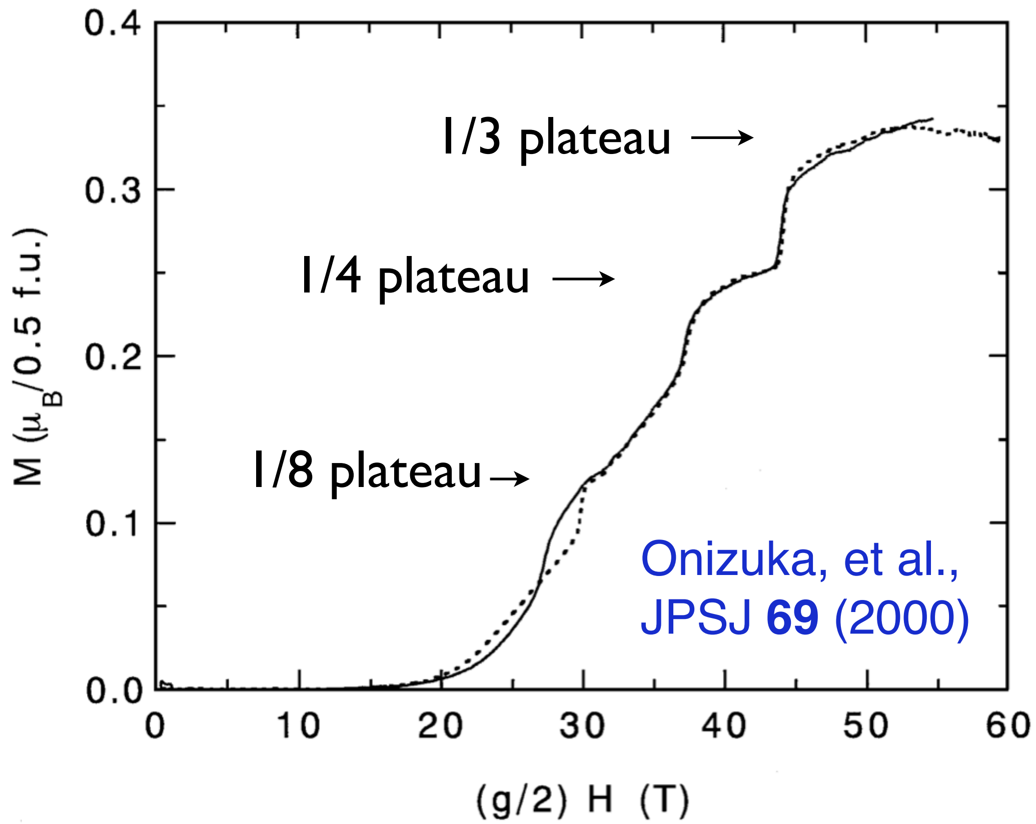

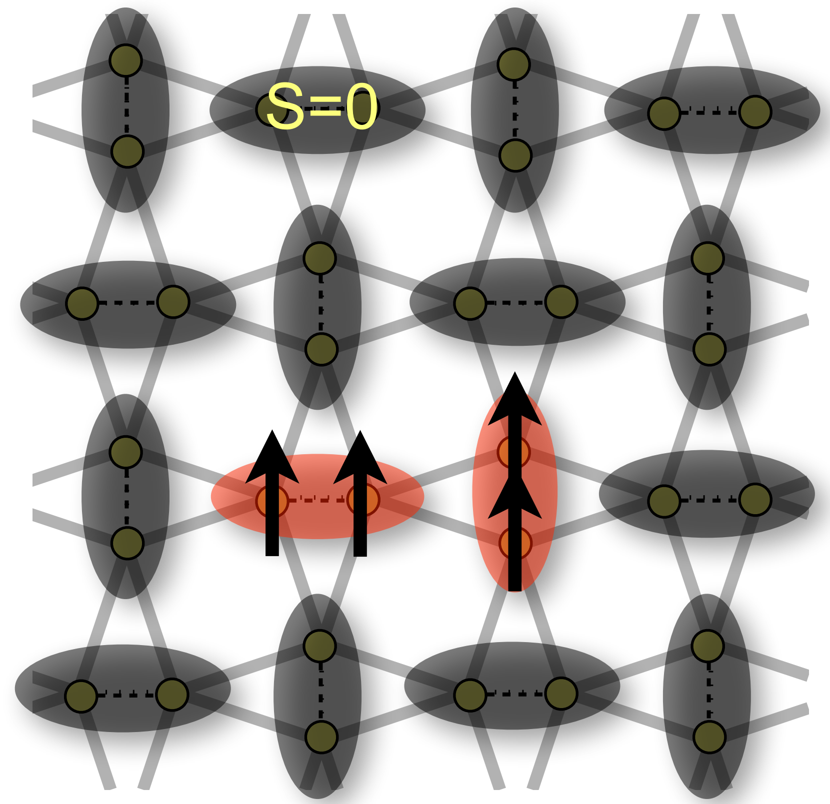

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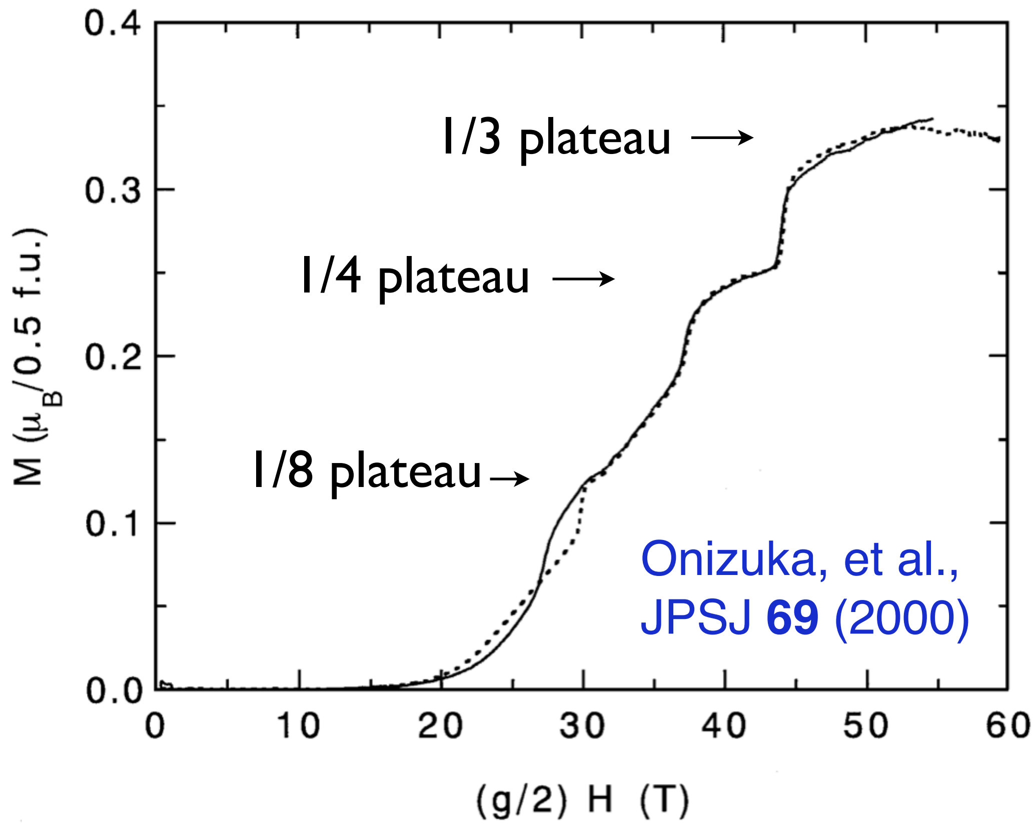

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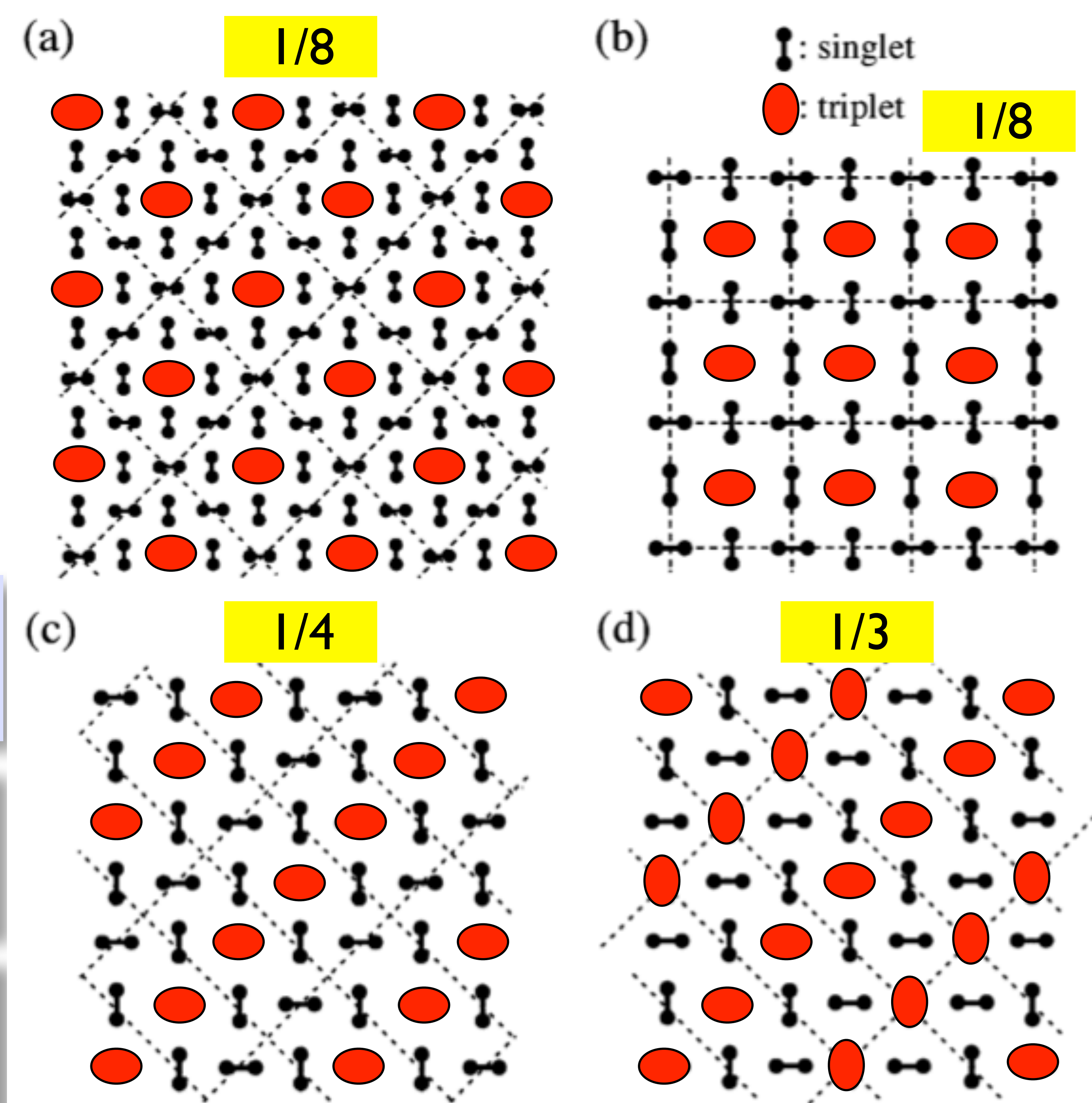

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★ Ideal problem for iPEPS: simulating large unit cell embedded in infinite system and compare variational energies of the proposed crystals

BUT!

SURPRISE!

iPEPS simulations of the SSM in a magnetic field

PC, F. Mila, PRL **112** (2014)

- The assumption that plateaus correspond to crystals of triplets is wrong!

(for the plateaus below 1/4)

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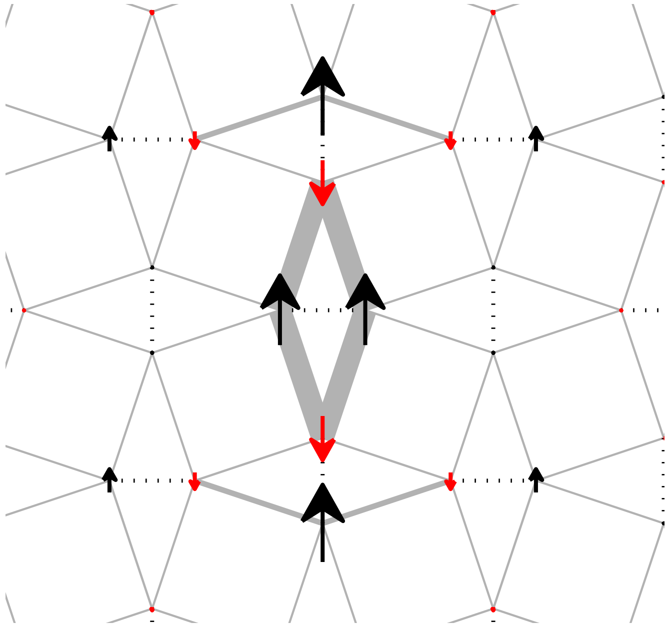

spin structure of 1
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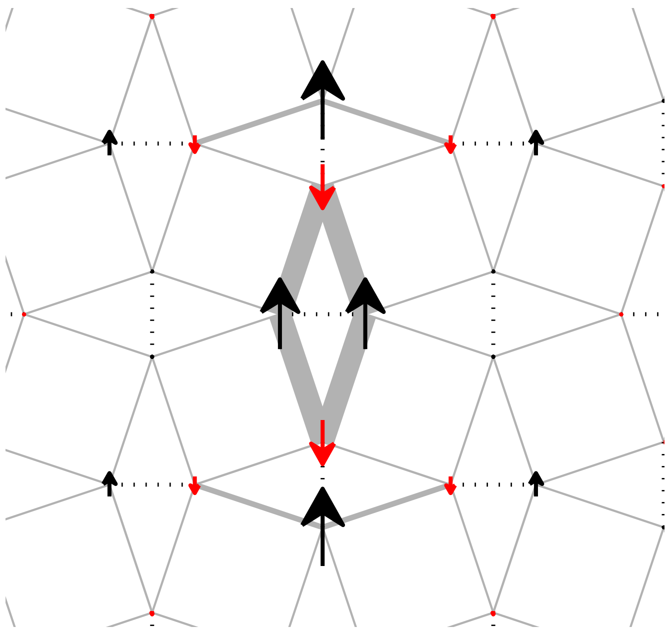

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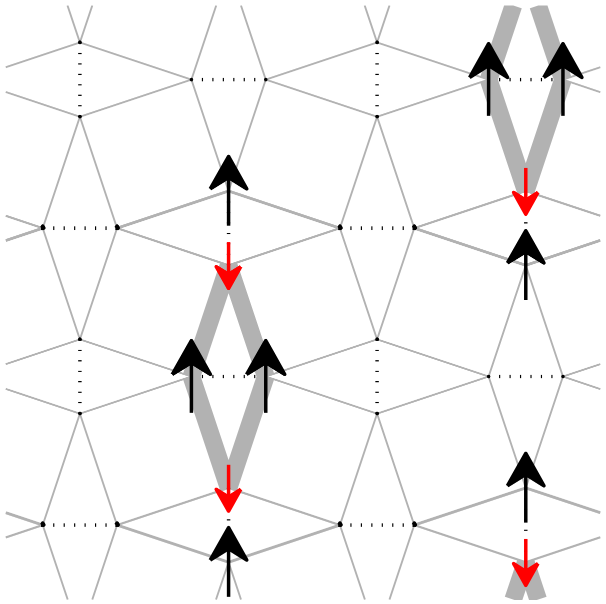

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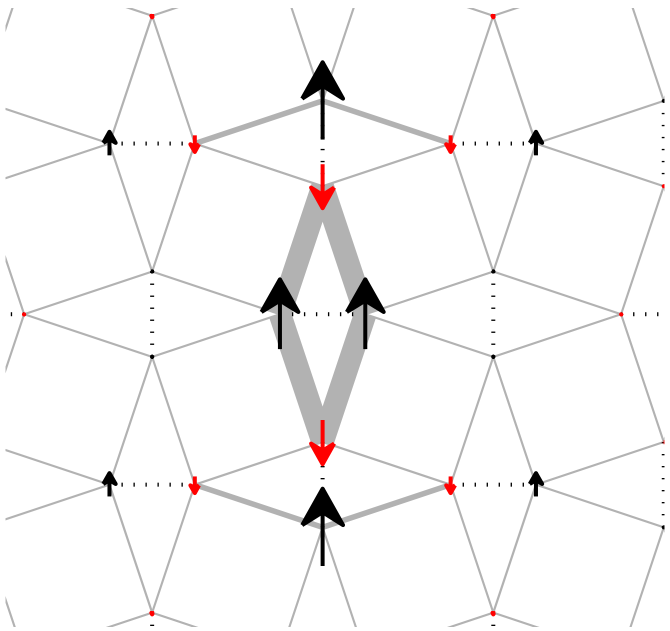

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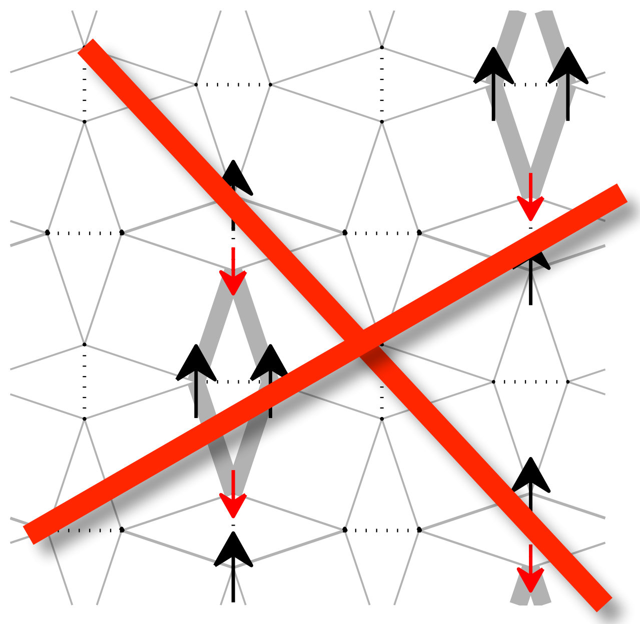

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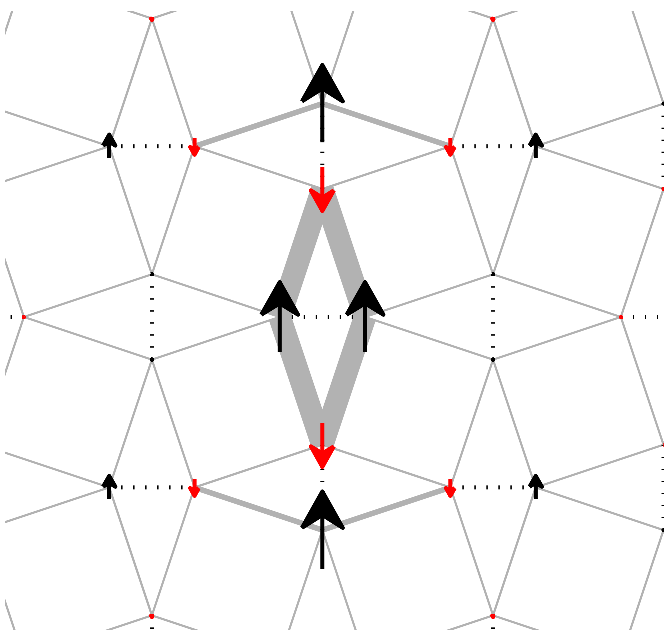

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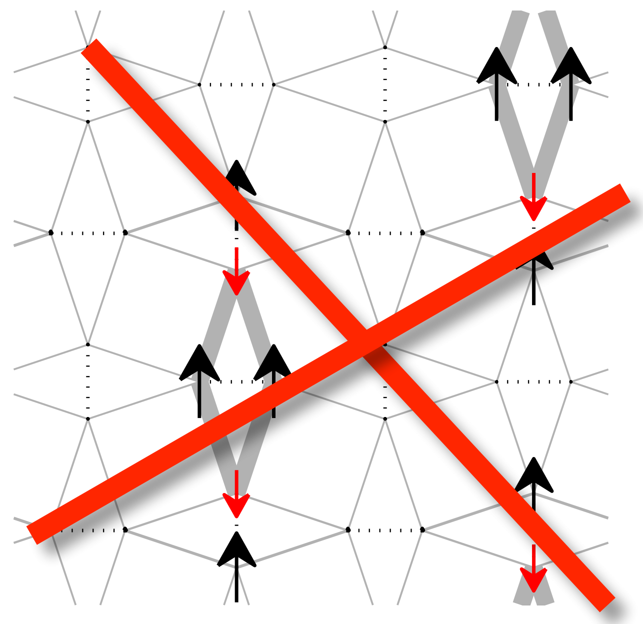

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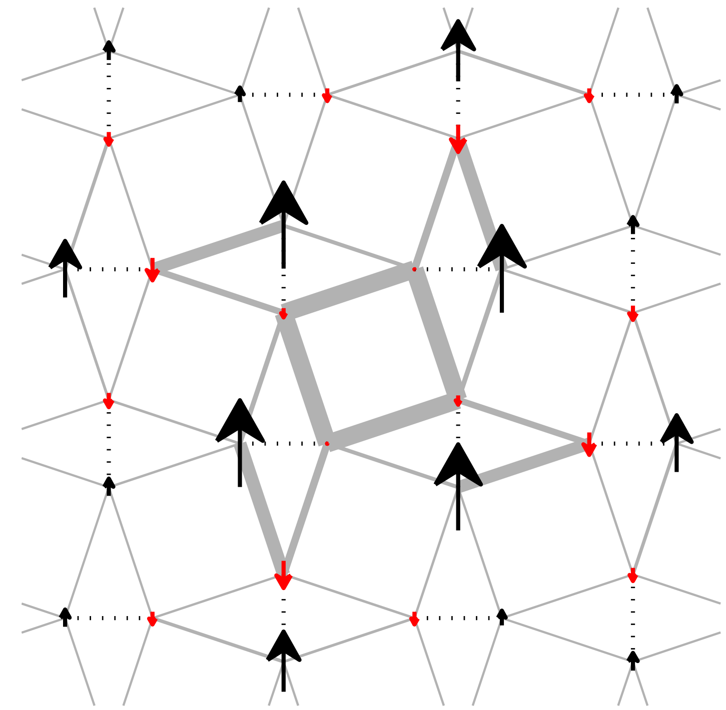

spin structure of a Sz=2 excitation in a 4x4 cell

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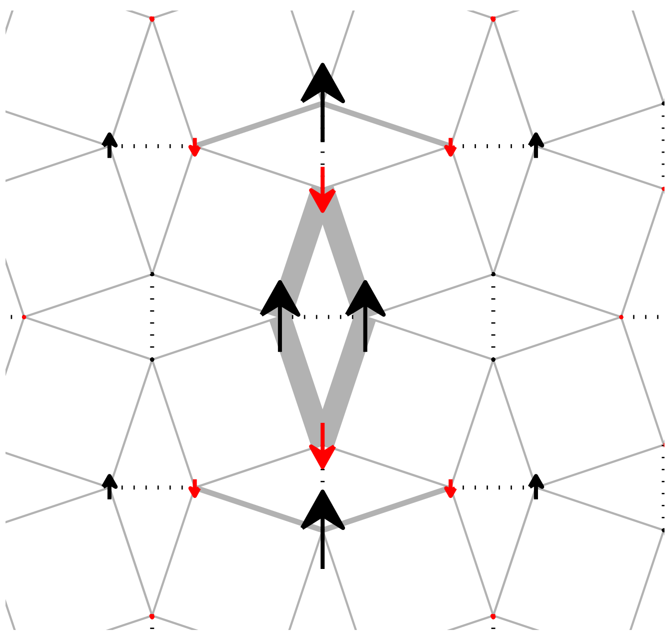

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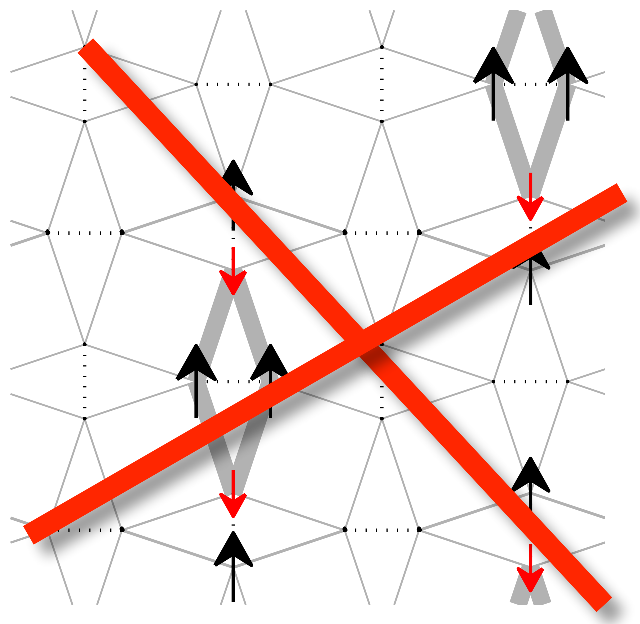

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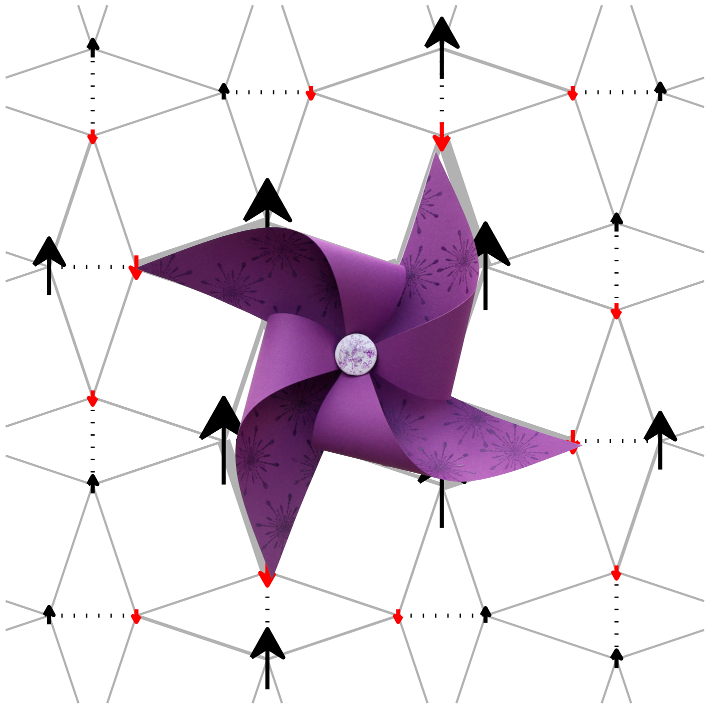

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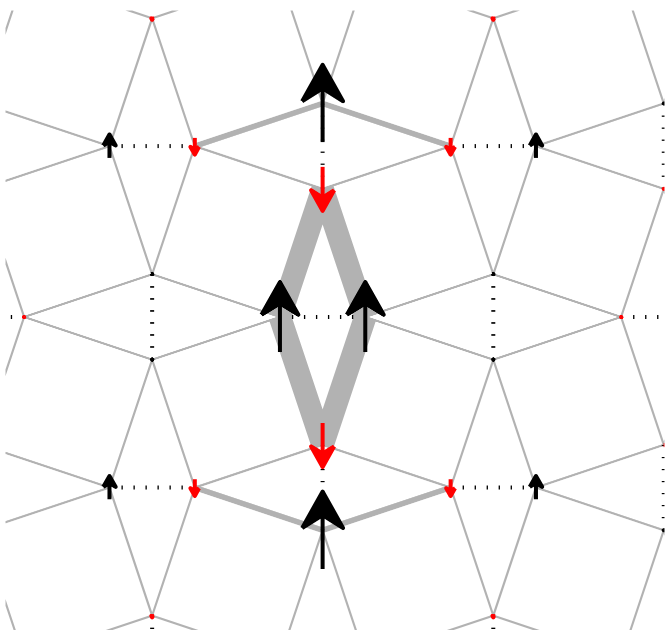

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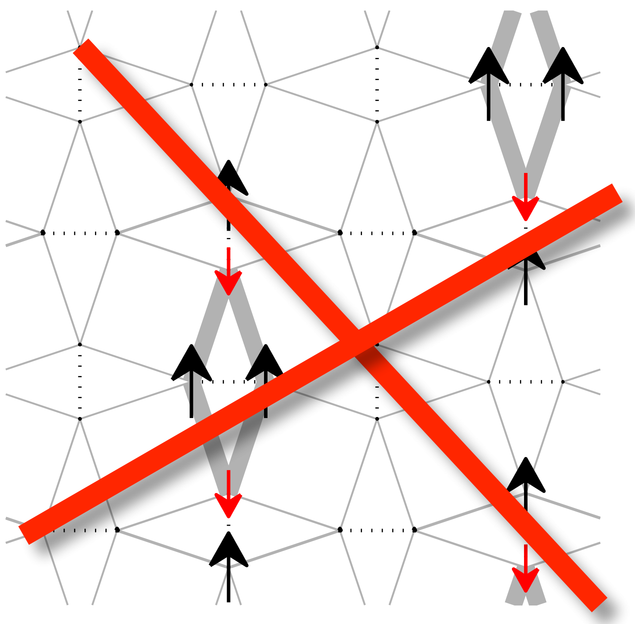

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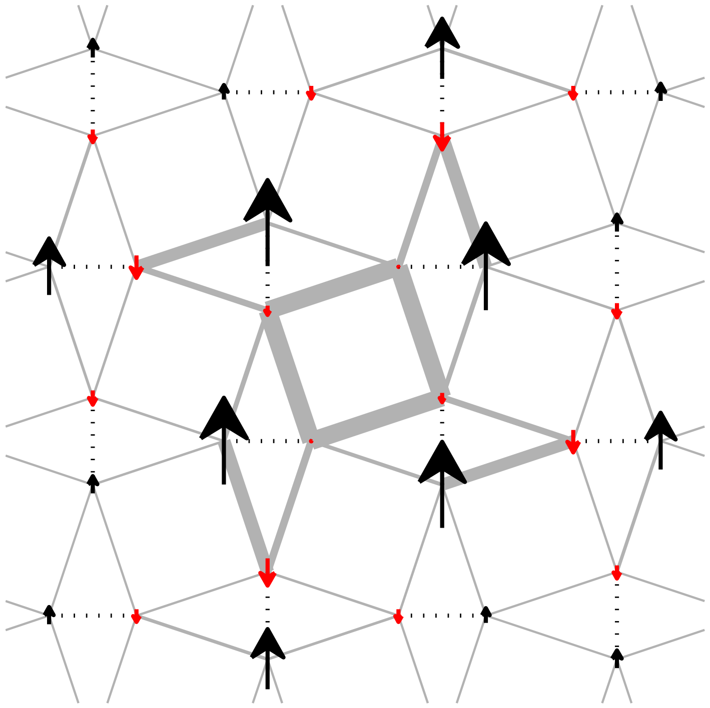

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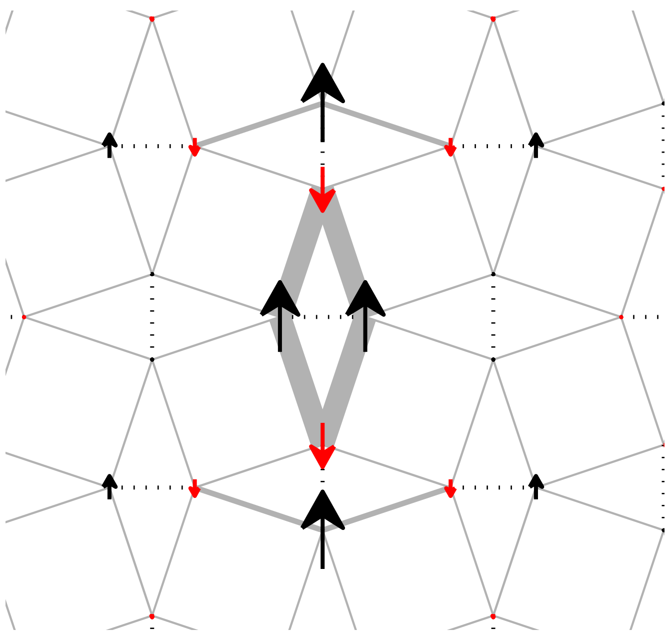
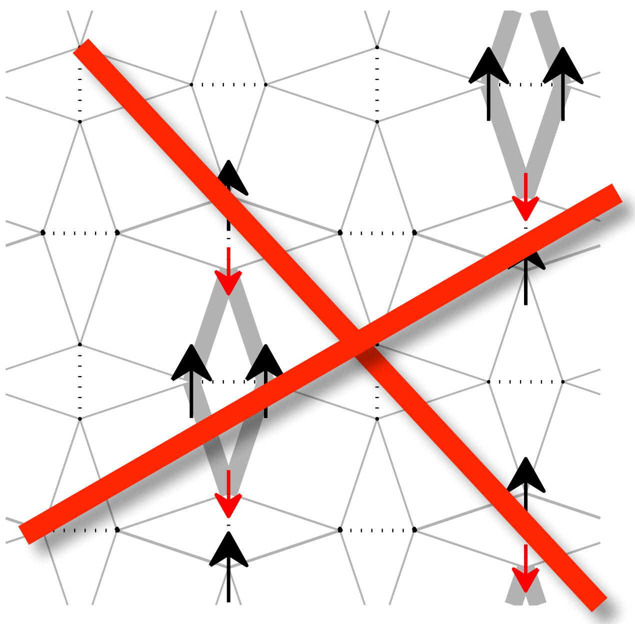
PC, F. Mila, PRL **112** (2014)

- The assumption that plateaus correspond to crystals of triplets is wrong!

(for the plateaus below 1/4)

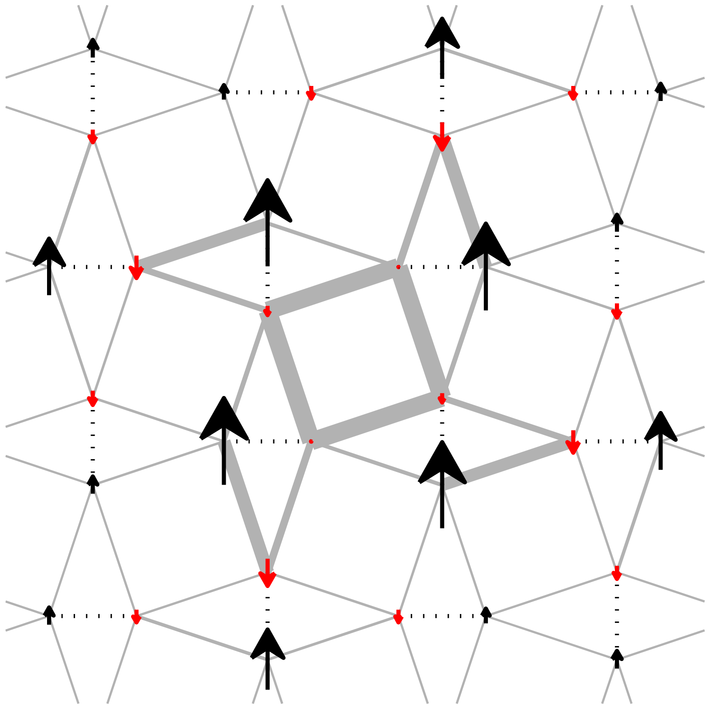


spin structure of 1 localized triplet in a 4x4 cell



expected spin structure of 2 localized triplets in a 4x4 cell

small D (mean-field result)



spin structure of a Sz=2 excitation in a 4x4 cell

obtained with iPEPS for D>4

Bound state of two triplets!

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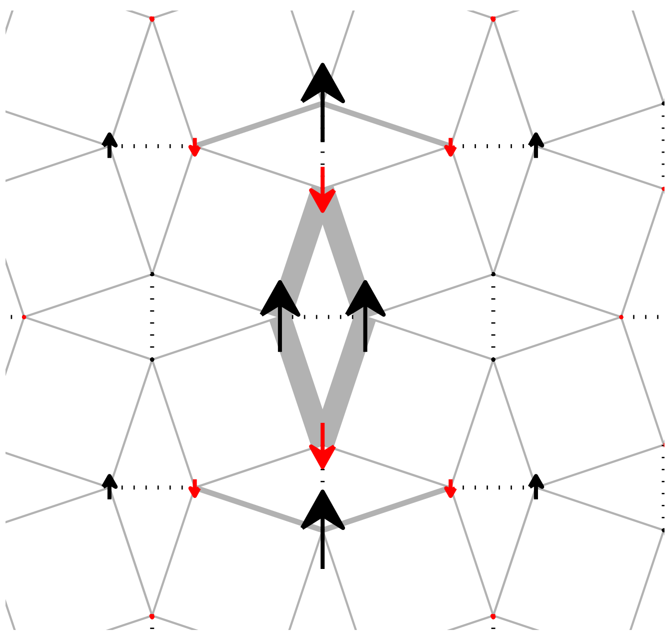
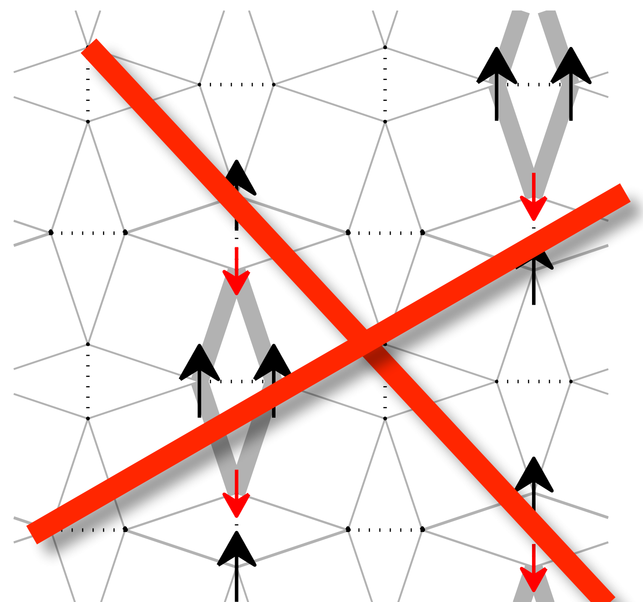


spin structure of 1 localized triplet in a 4x4 cell



expected spin structure of 2 localized triplets in a 4x4 cell

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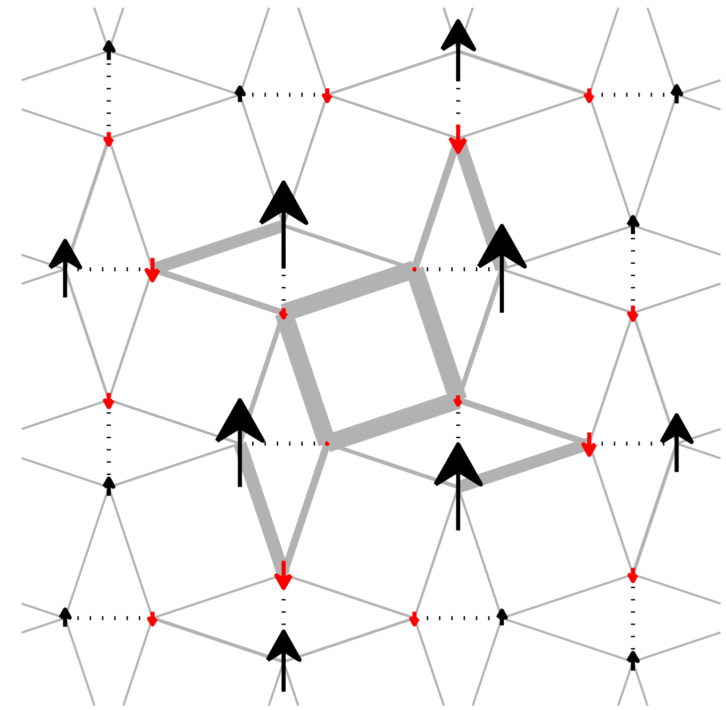


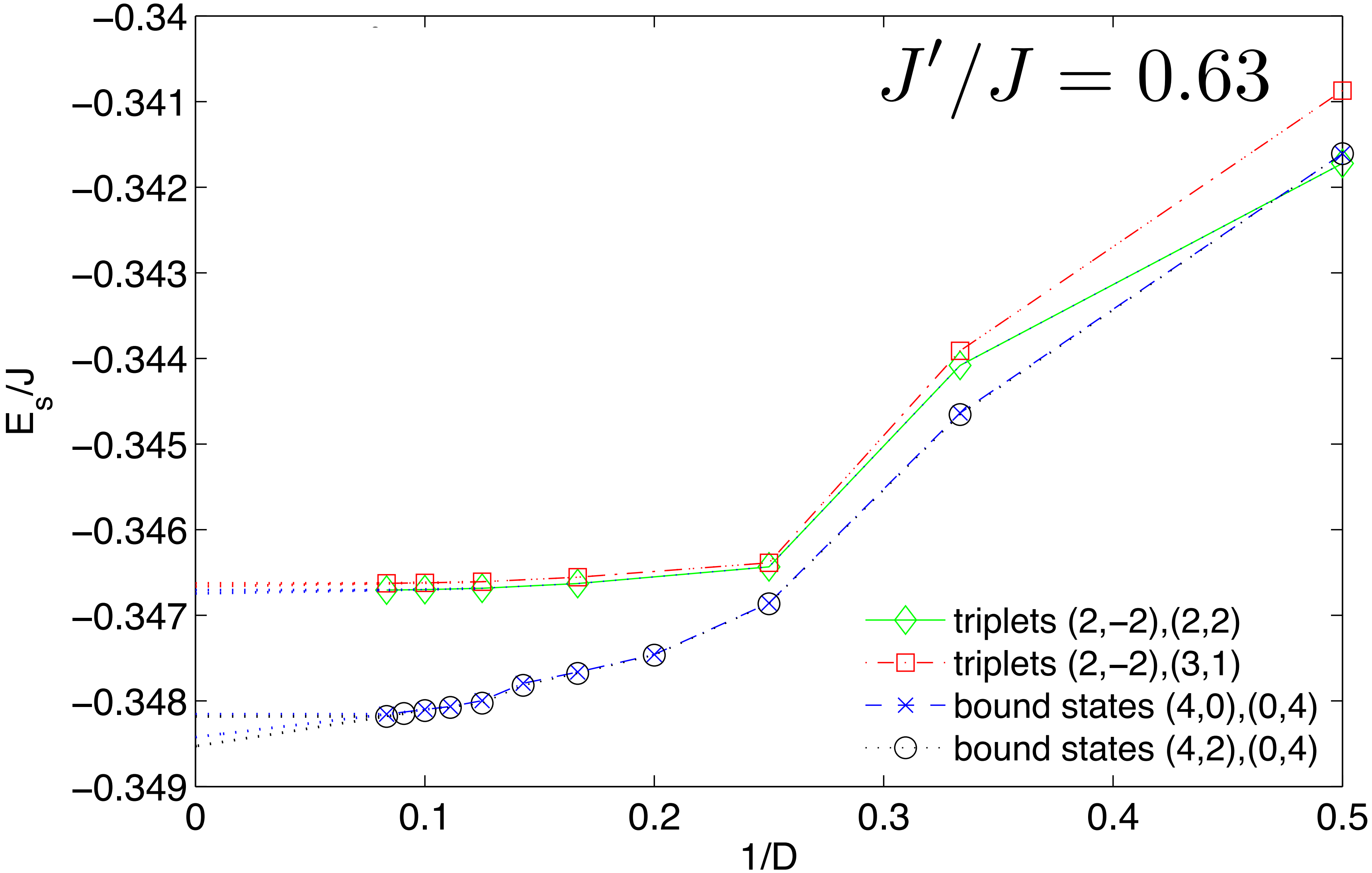
spin structure of a Sz=2 excitation in a 4x4 cell

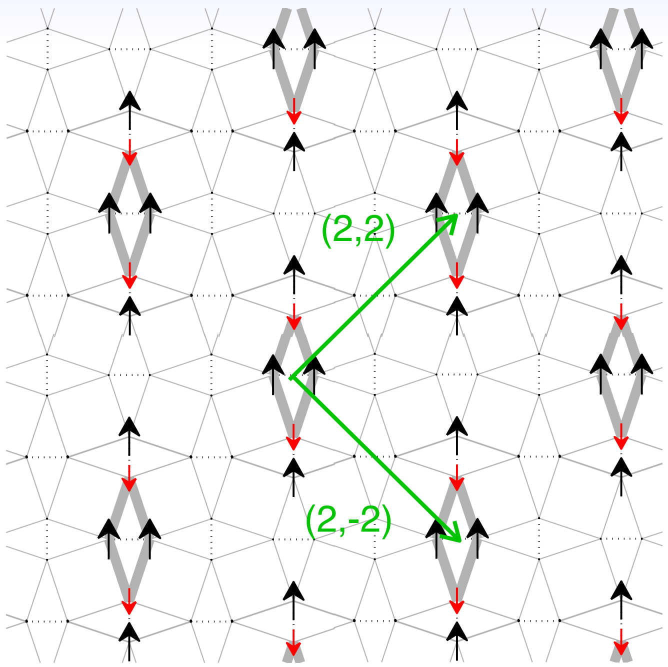
obtained with iPEPS for D>4

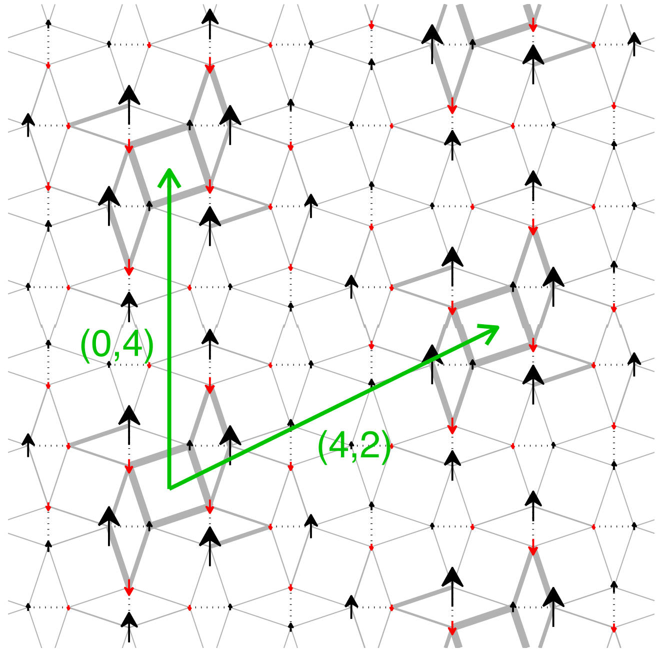
Bound state of two triplets!

- Crystals of bound states instead of crystals of triplets!!

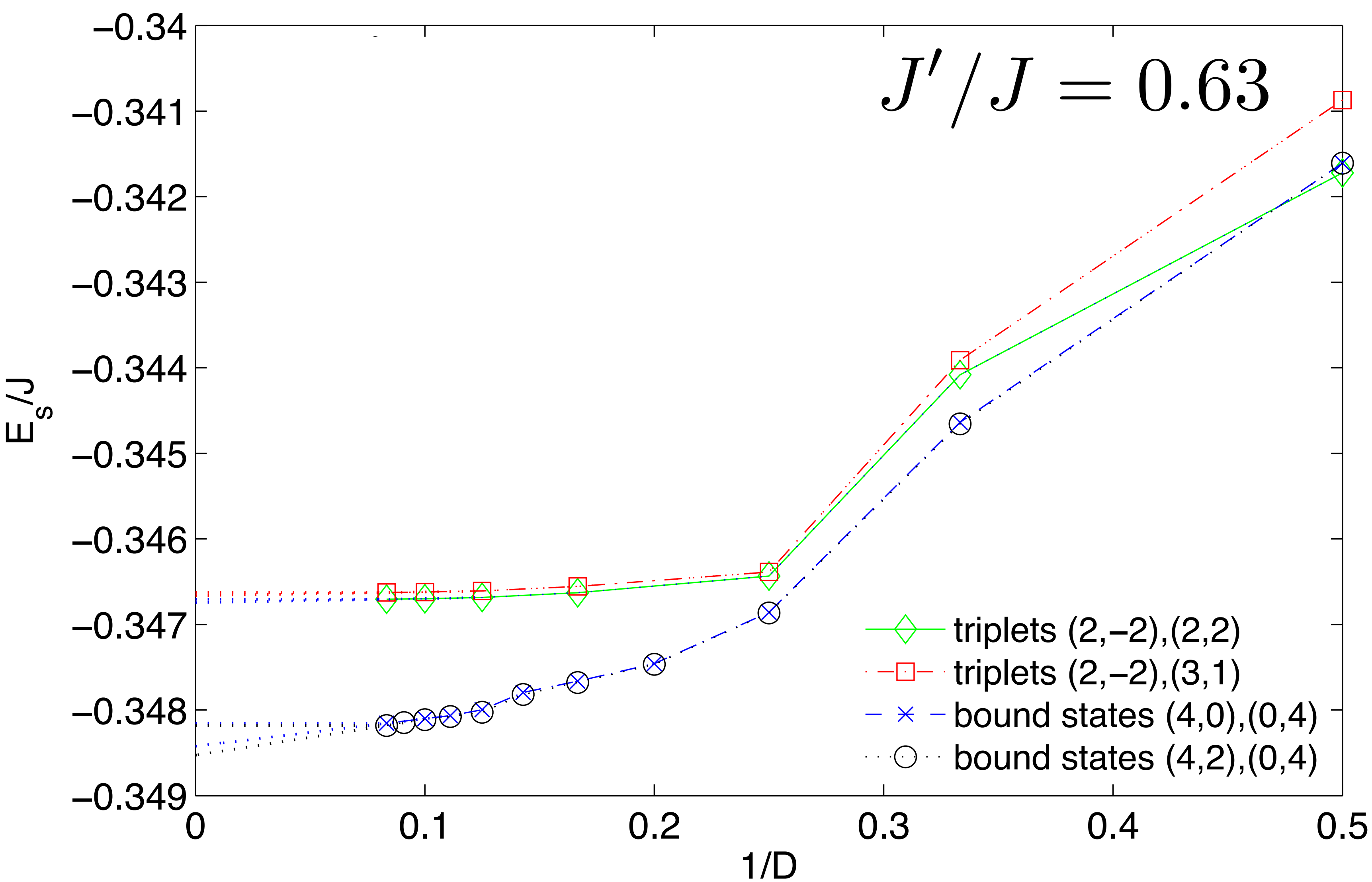
Example: 1/8 plateau

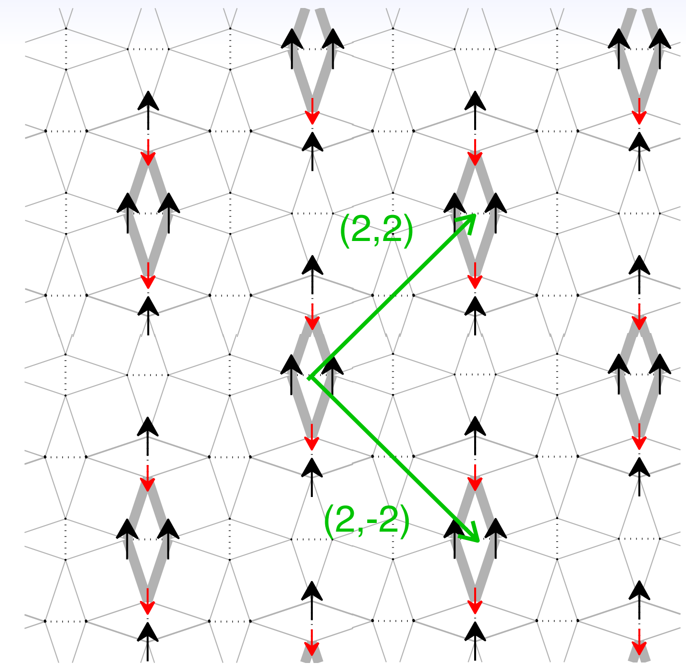


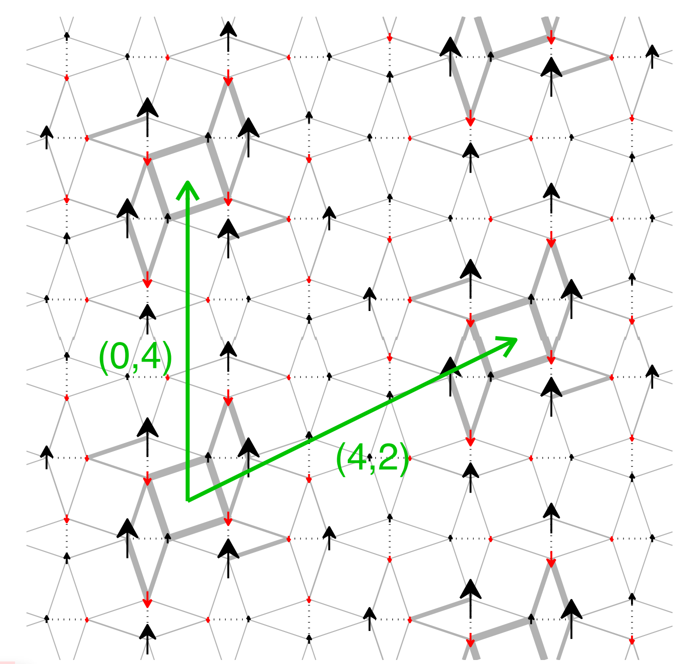




Example: 1/8 plateau

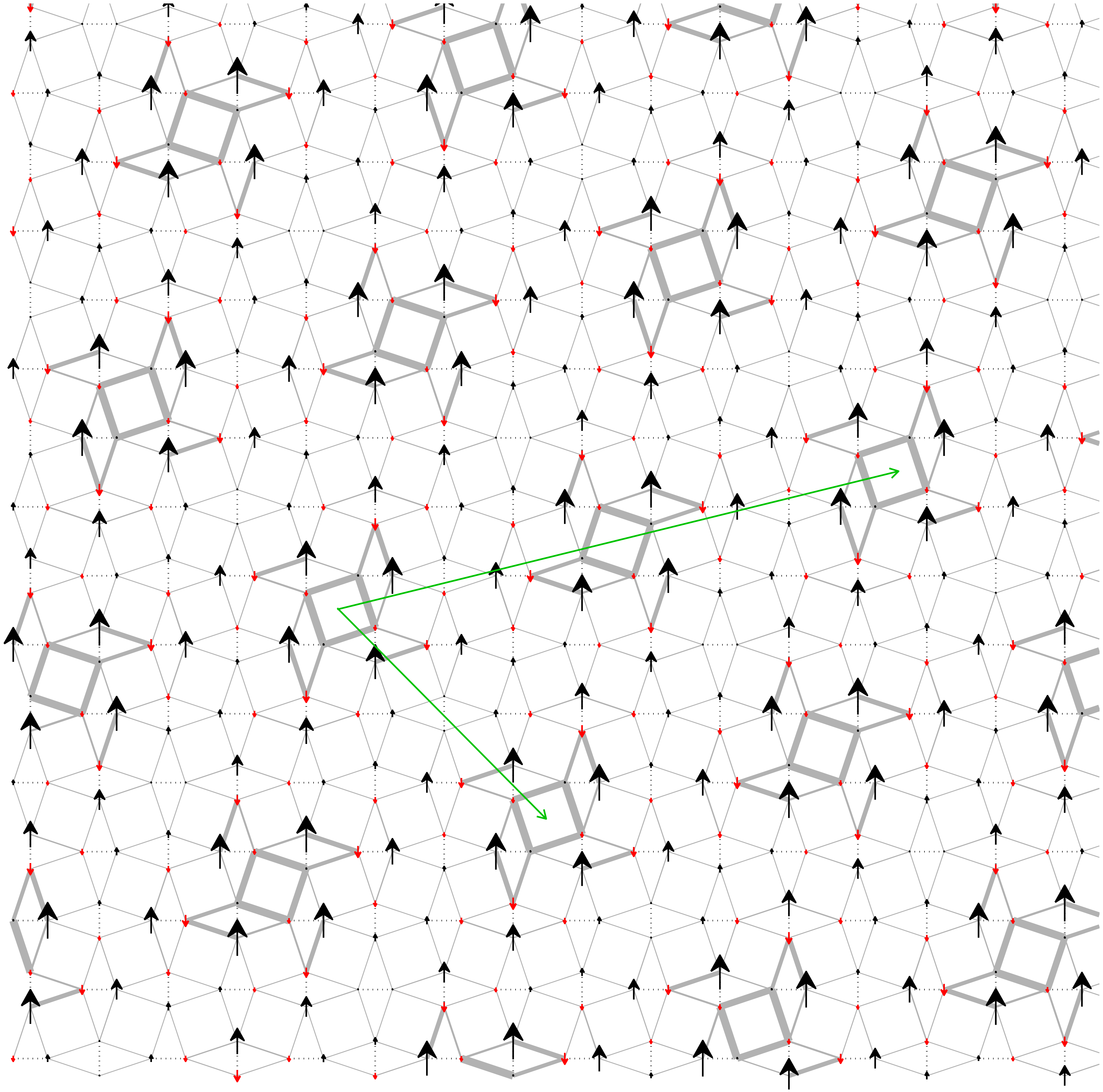






- All the proposed triplet crystals have a higher energy than the crystals made of bound states!
- Similar results found for other plateaus below 1/4

2/15 plateau

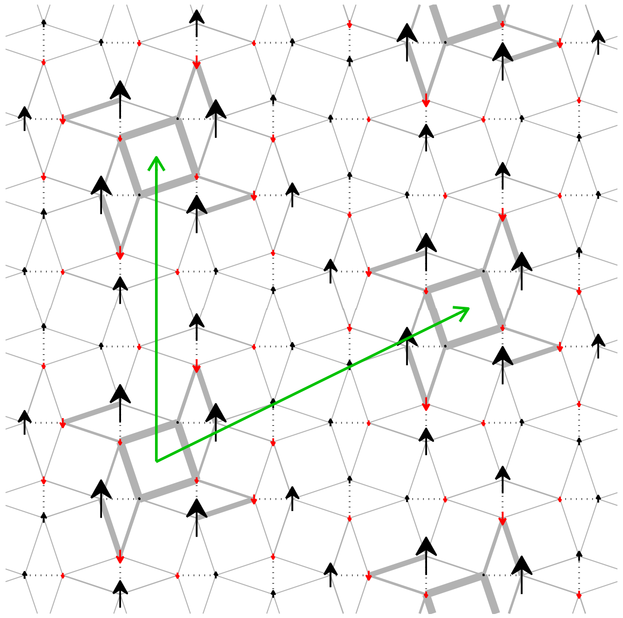


Unit cell with 30 tensors (60 sites)

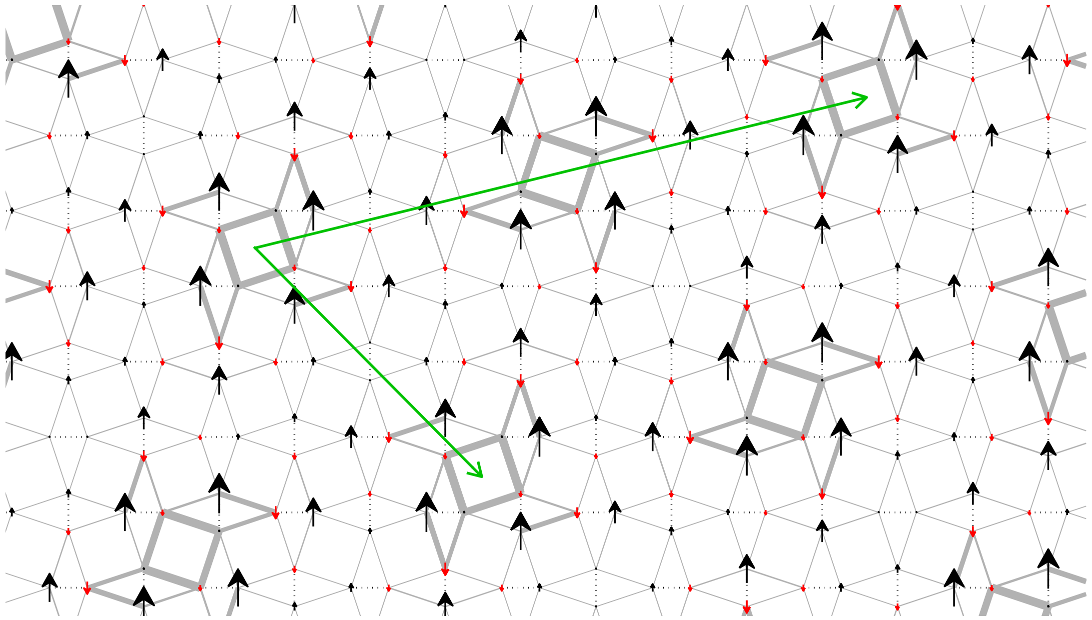
Regular pattern of bound states!

Computing the energies of all possible crystals

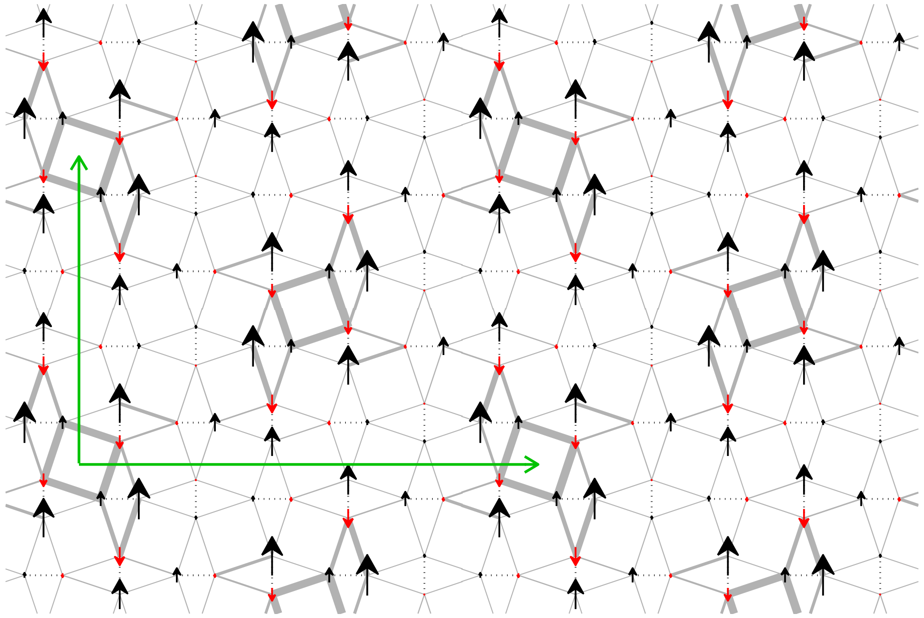
1/8 rhomboid : (4,2),(0,4)



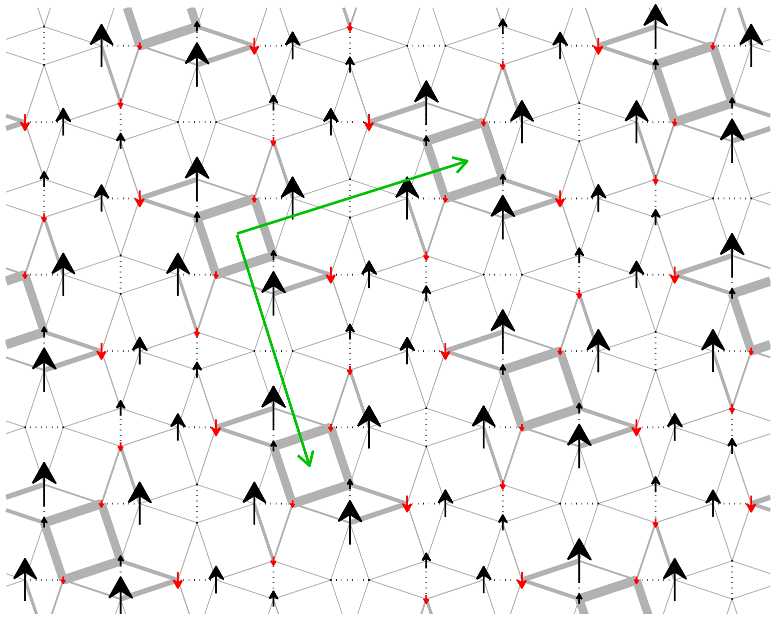
2/15 : (3,-3),(8,2)



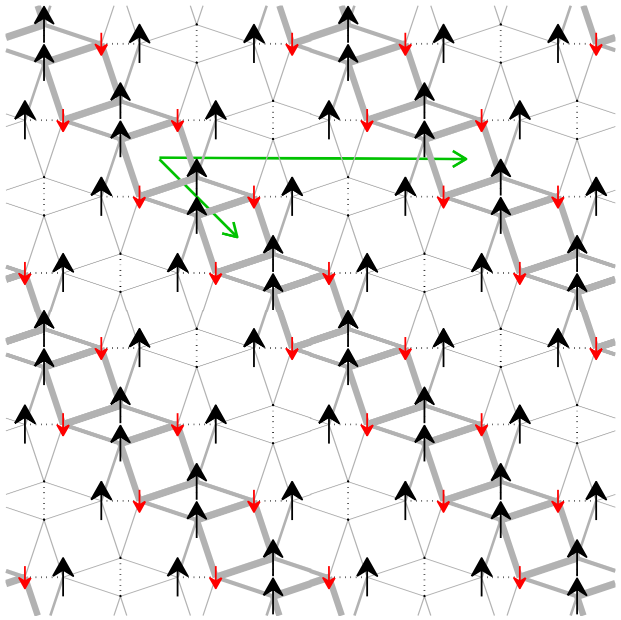
1/6 rectangular : (6,0),(0,4)



1/5 : (1,-3),(3,1)

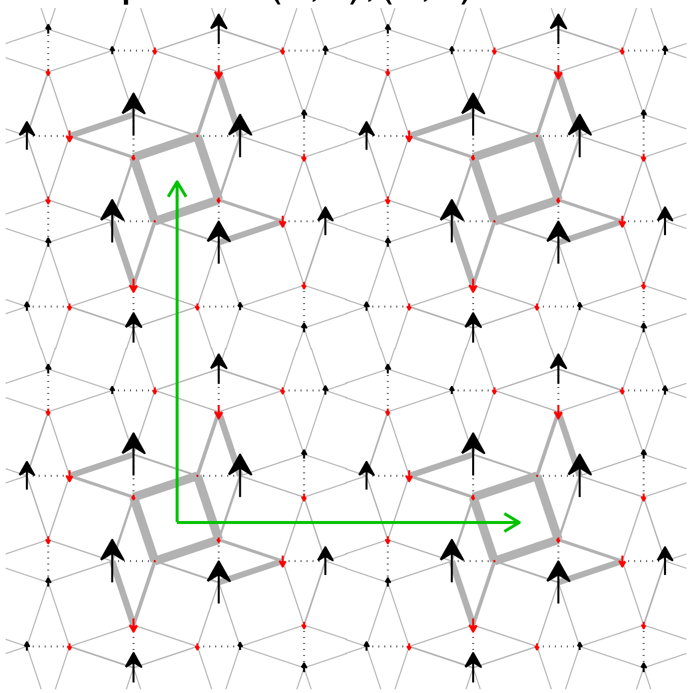


1/4 : (1,-1),(4,0)

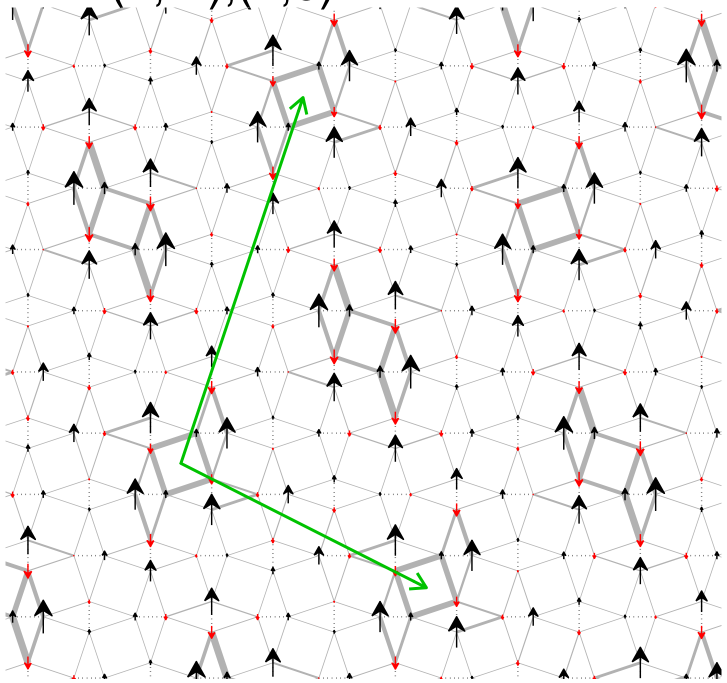


Computing the energies of all possible crystals

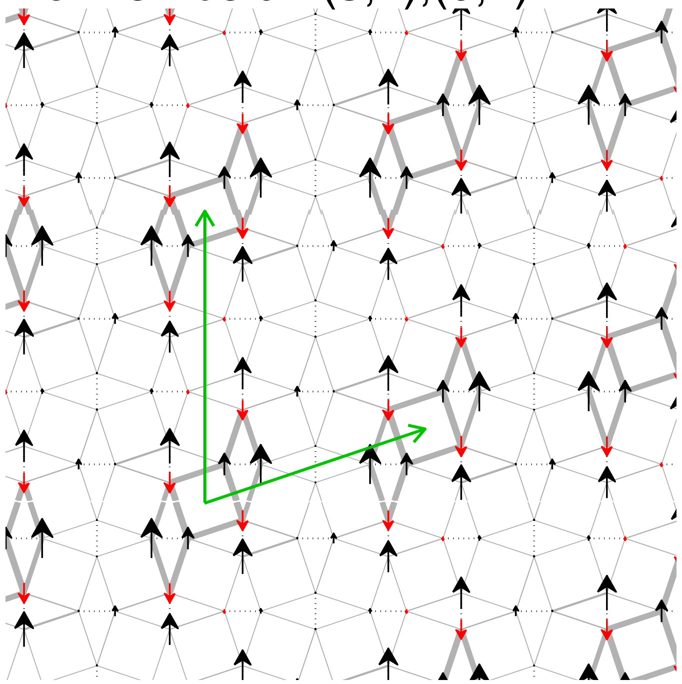
1/8 square : (4,0),(0,4)



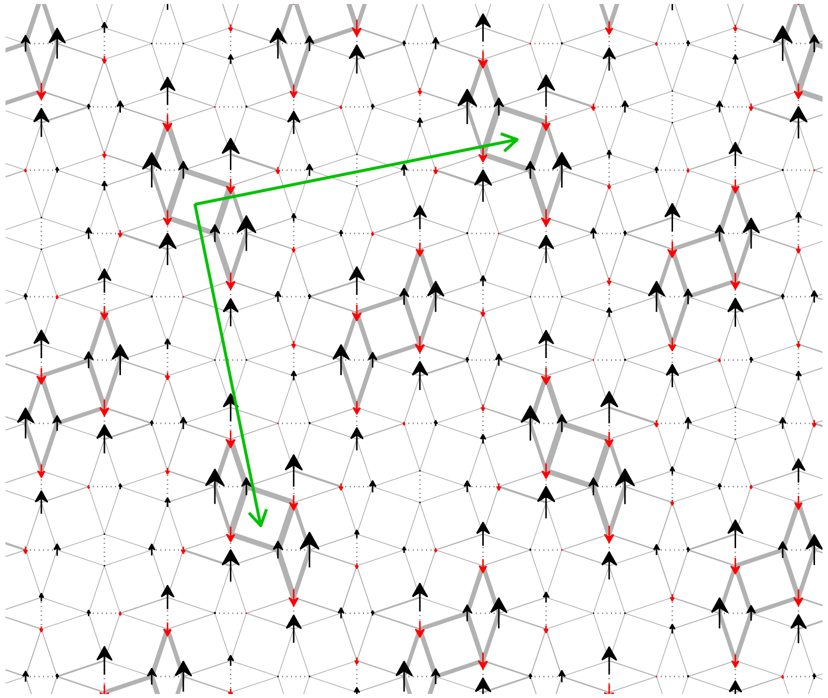
1/7 : (4,-2),(2,6)



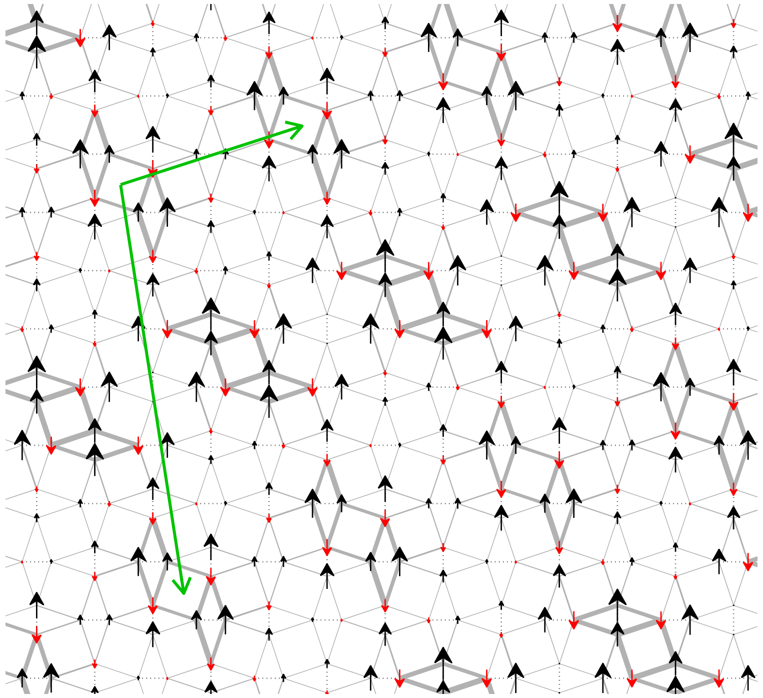
1/6 rhomboid : (3,1),(0,4)



2/13 : (1,-5),(5,1)

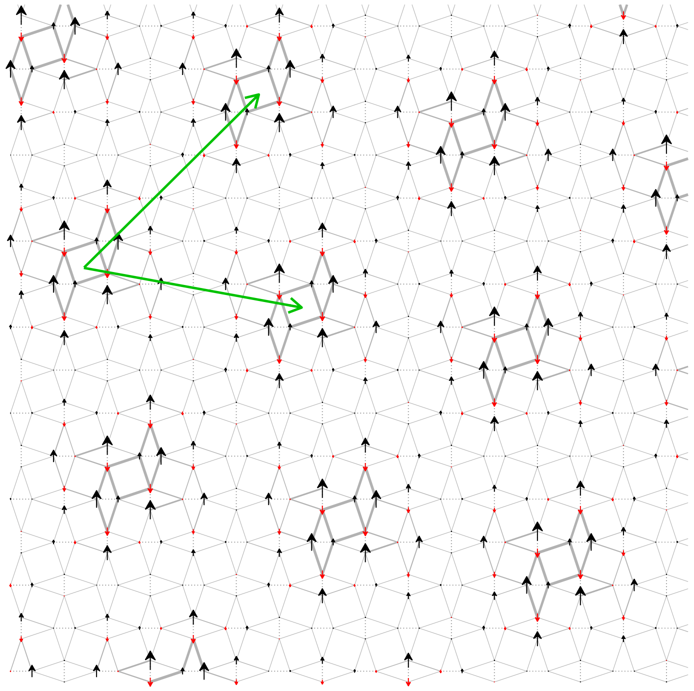


2/11 : (1,-7),(3,1)

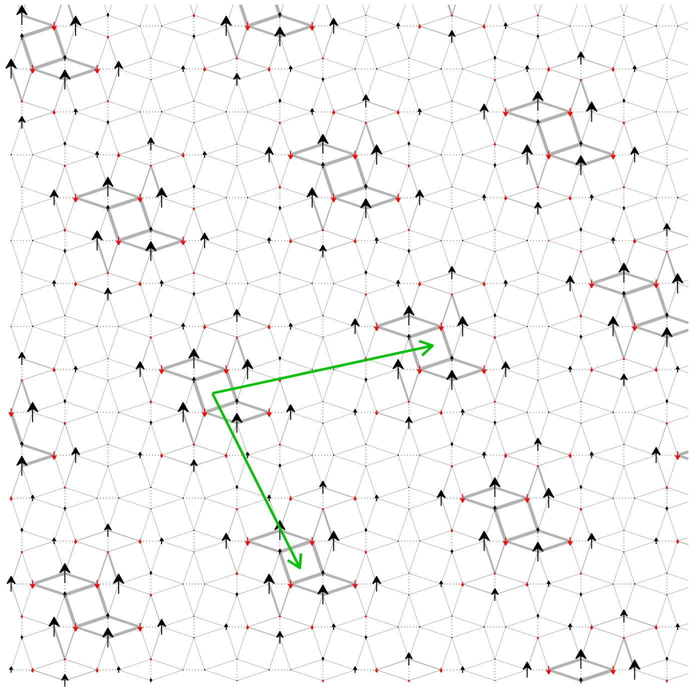


Computing the energies of all possible crystals

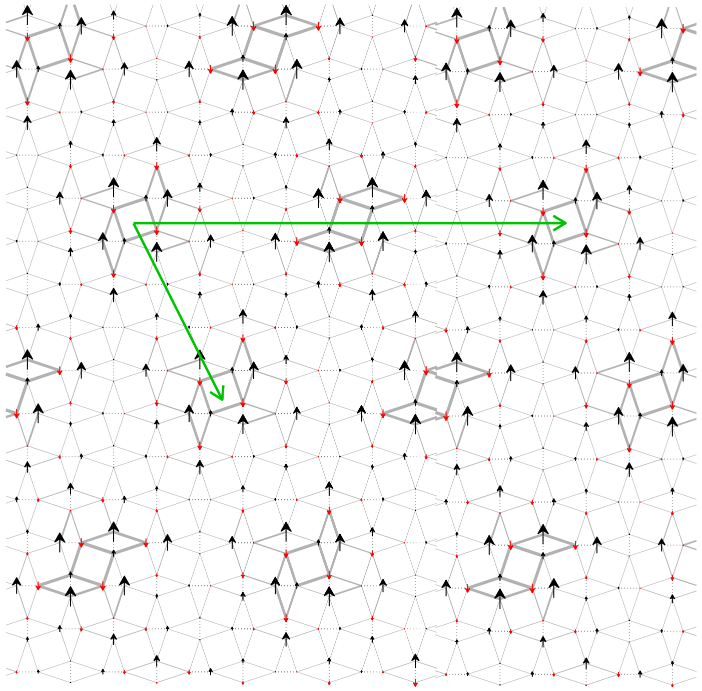
1/12 : (1,-5),(5,-1)



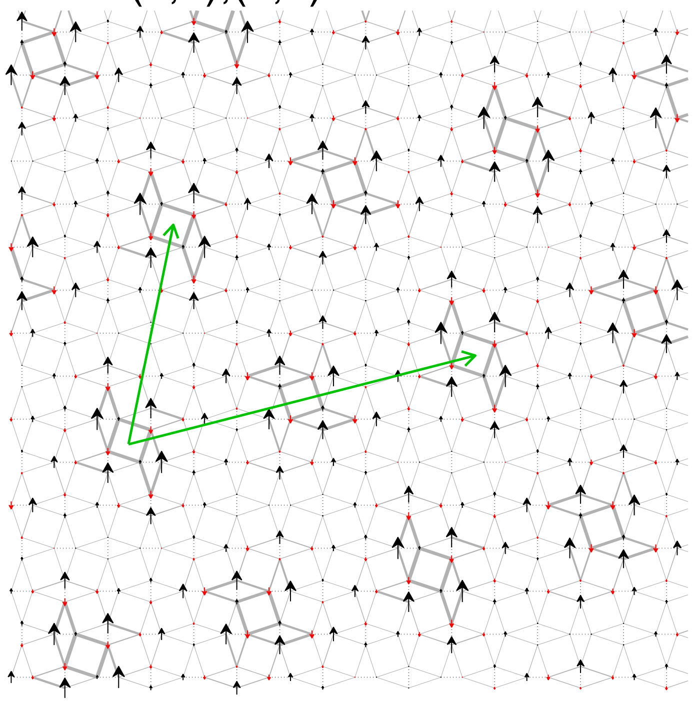
1/11 : (2,-4),(5,1)



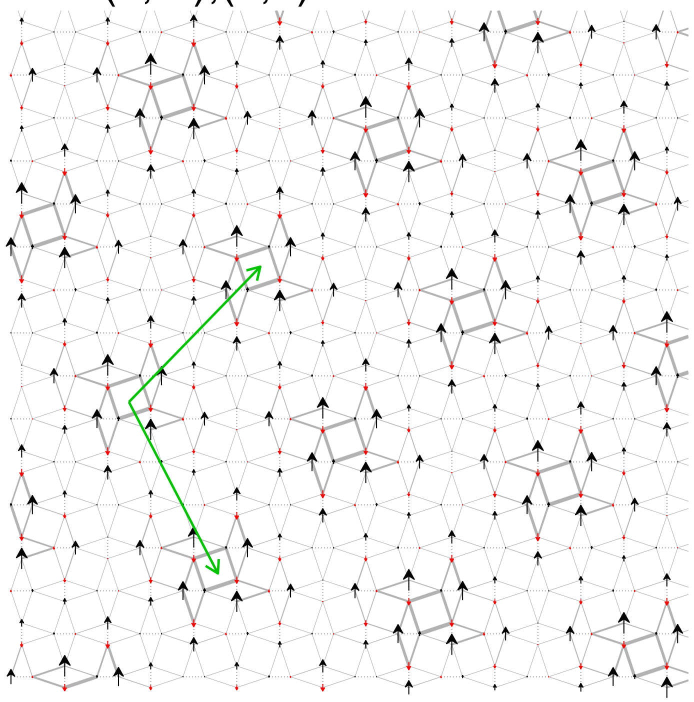
1/10 : (2,-4),(10,0)



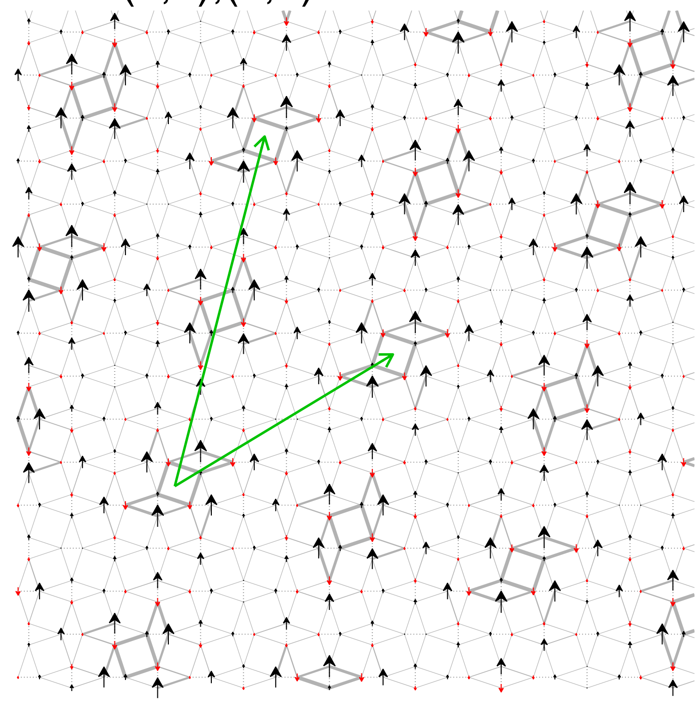
2/19 : (8,2),(1,5)



1/9 : (2,-4),(3,3)

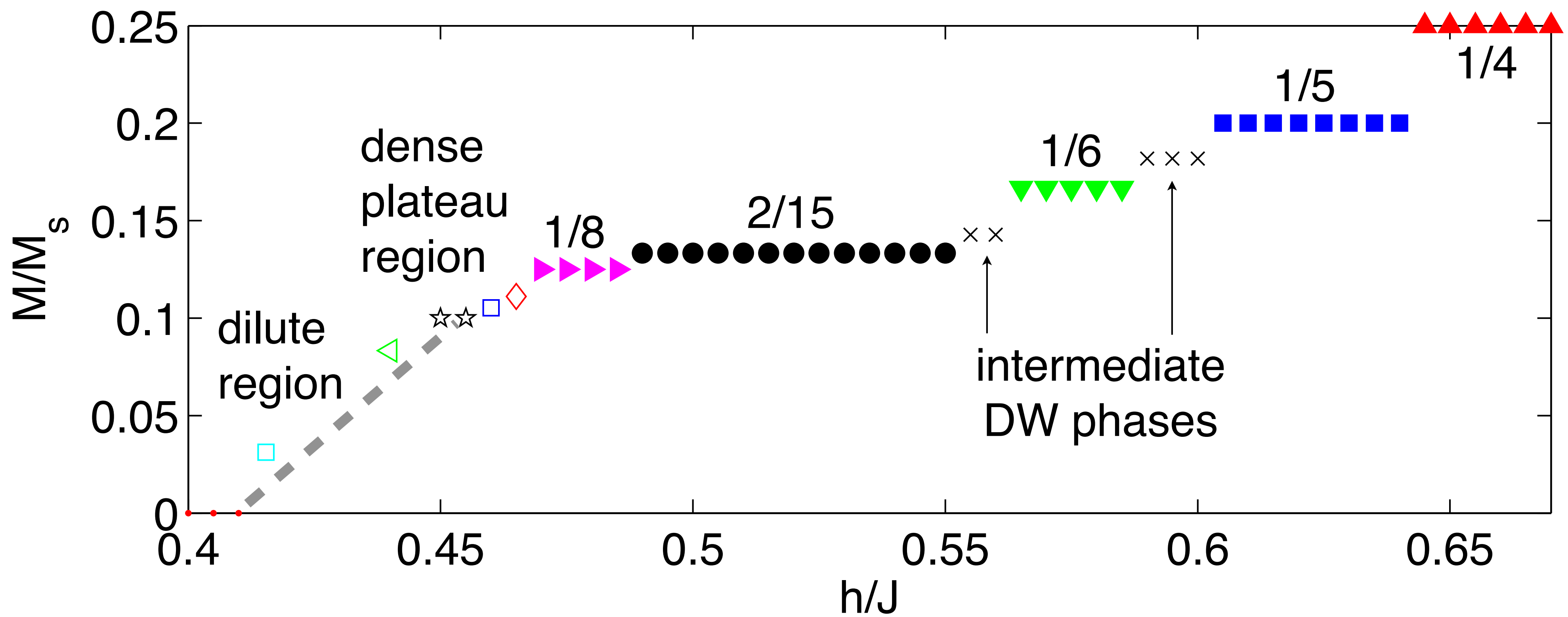


2/17 : (5,3),(2,8)



Magnetization curve obtained with iPEPS

PC, F. Mila, PRL **112** (2014)



$$J'/J = 0.63$$

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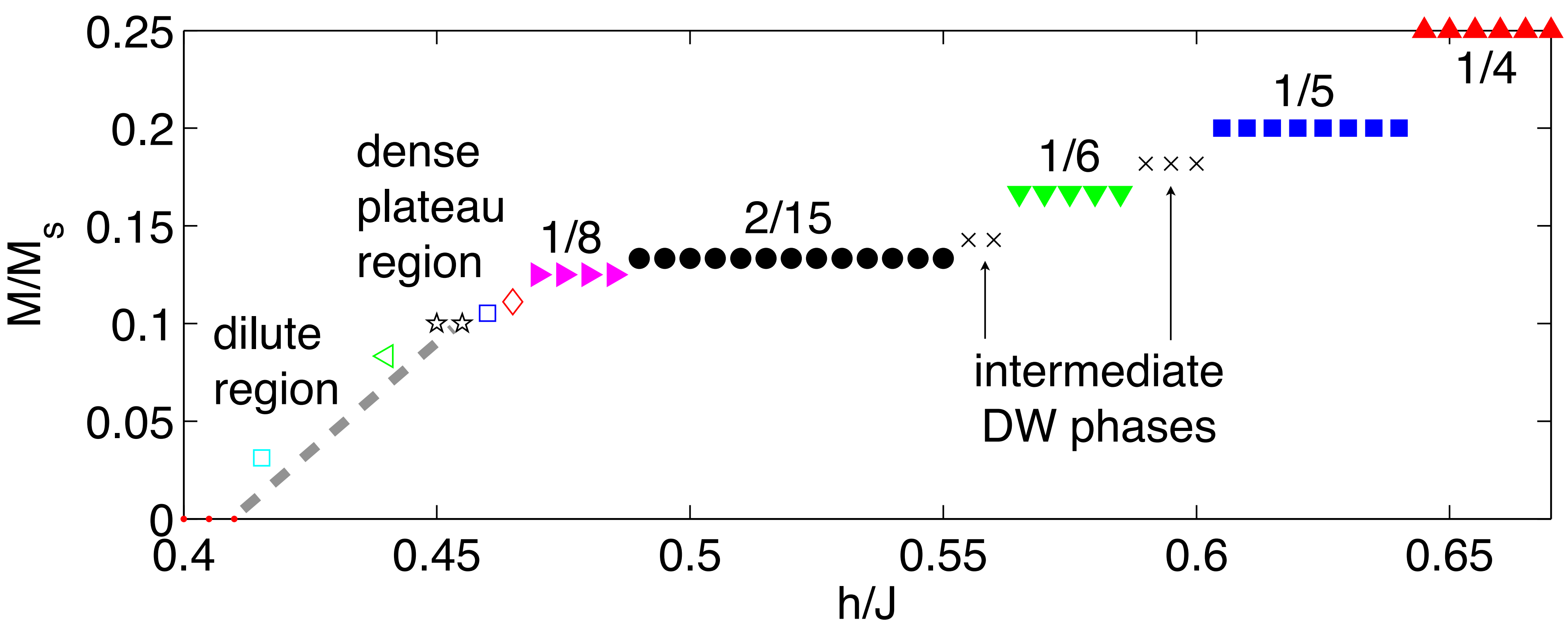

$J'/J = 0.63$

★ Sizable plateaus found at: 1/8, 2/15, 1/6, 1/5, 1/4, 1/3, 1/2

[1/5 plateau vanishes upon adding a small (but realistic) DM interaction]

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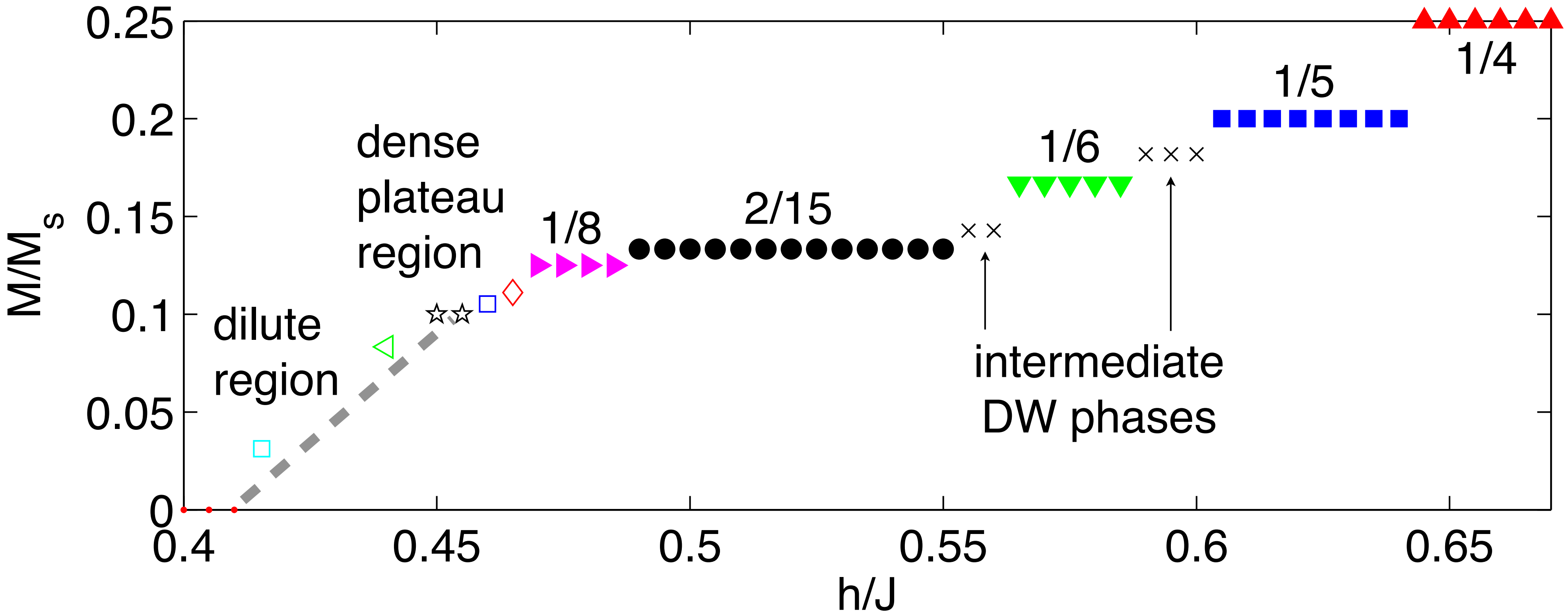

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★ **Sequence in agreement with experiments**

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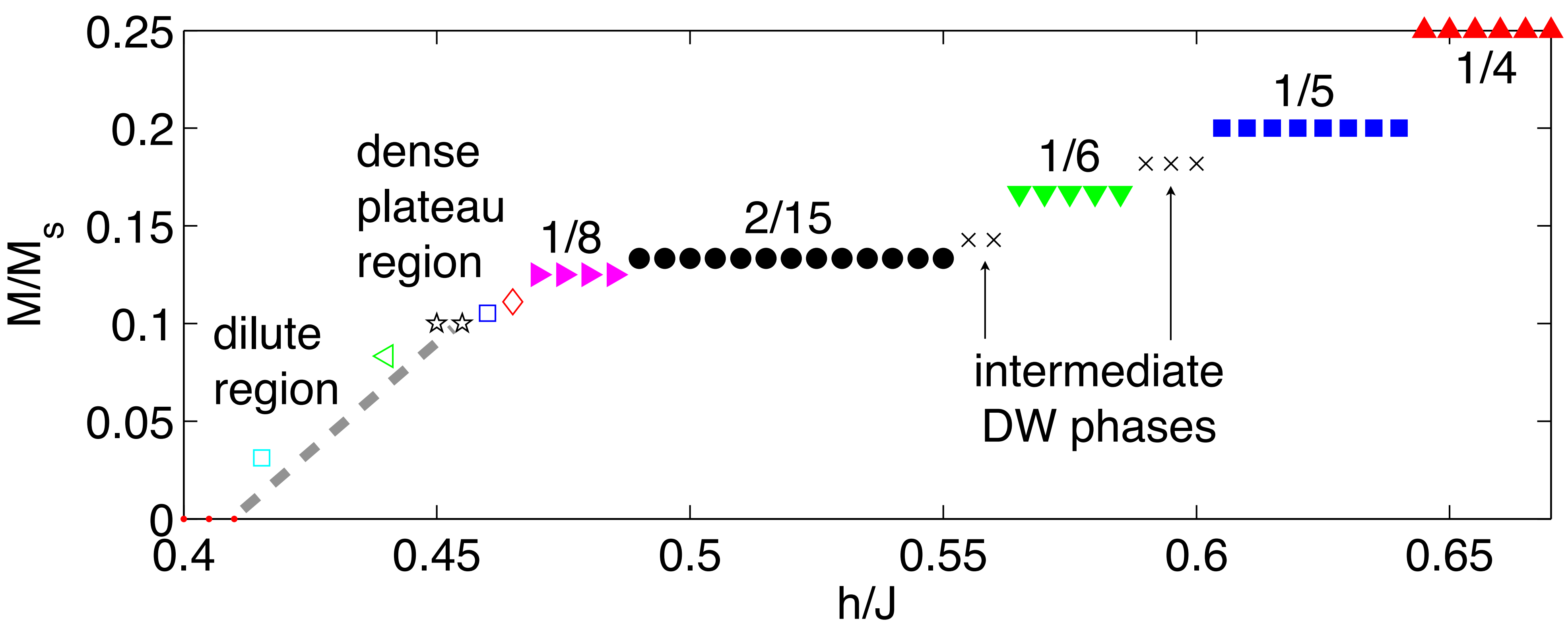

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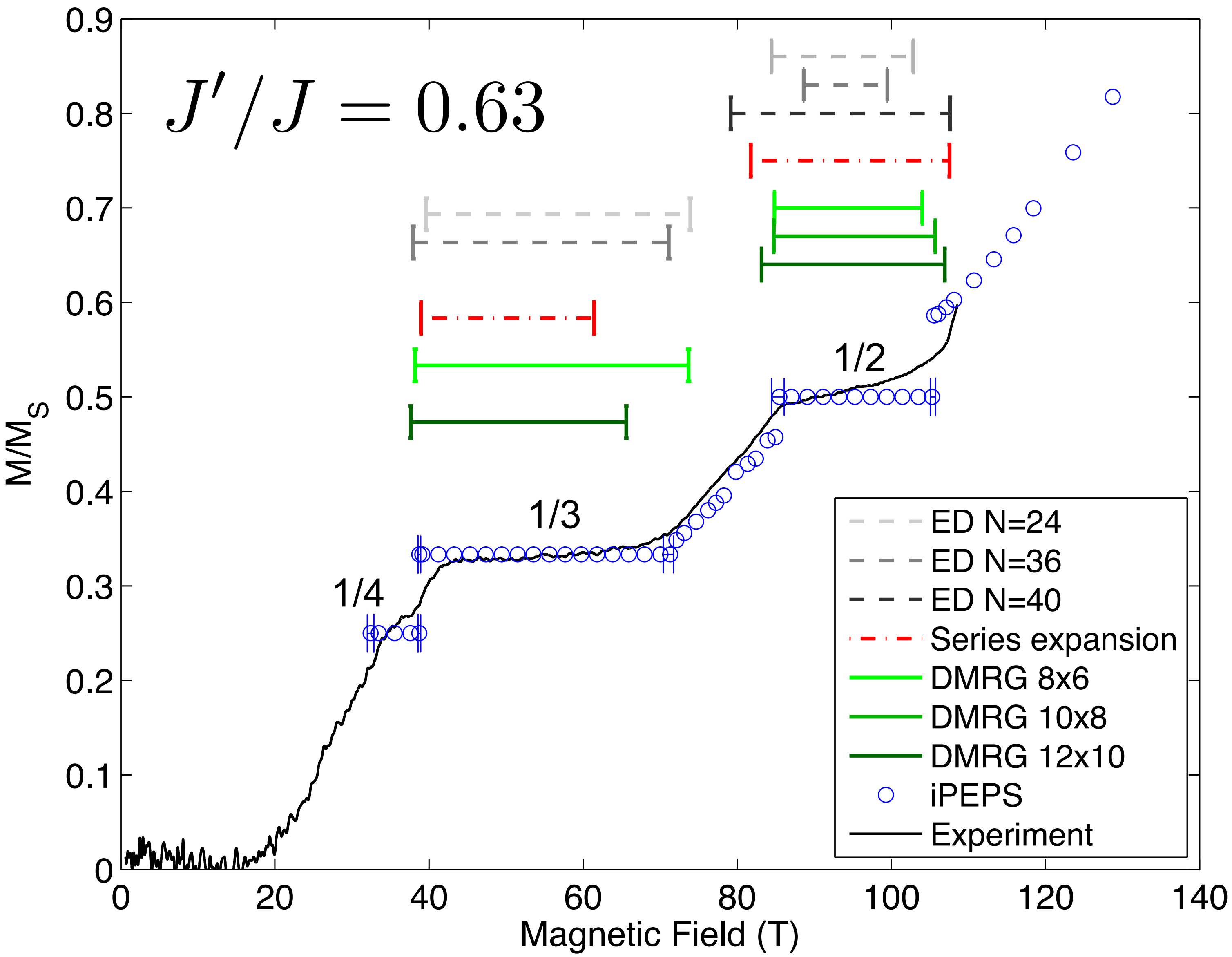
★ **Sequence in agreement with experiments**

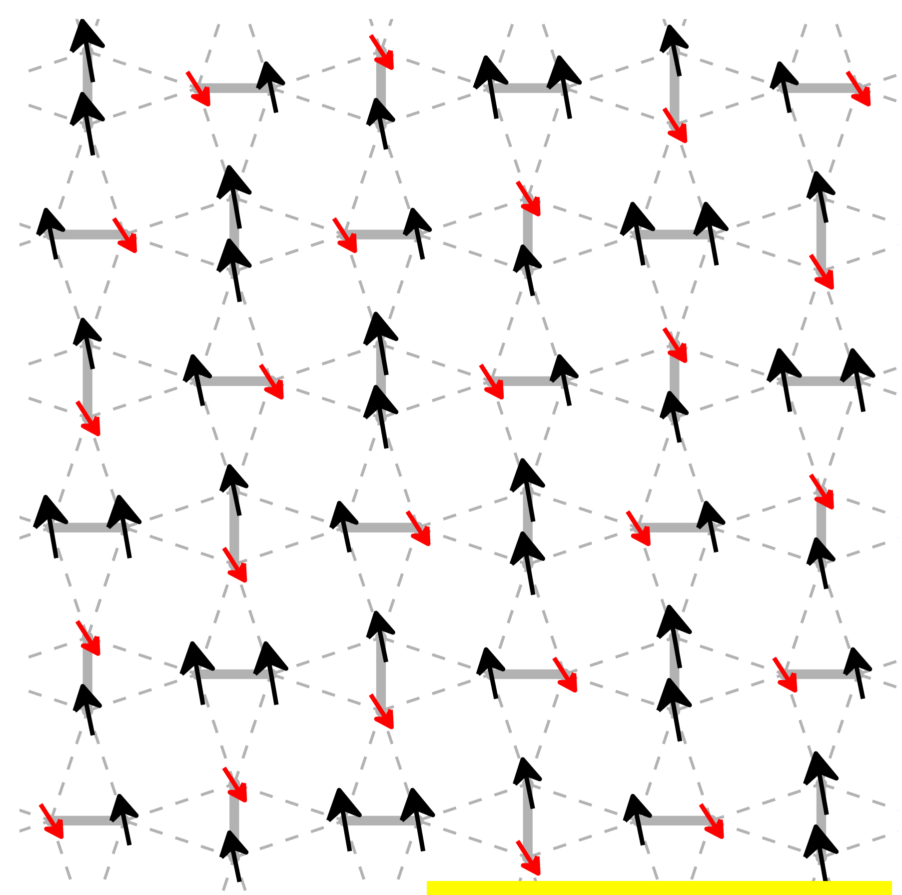
★ New understanding of the magnetization process in $SrCu_2(BO_3)_2$

$SrCu_2(BO_3)_2$ in ultra-high magnetic fields up to 118T

Matsuda, Abe, Takeyama, Kageyama, PC, Honecker, Manmana, Foltin, Schmidt & Mila, PRL 111 (2013)



- Best fit with experiments for J'/J = 0.63 using iPEPS, DMRG, ED, series expansion
- Supersolid phases at high fields

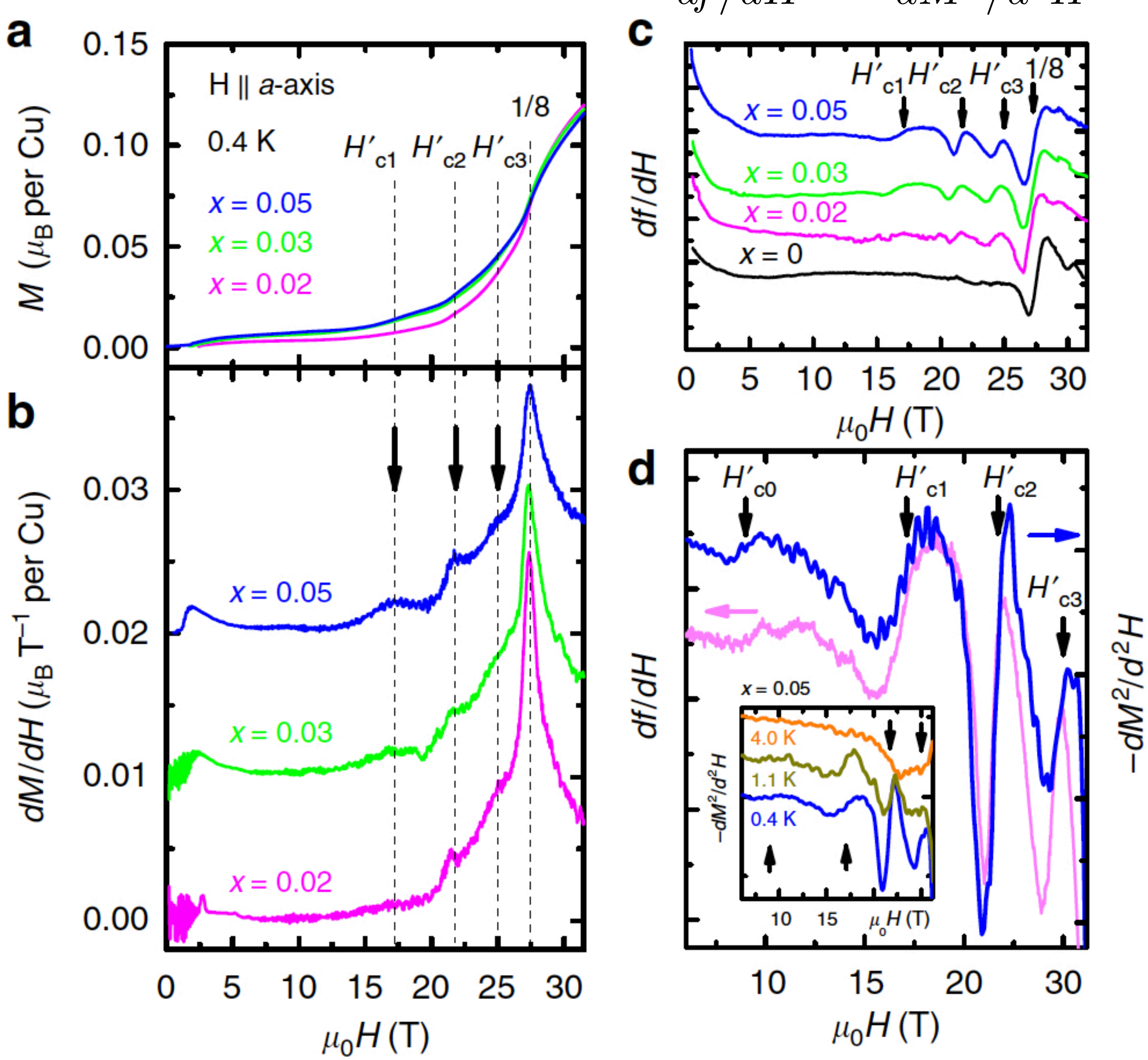


1/3 supersolid

$SrCu_{2-x}Mg_x(BO_3)_2$ in a magnetic field

Shi, Steinhardt, Graf, PC, Weickert, Harrison, Jaime, Marjerrison, Dabkowska, Mila, Haravifard, Nature Communications 10, 2439 (2019).

$$df/dH \sim -dM^2/d^2H$$



★ New anomalies appearing below the 1/8 plateau at fields which are absent at zero doping

★ Use iPEPS to gain insights into the nature of these anomalies

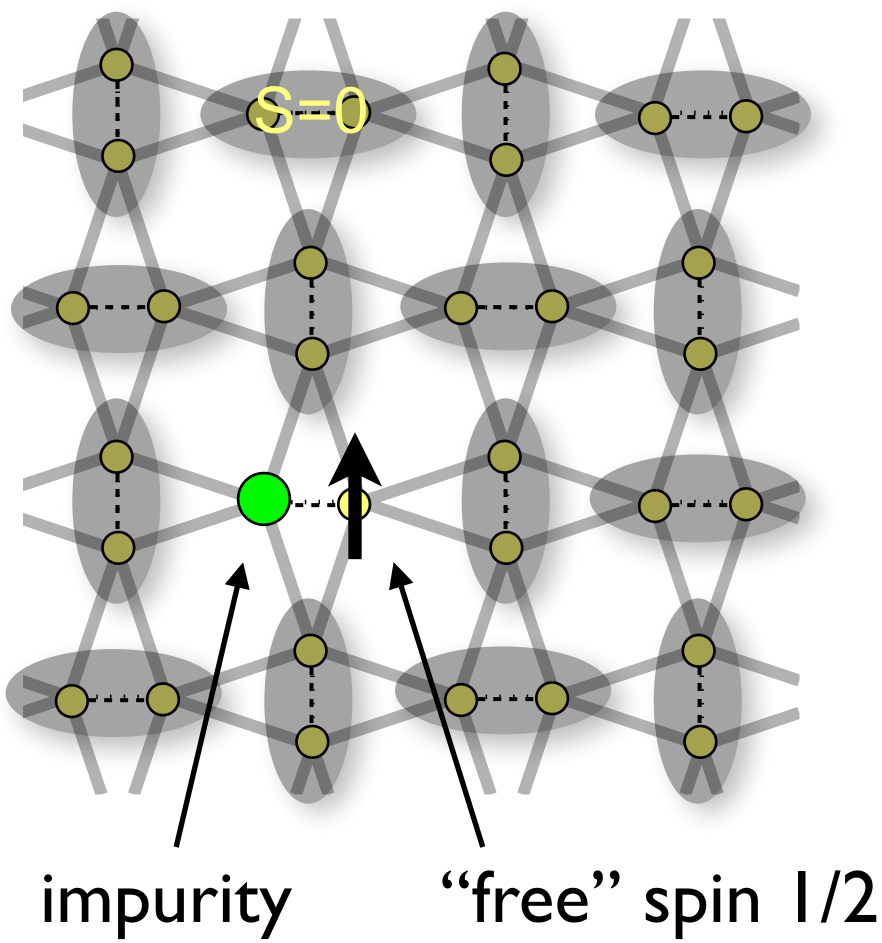
$$H'_{C0} \sim 9T, \quad H'_{C1} \sim 17.1T, \quad H'_{C2} \sim 21.7T, \quad H'_{C3} \sim 25T$$

$SrCu_{2-x}Mg_x(BO_3)_2$ in a magnetic field

Shi, Steinhardt, Graf, PC, Weickert, Harrison, Jaime, Marjerrison, Dabkowska, Mila, Haravifard, Nature Communications 10, 2439 (2019).

$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j - h \sum_i S_i^z$$

with non-magnetic impurities



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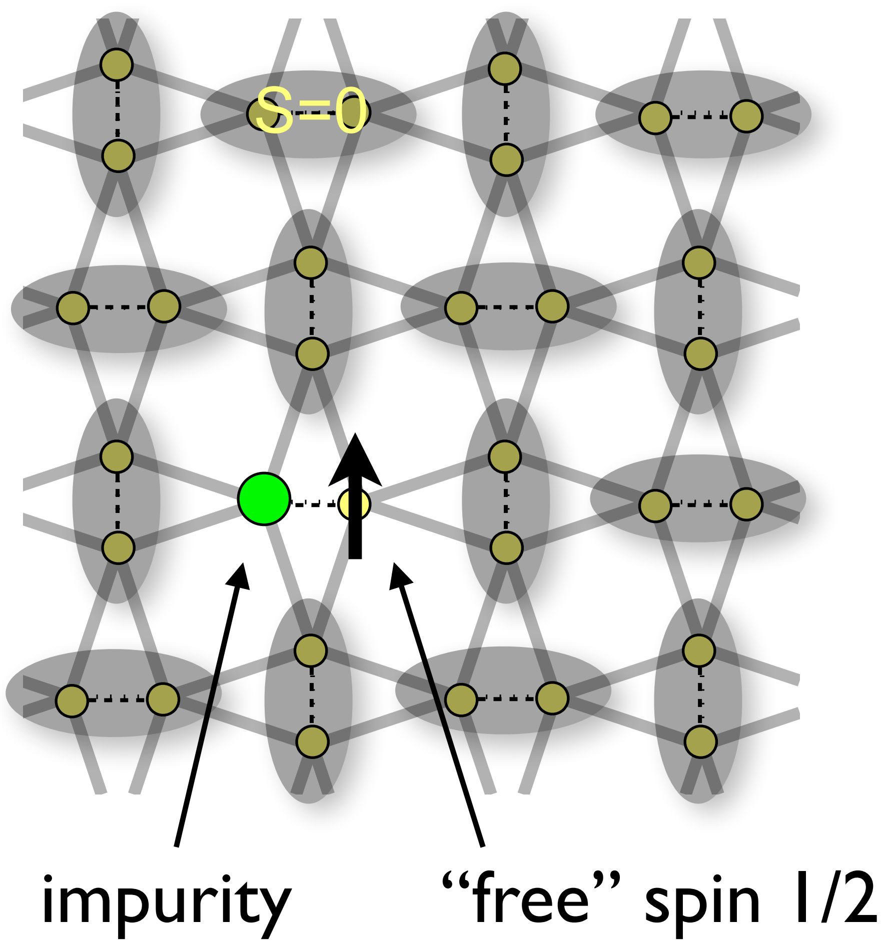

★ The free spin next to an isolated impurity aligns with an arbitrarily small field

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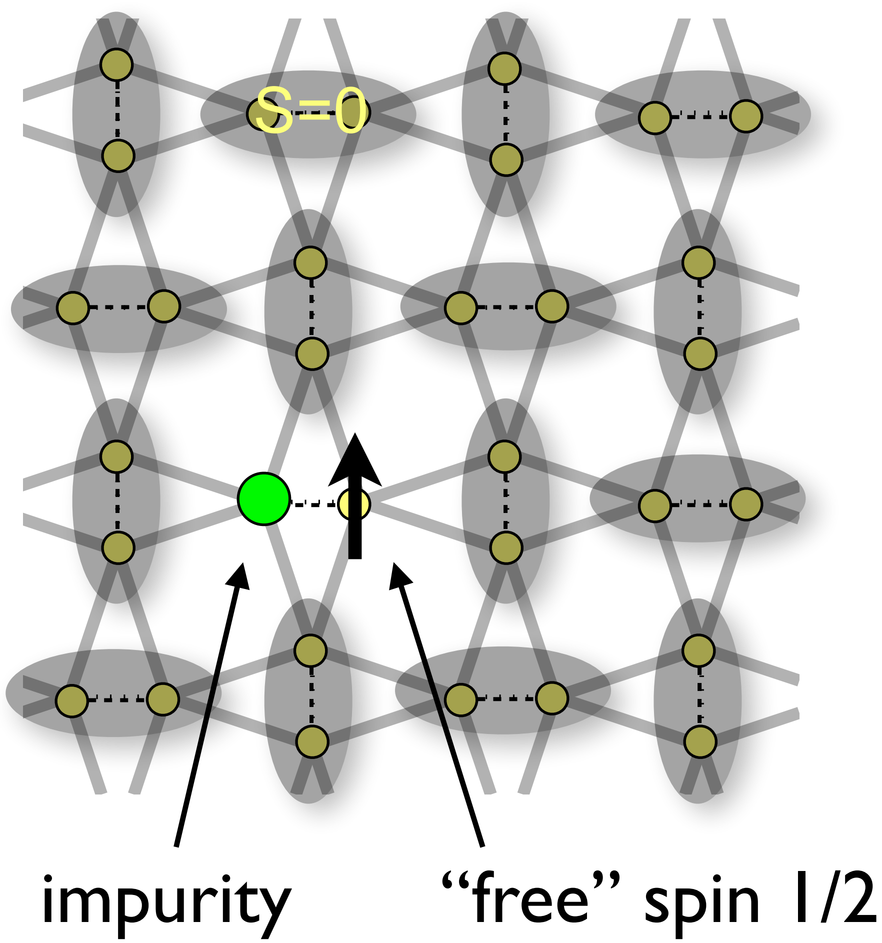

★ The free spin next to an isolated impurity aligns with an arbitrarily small field

★ Magnetization process in the presence of the impurities?

Key question 1: Bound states attracted or repelled?

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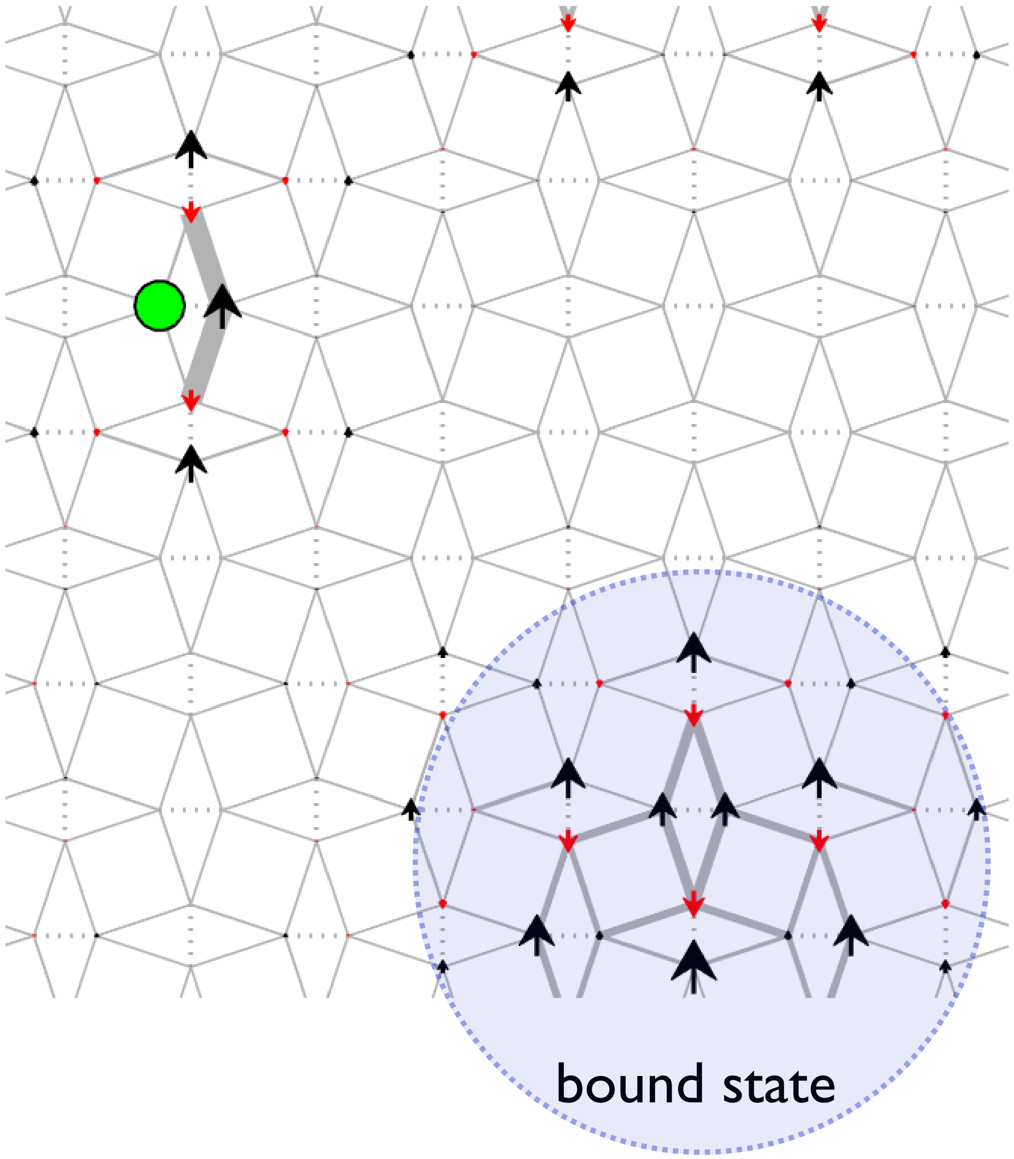
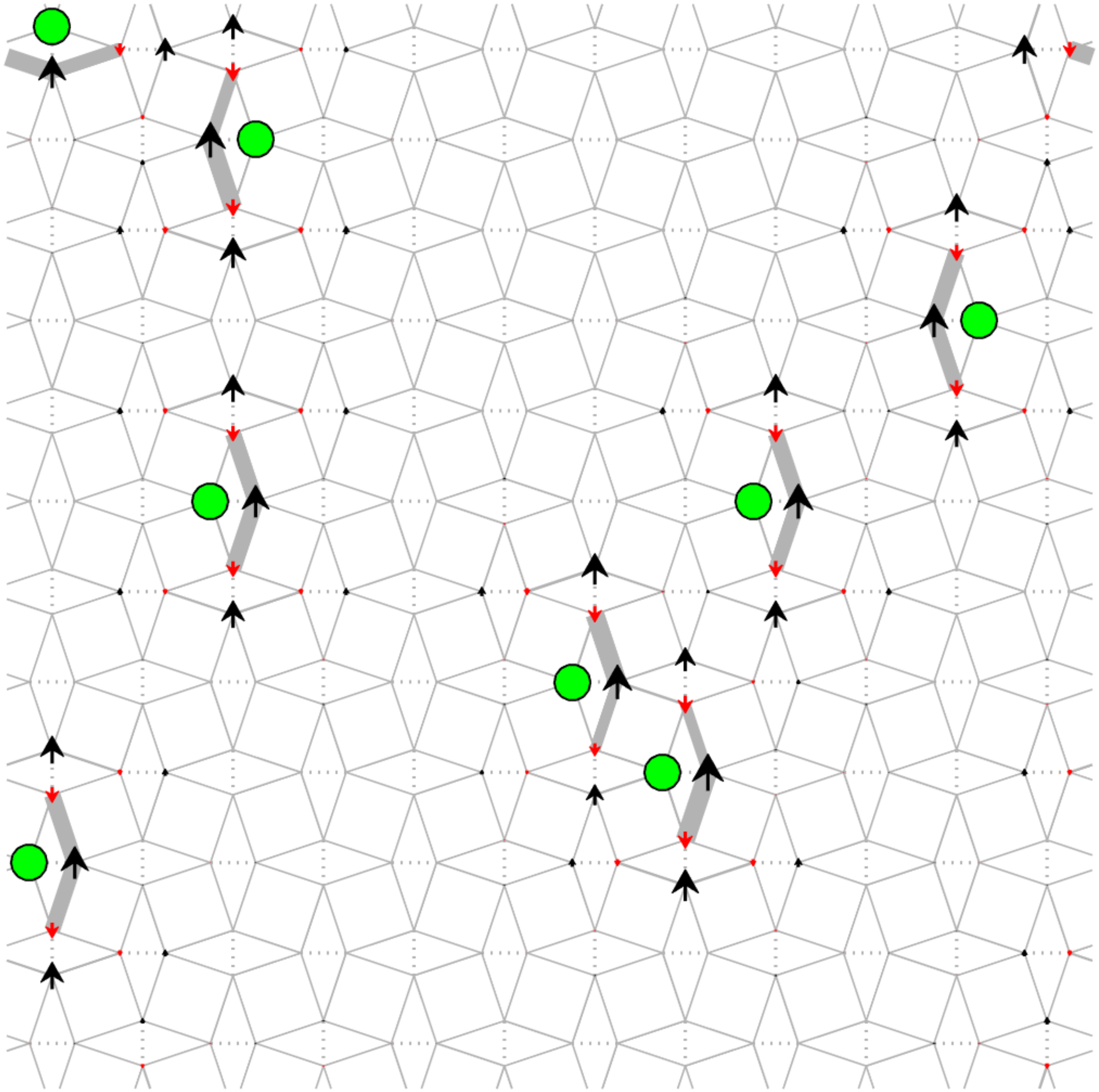
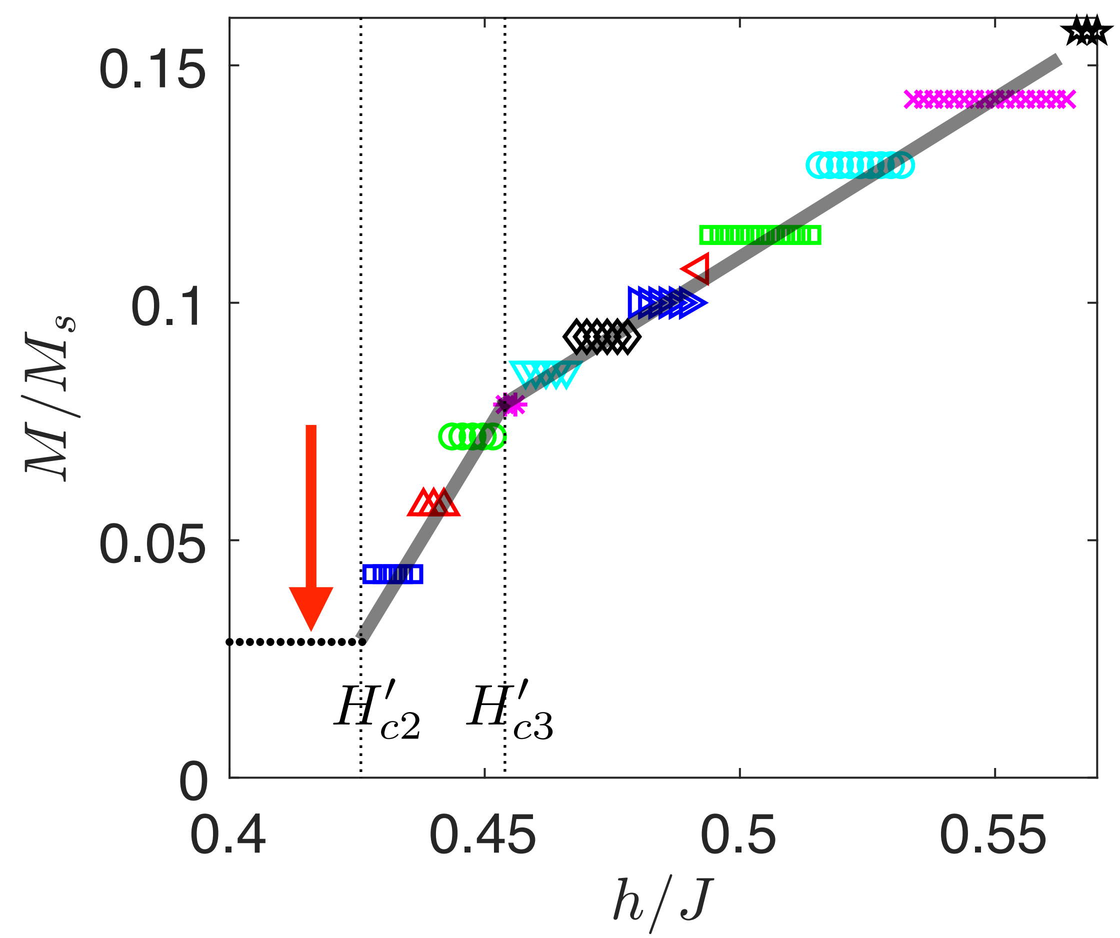


★ A bound state gets repelled by an impurity site

Key question 2: how does the lattice get filled?





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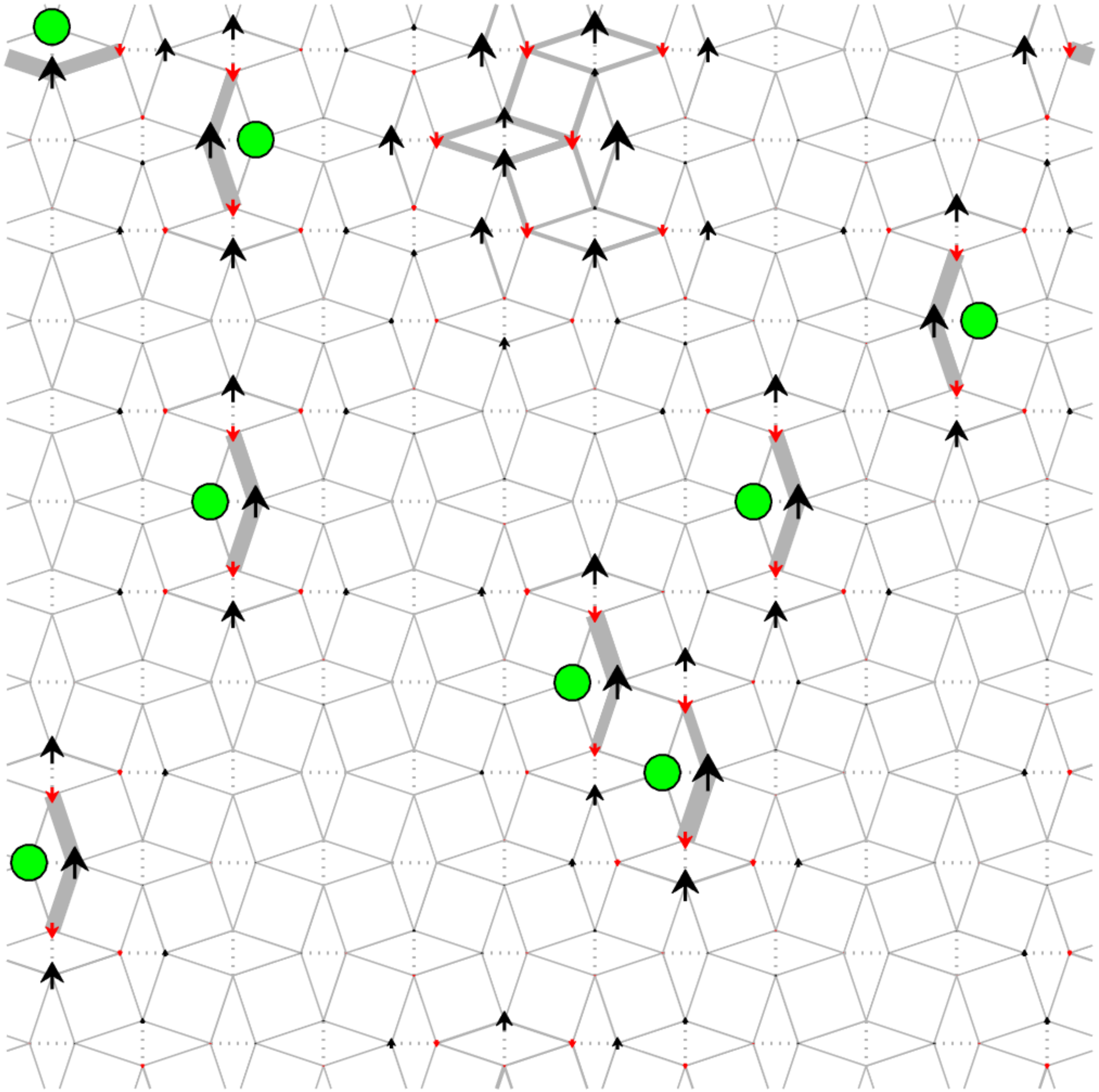
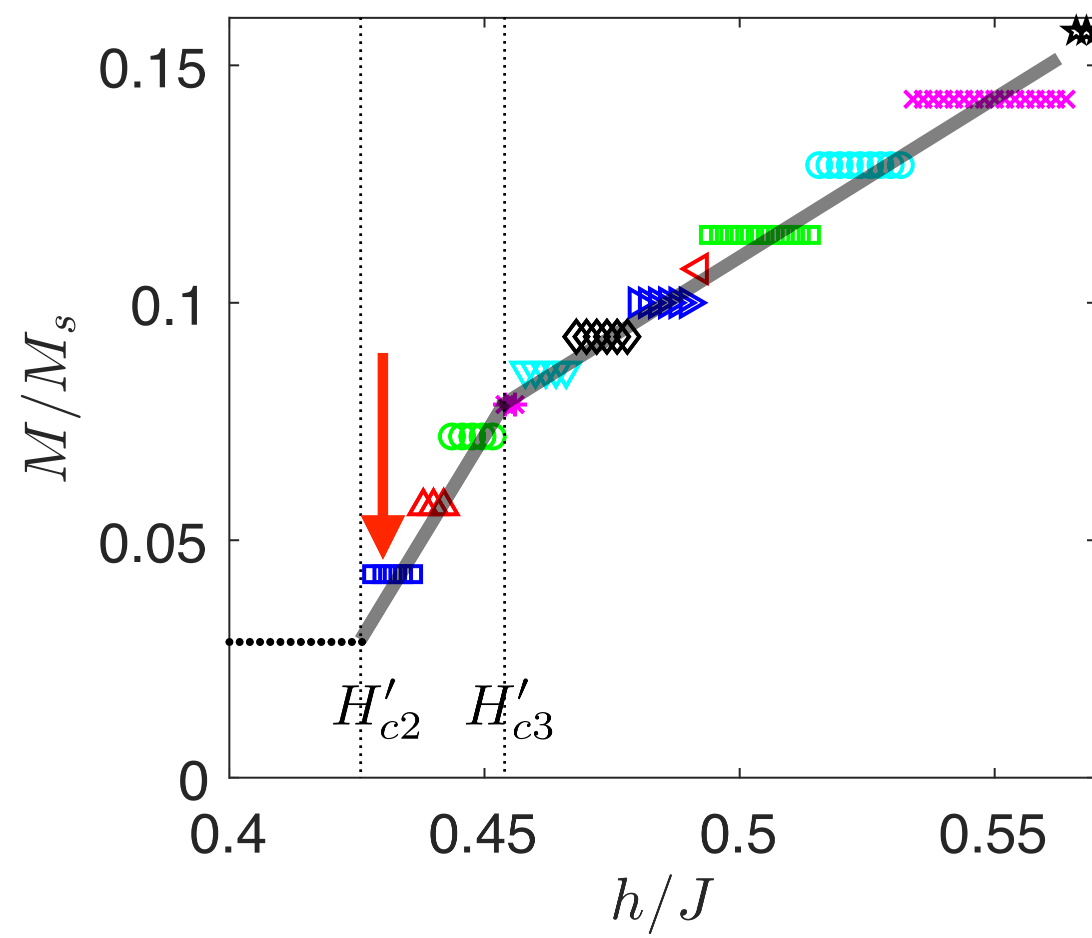
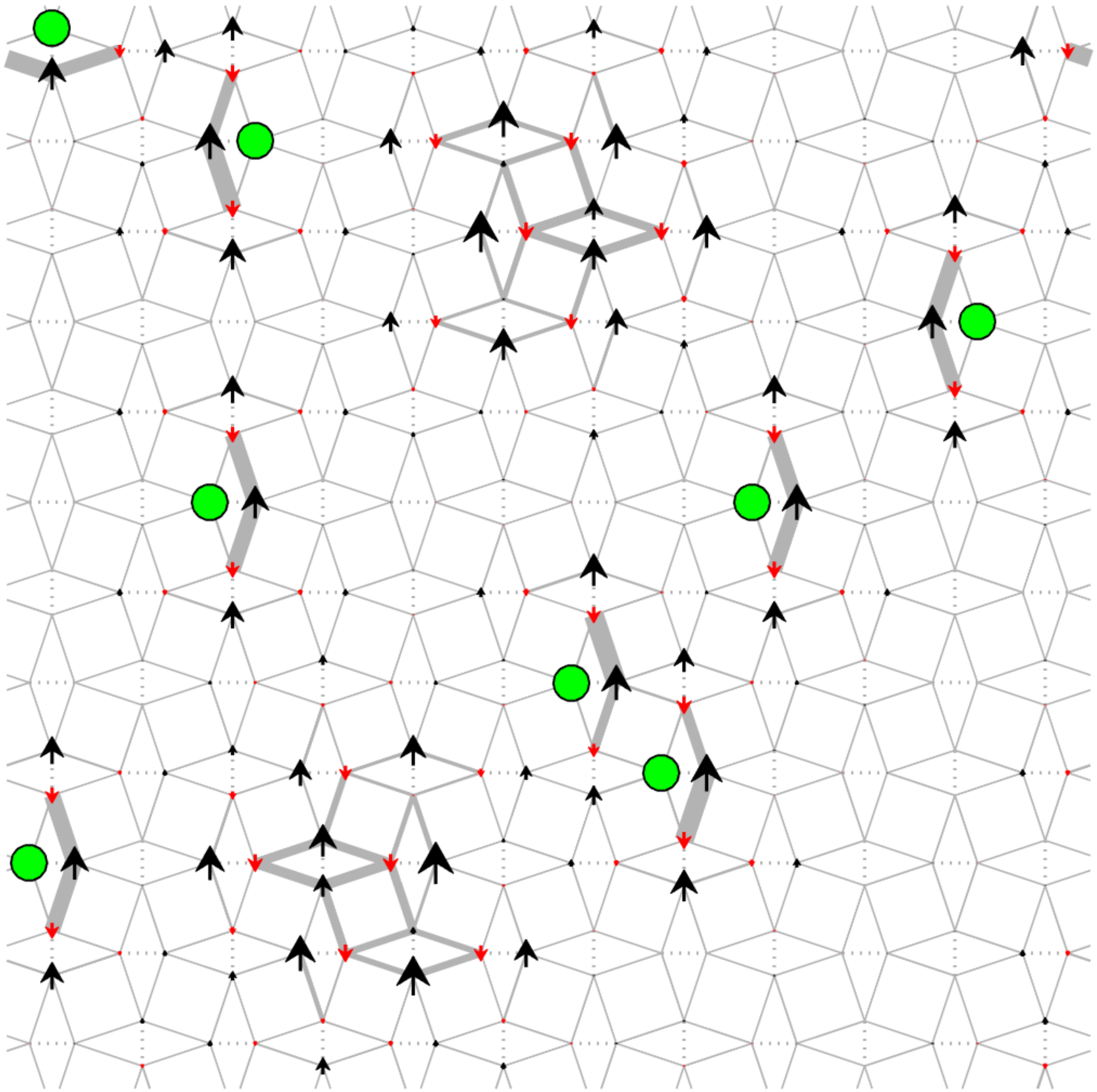


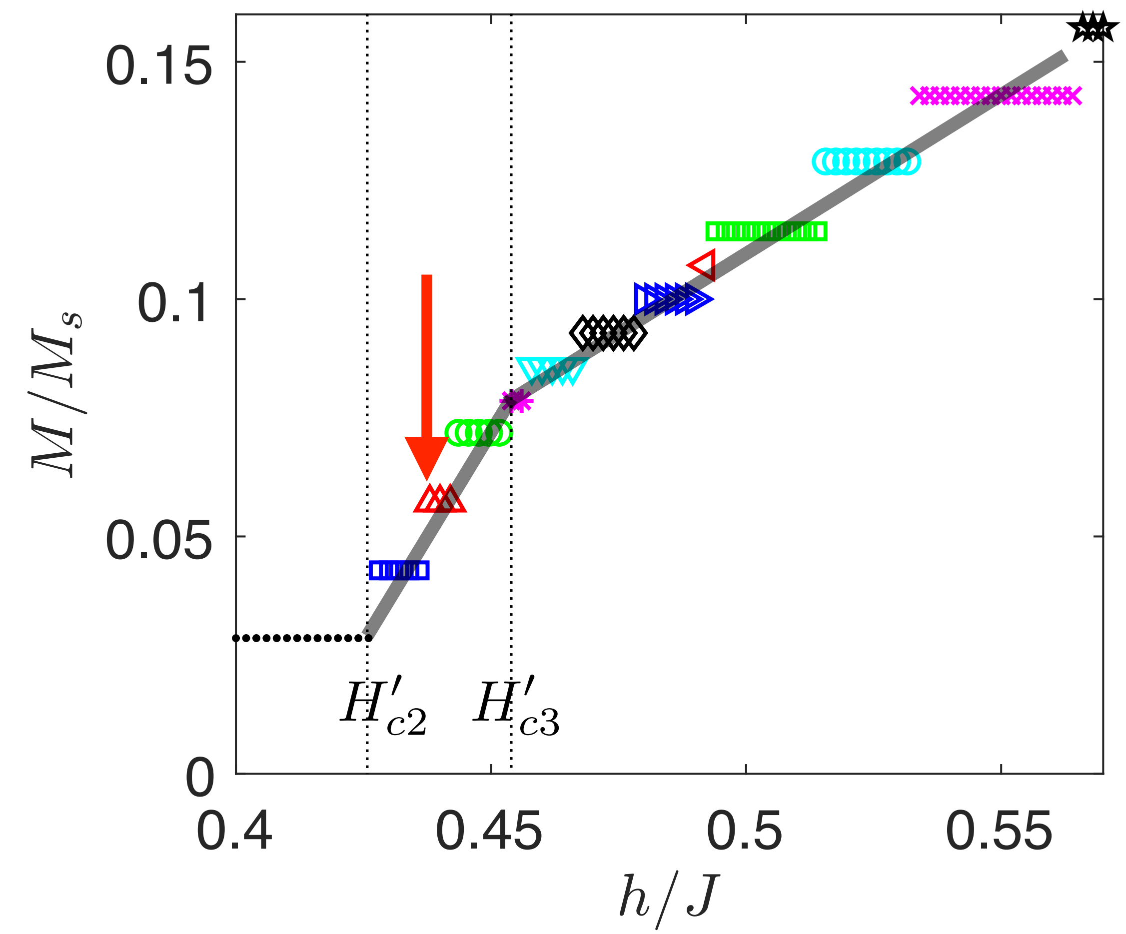


★ At $H'_{c2} \sim 21.8T$: appearance of first bound states

Jump in magnetization leads to anomaly in experiments at $H'_{c2} \sim 21.7T$

Key question 2: how does the lattice get filled?





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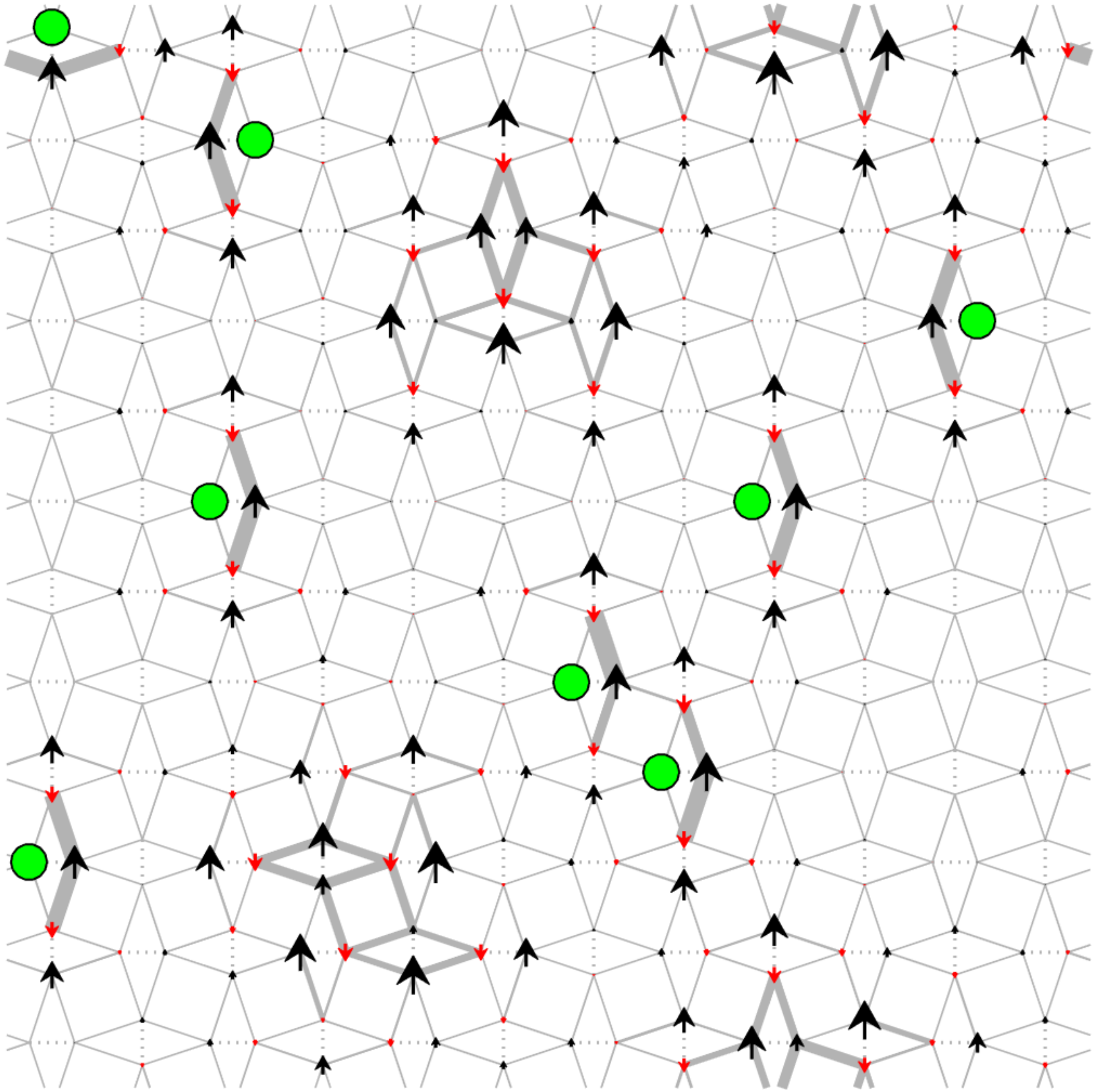

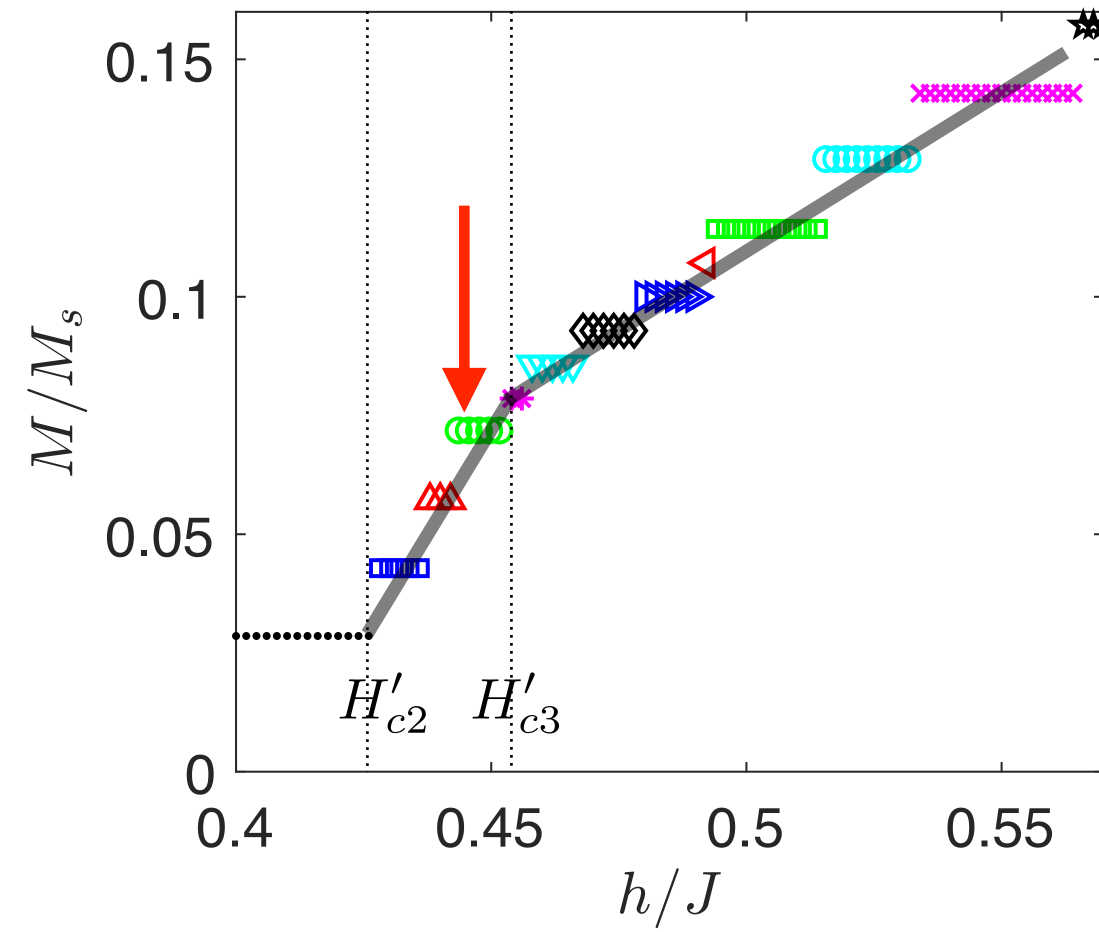

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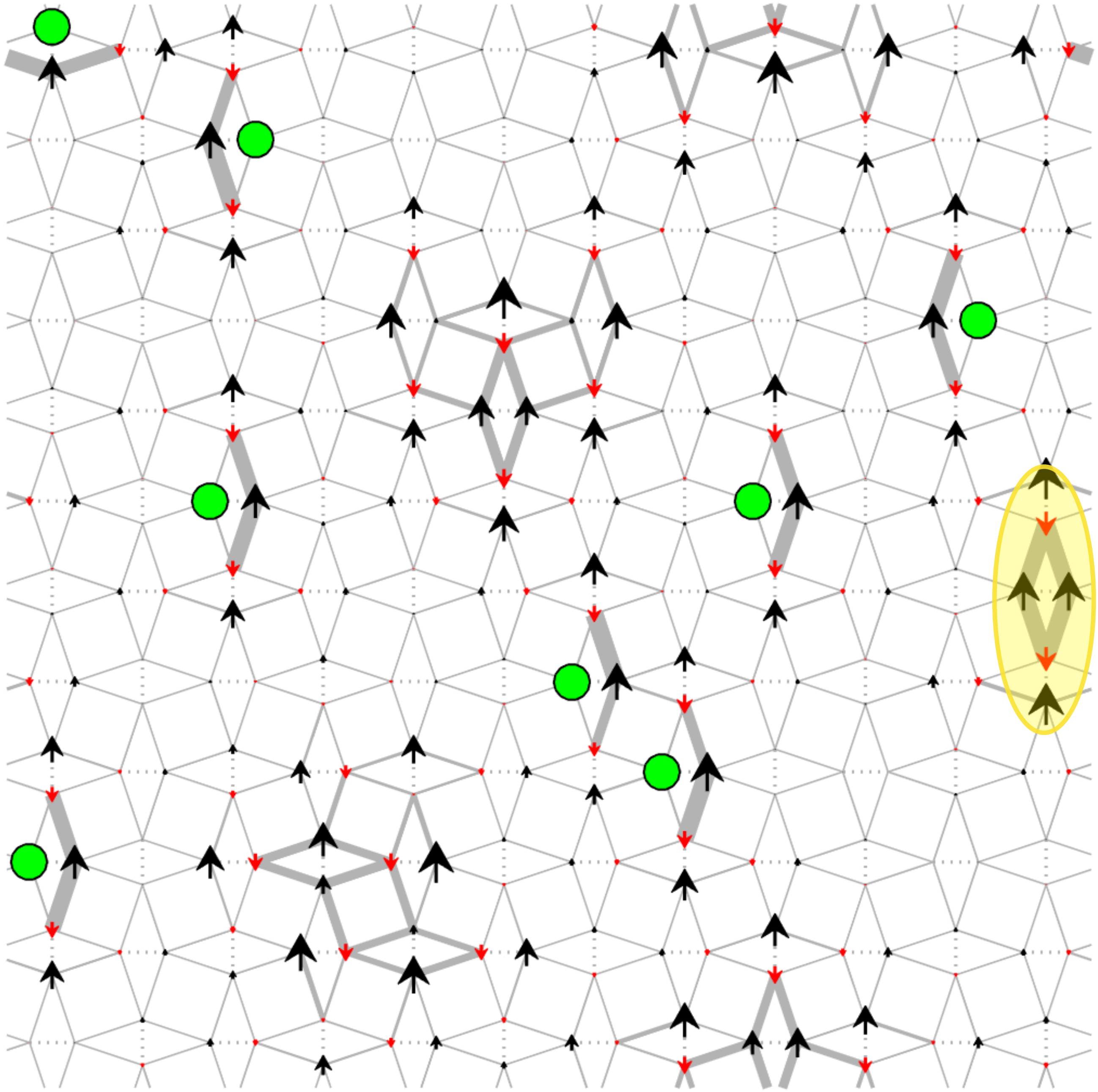
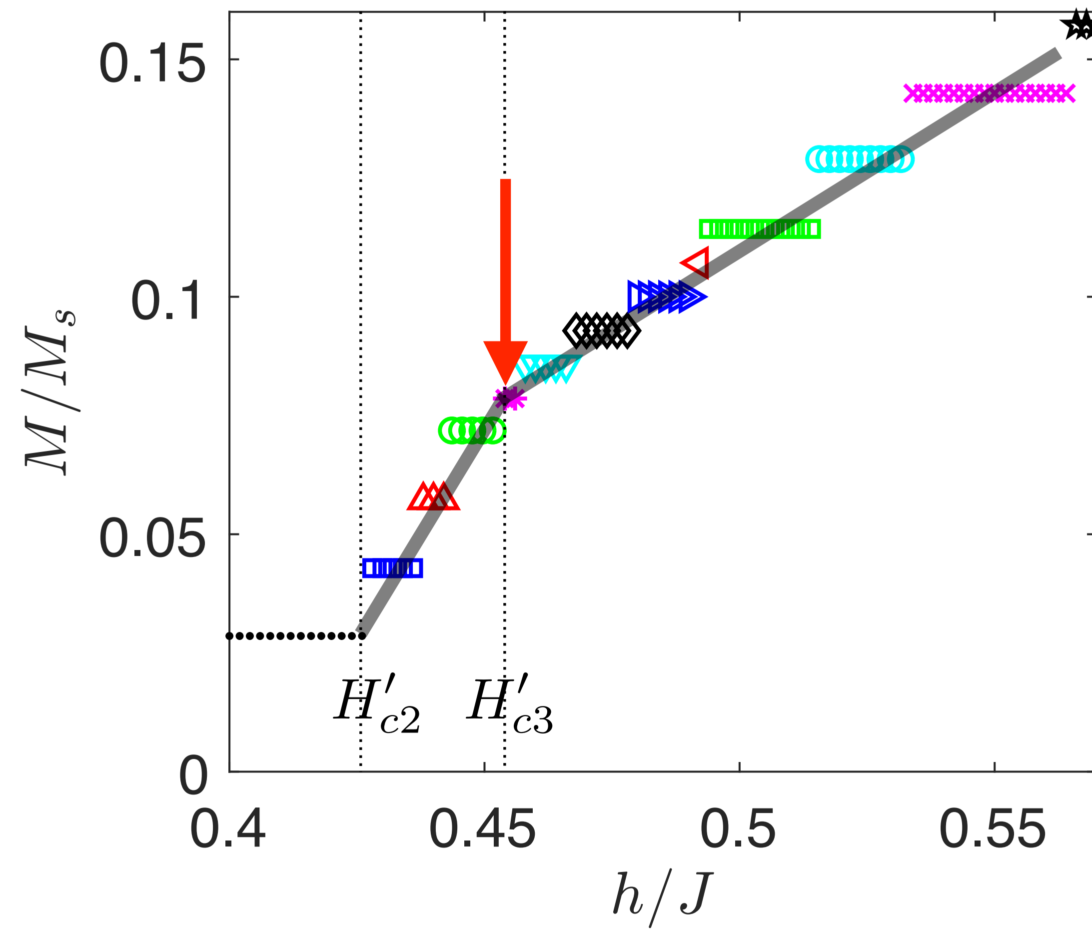
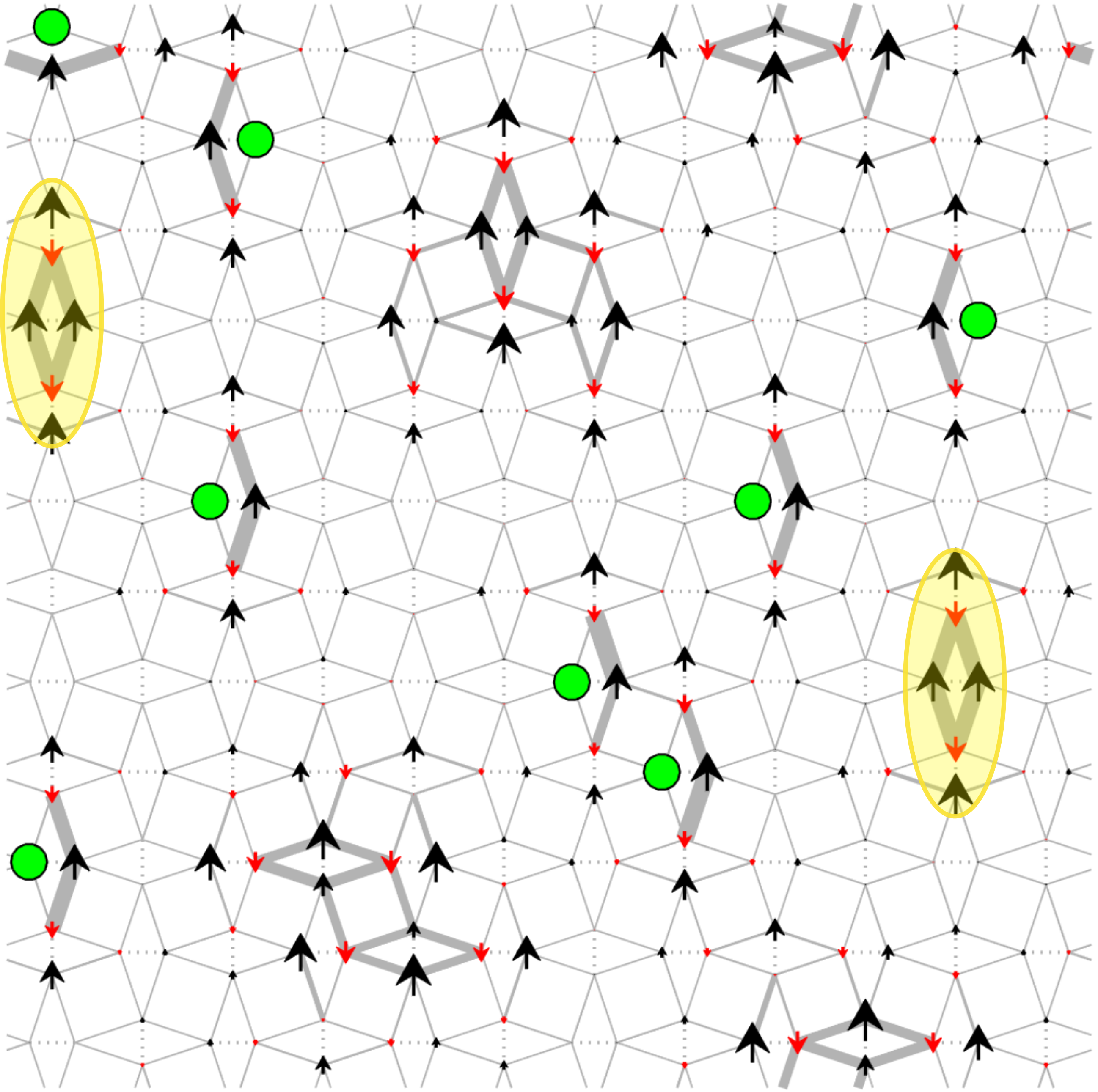


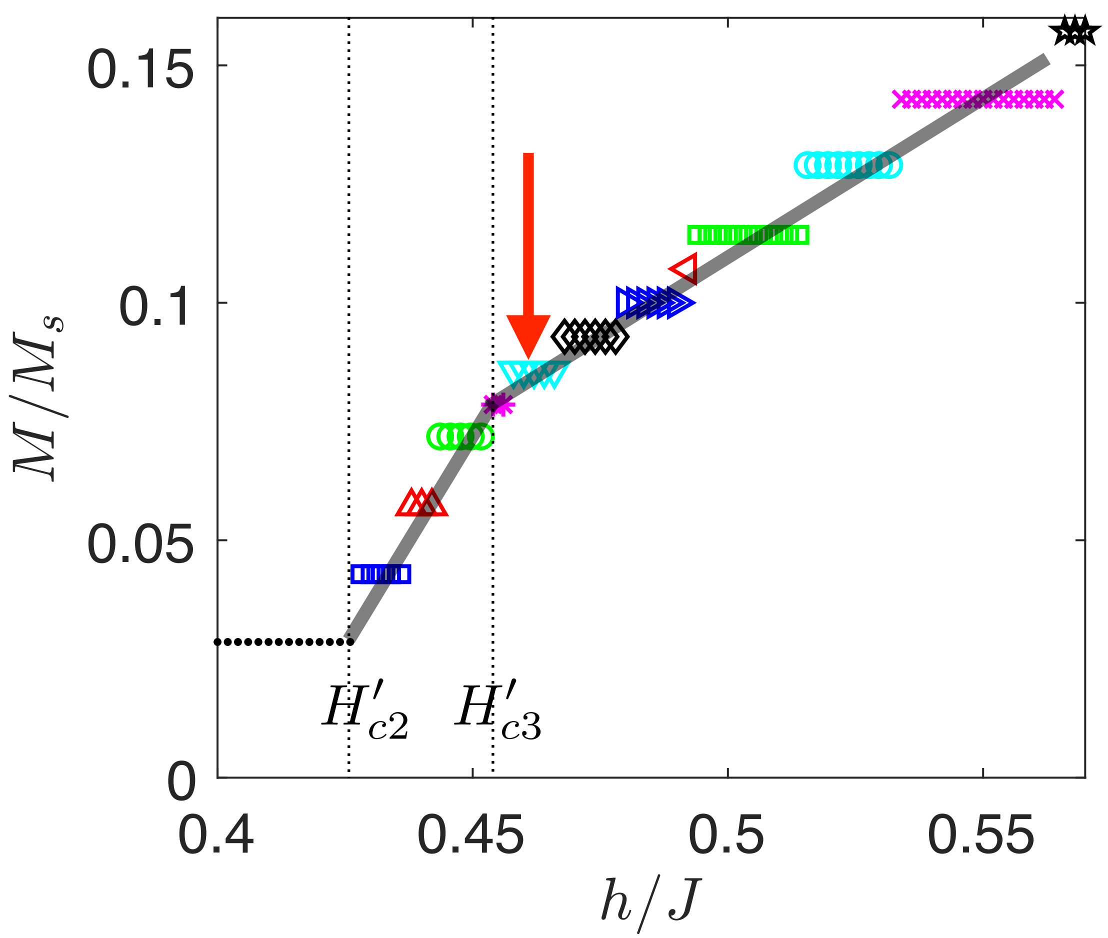


★ At $H'_{c3} \sim 23.2T$: appearance of additional triplets

Anomaly in experiment at $H'_{c3} \sim 25T$ due to change of slope

Key question 2: how does the lattice get filled?





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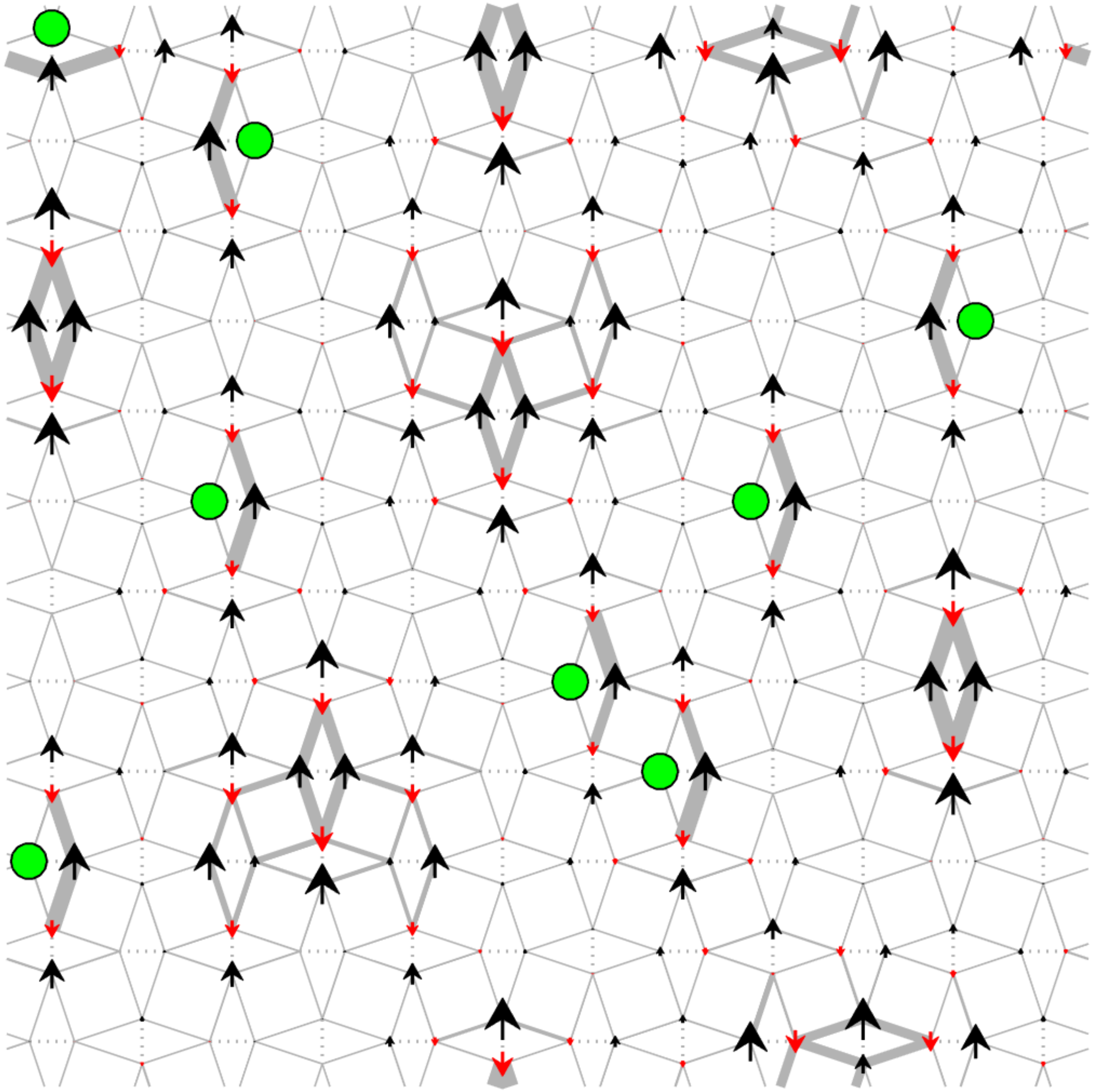

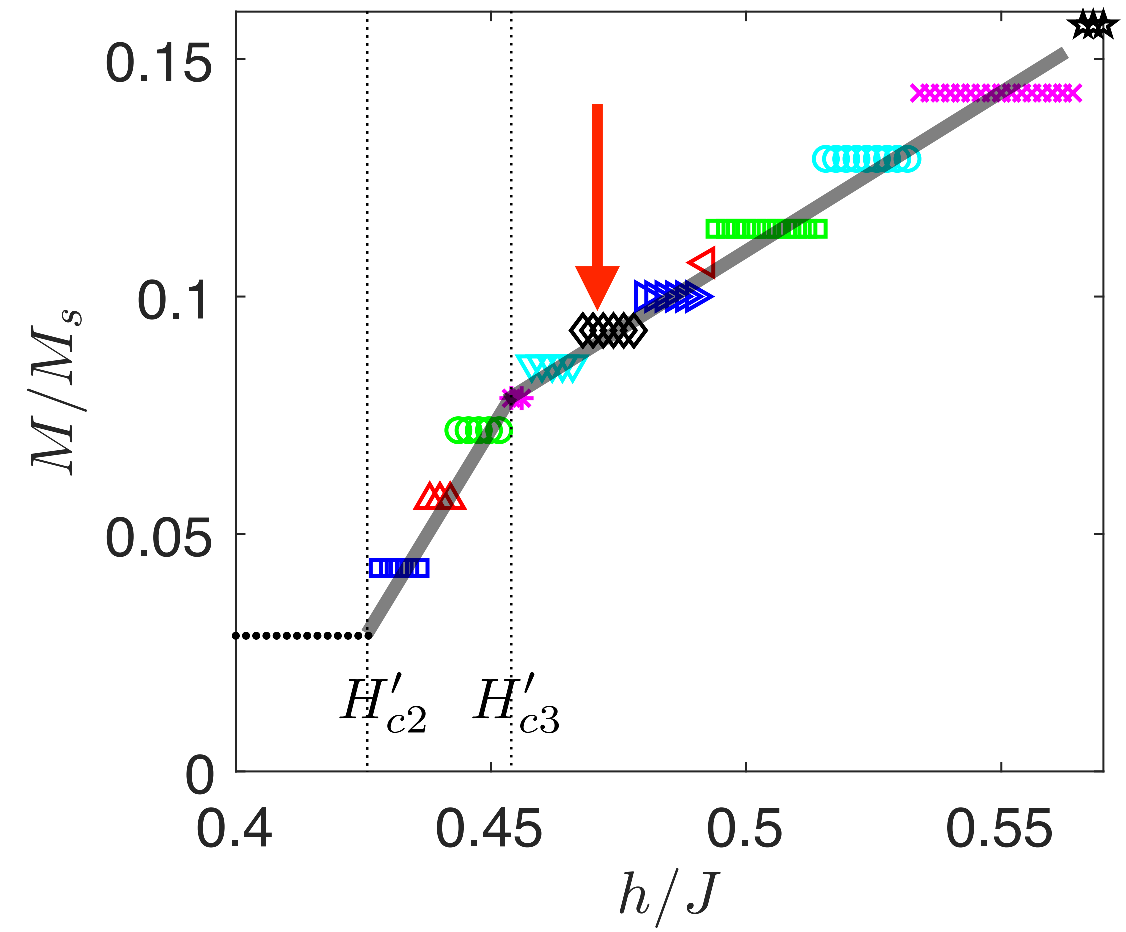

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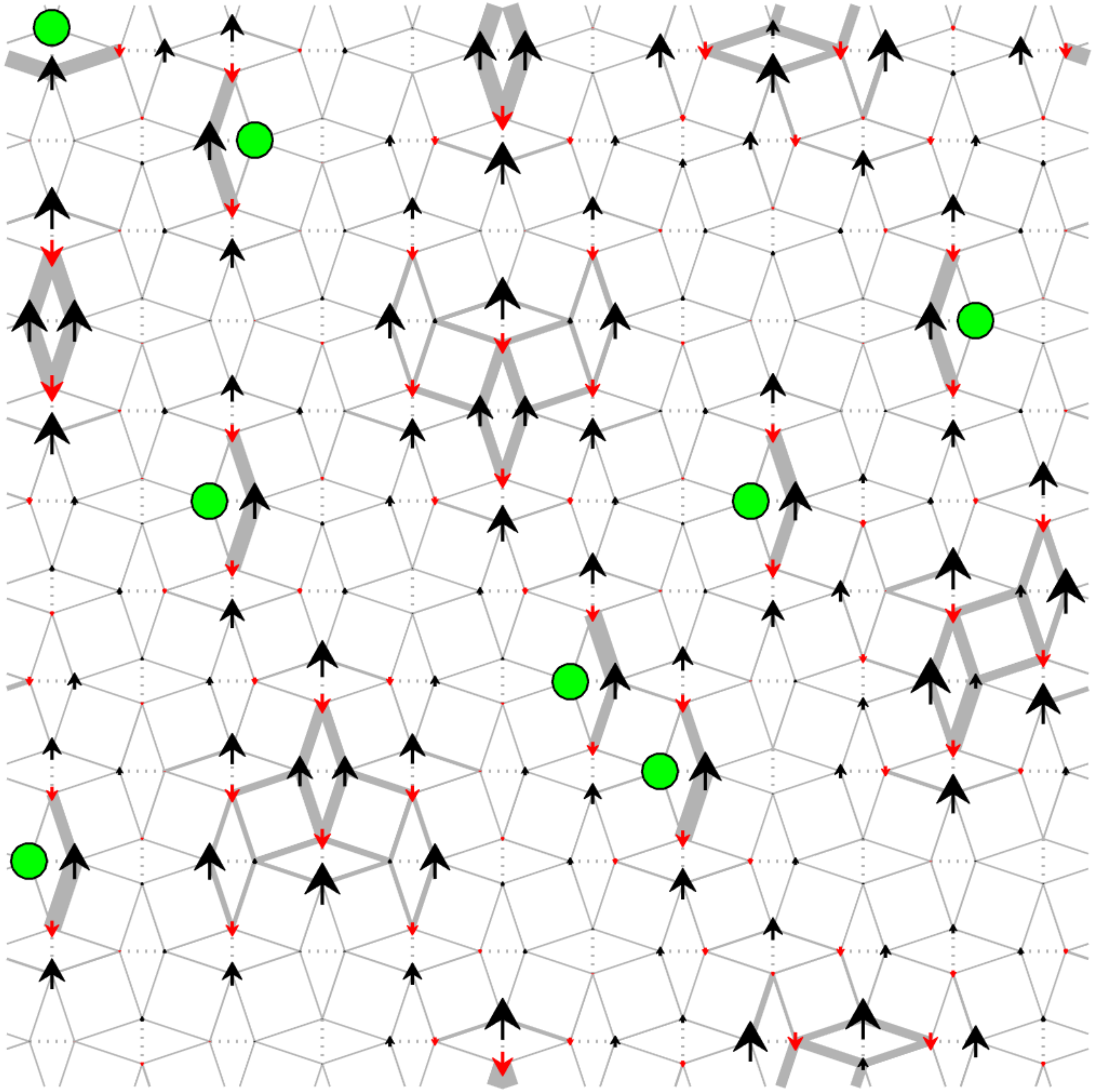

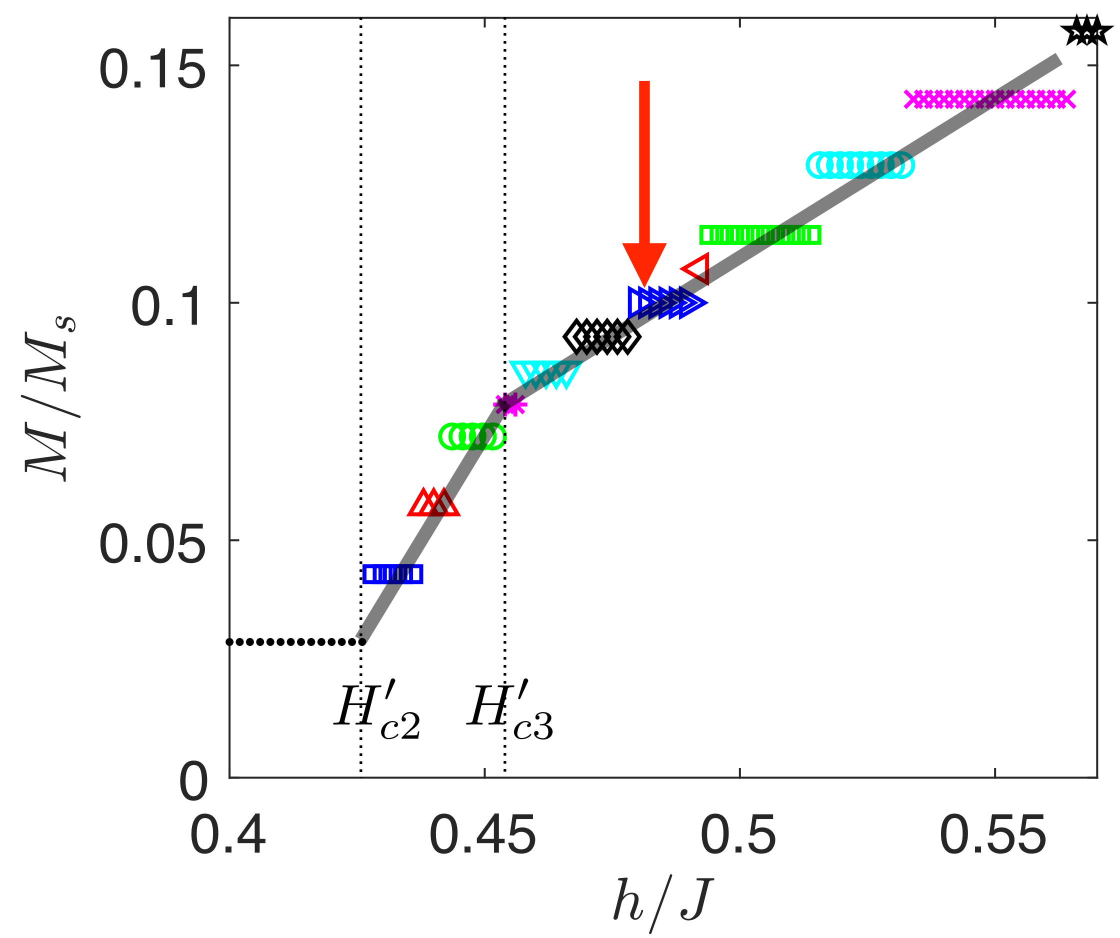

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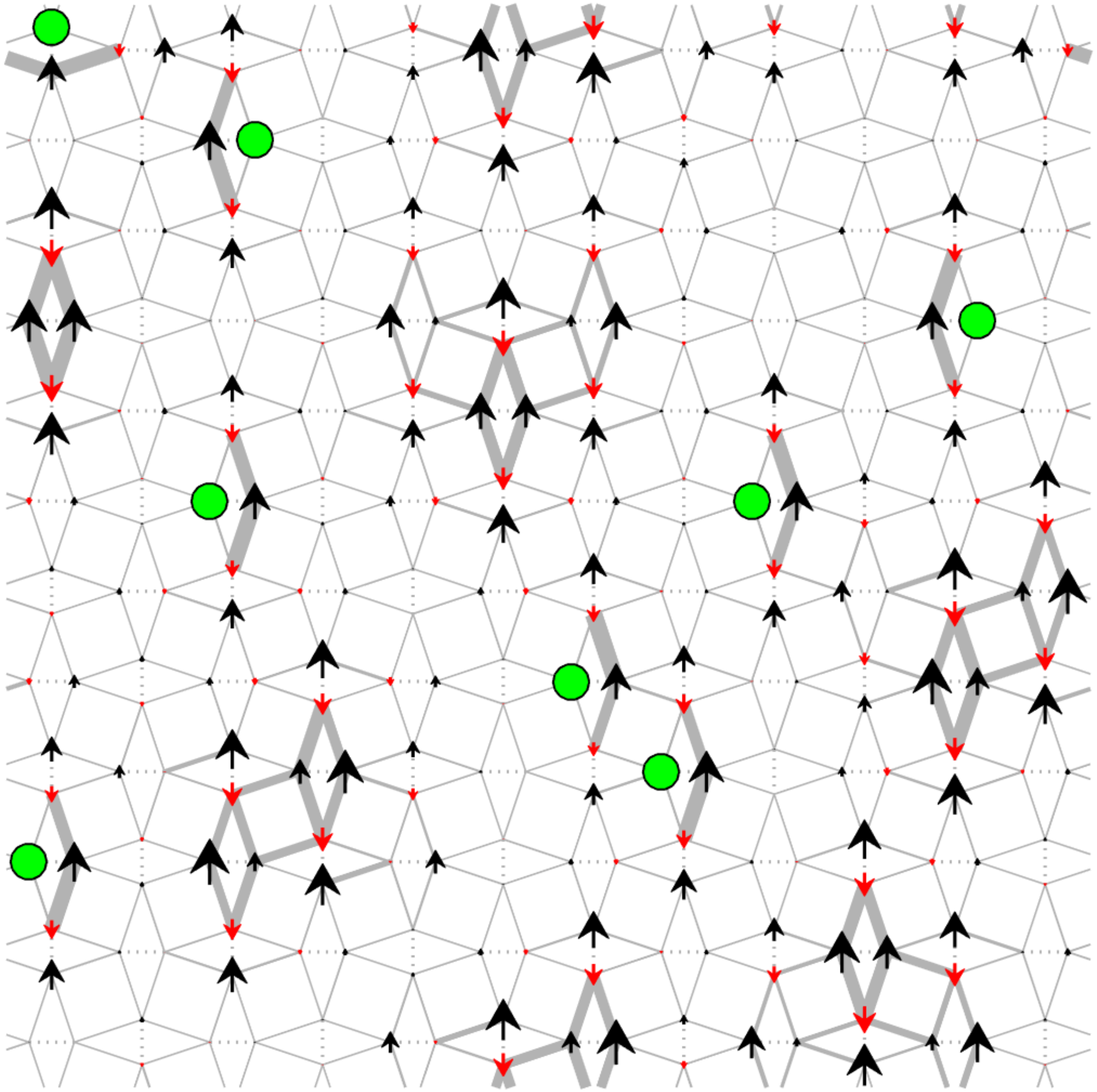

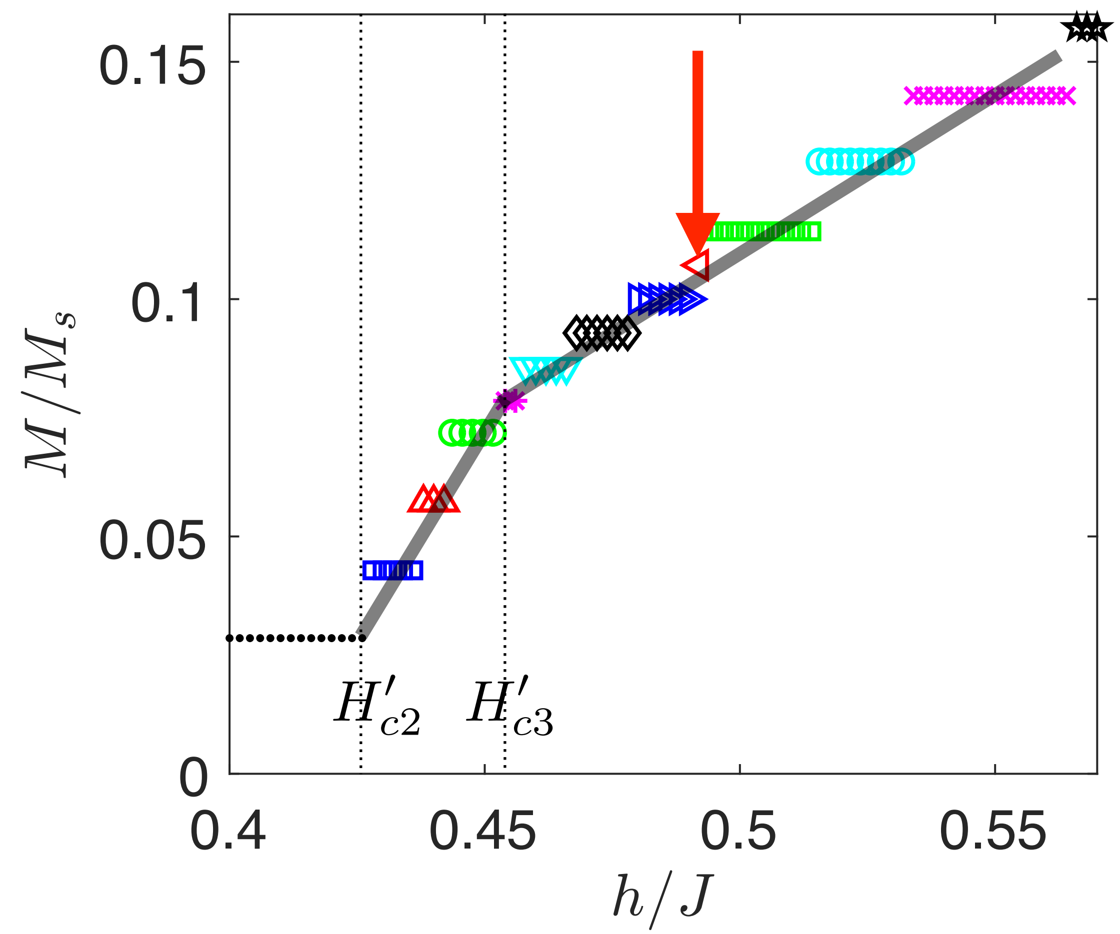

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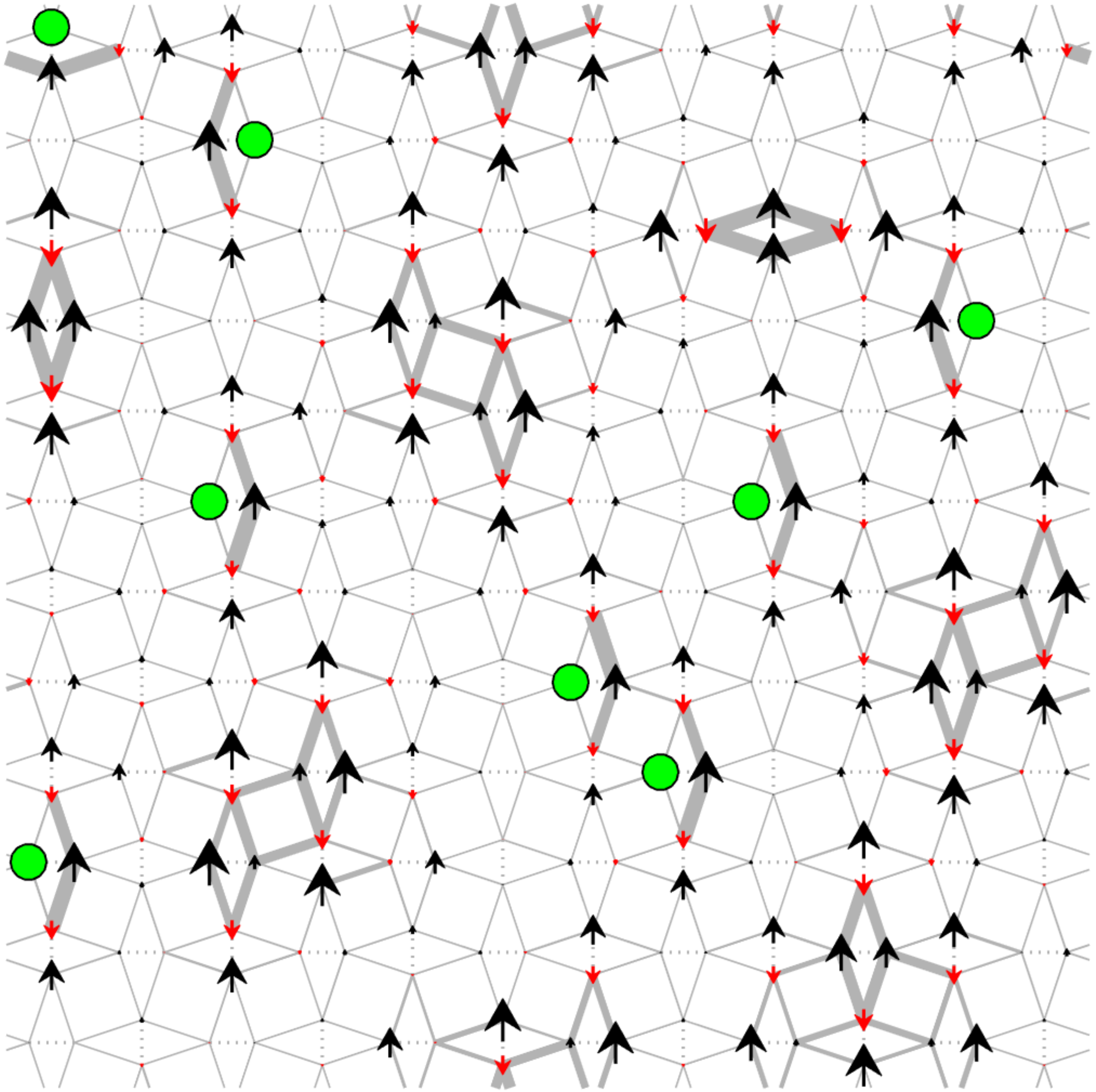

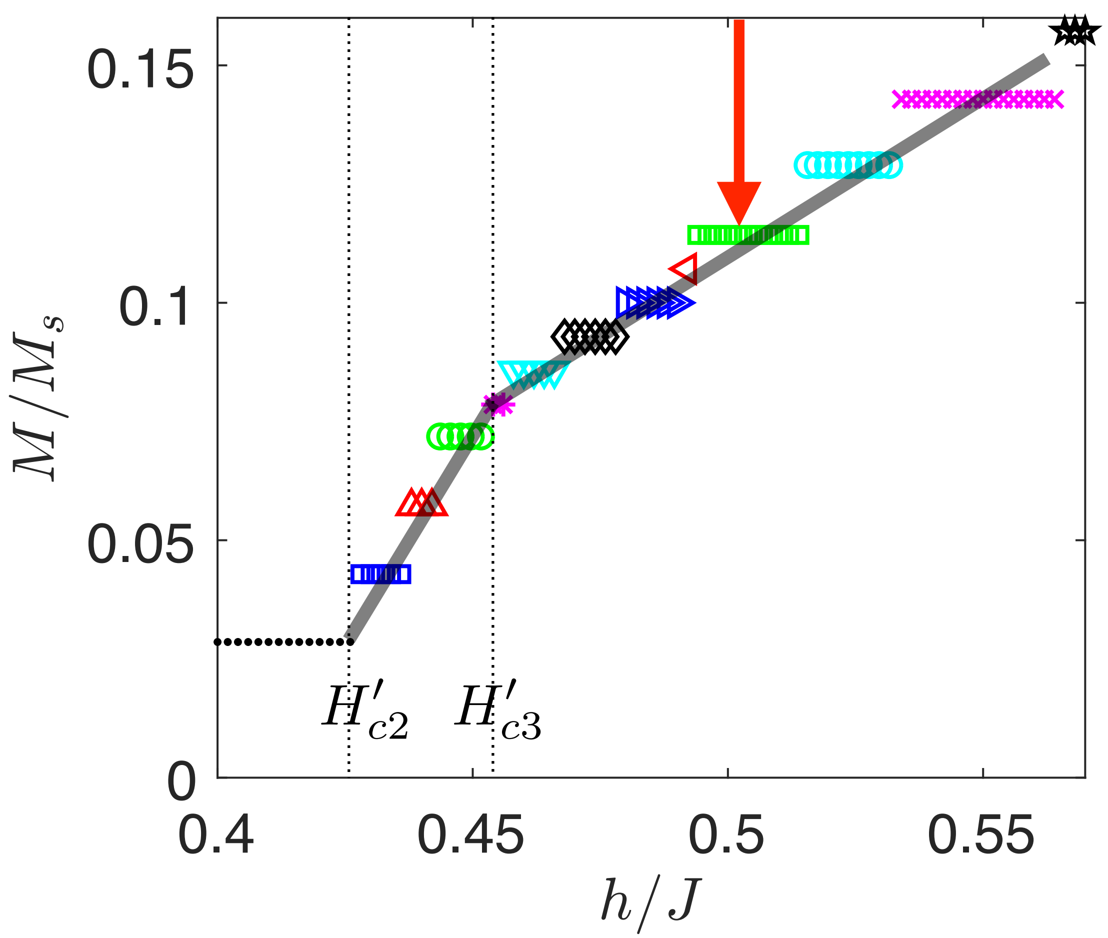

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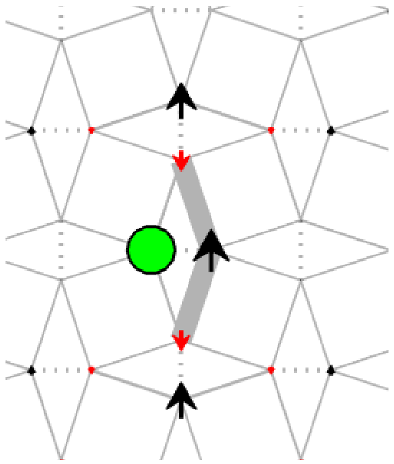

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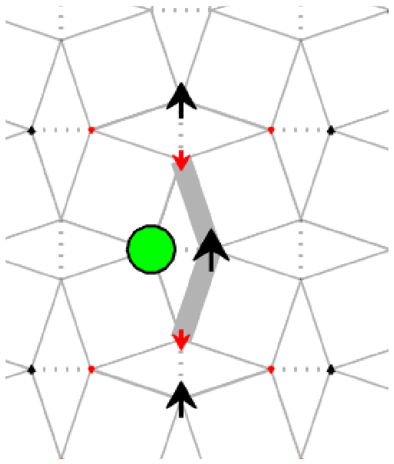

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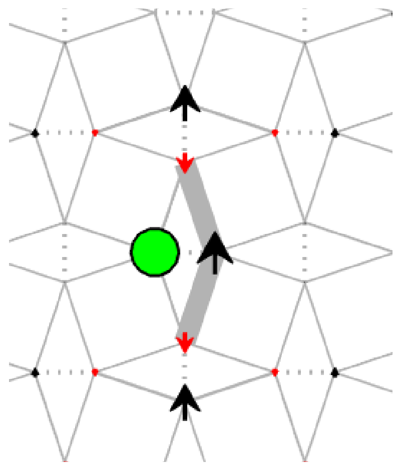

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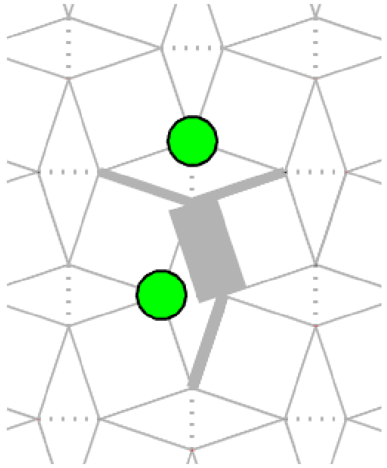

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- It takes a finite energy to excite this impurity pair configuration, i.e. only beyond a certain critical value of h

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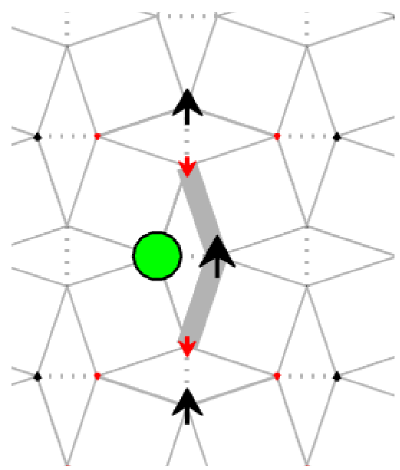

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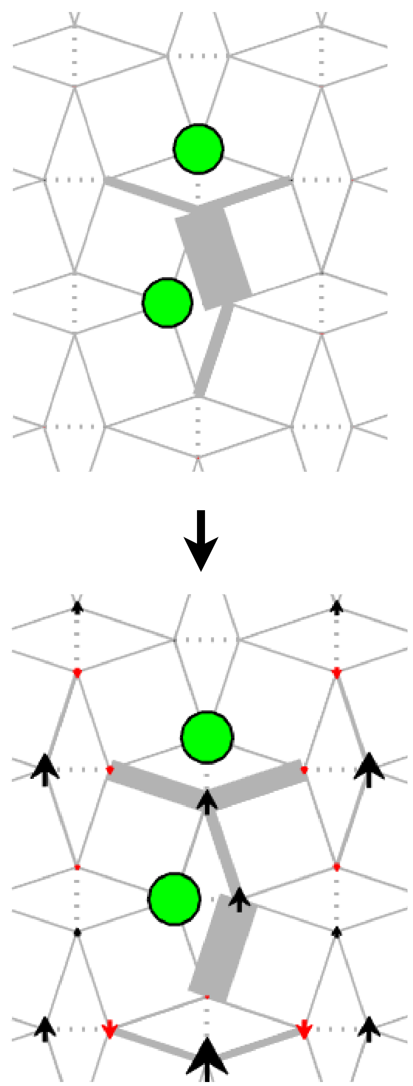

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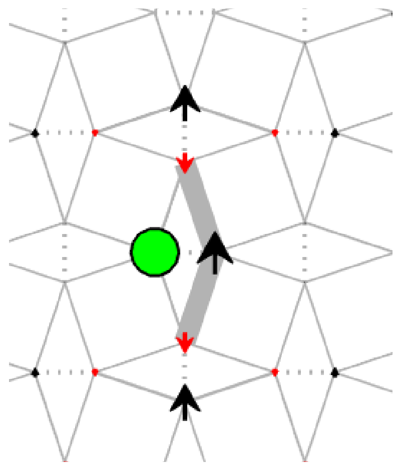

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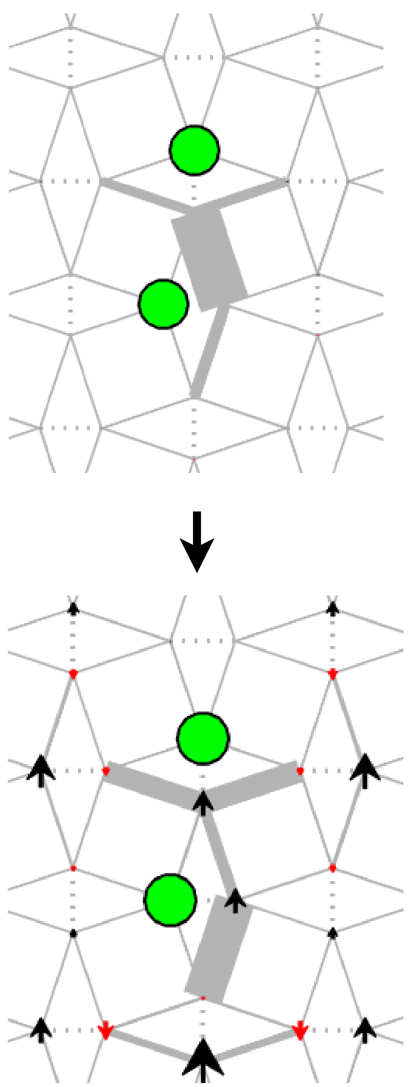

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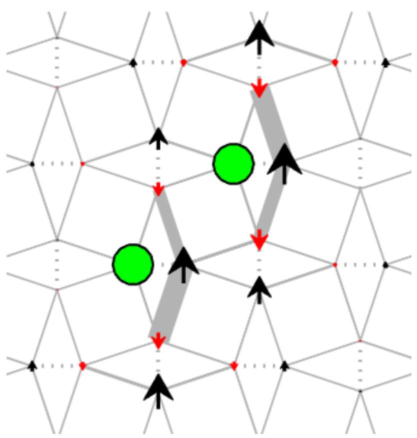
well below H'_{C2}!

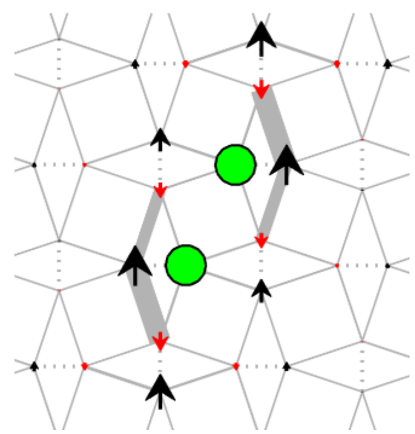
★ Lower than experimental value ($H'_{C1} \sim 17.1T$),
but, additional impurities will increase theoretical value

Key question 3: what are the anomalies below H'$_{C2}$?

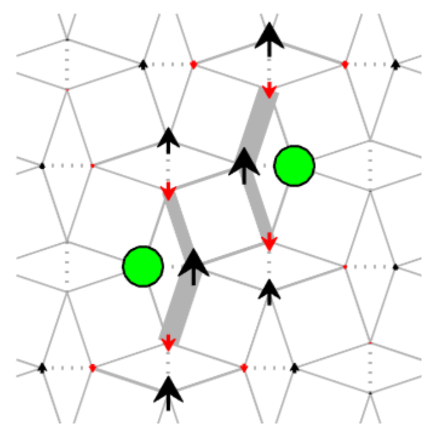
★ More 2-impurity configurations with lower excitation energies:



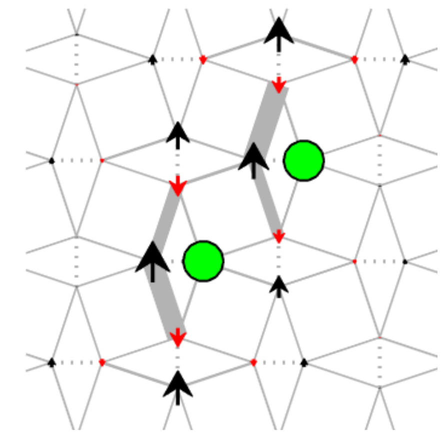
ΔE = 0.10J
(~5.1T)



ΔE = 0.012J
(~0.6T)



ΔE = 0.153J
(~7.8T)



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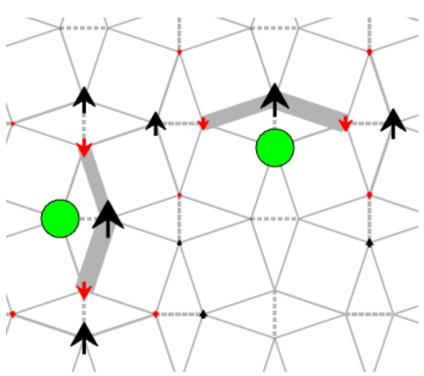
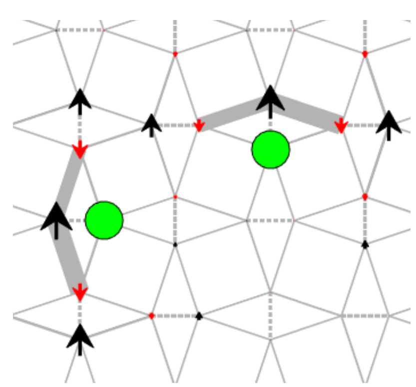
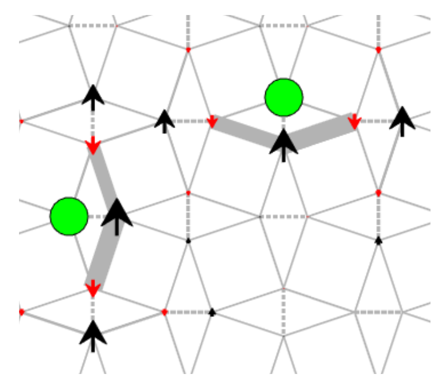


ΔE = 0.076J
(~3.86T)



ΔE = 0.064J
(~3.25T)



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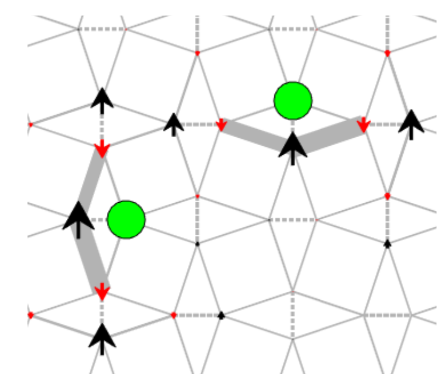

ΔE = 0.064J
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...

★ These values change in the presence of additional nearby impurities!

Summary: Mg-doped Shastry-Sutherland model

- ✓ Using large unit-cell iPEPS simulations we obtained a qualitative / semi-quantitative understanding of the novel anomalies observed in Mg-doped *$SrCu_2(BO_3)_2$*
- ✓ H'_{c0}, H'_{c1} : excitation of impurity-pair (multi-impurity) configurations
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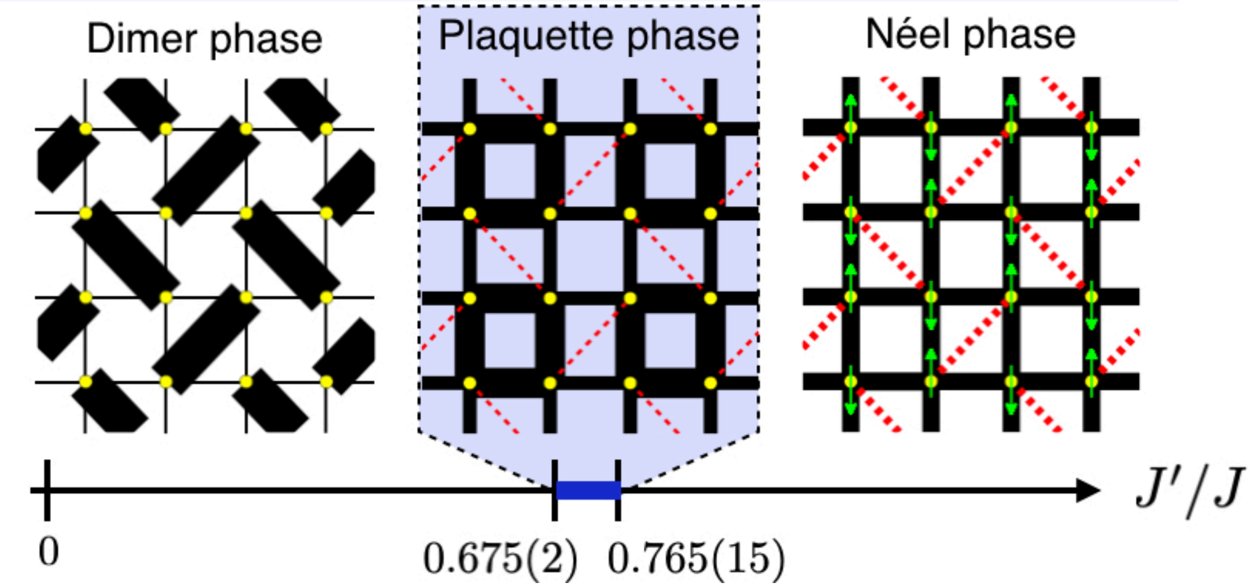
- ✓ *Room for improvement:*
  larger unit cells, taking disorder averages, more accurate model, …

$SrCu_2(BO_3)_2$ under pressure

- Applying pressure: *change ratio of J'/J*

$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$



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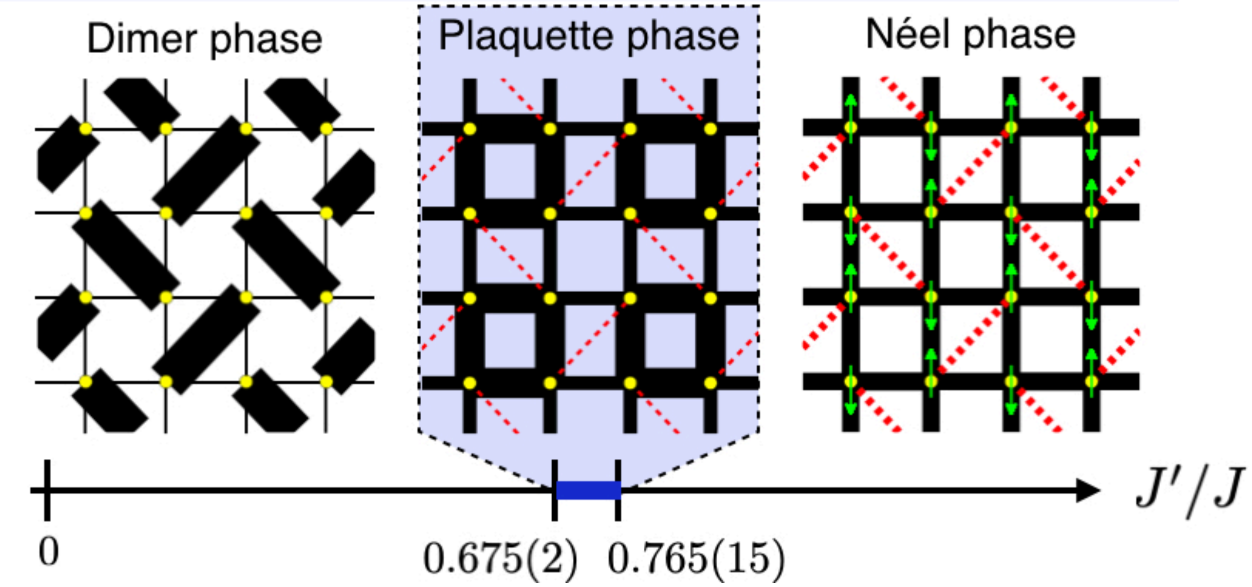
- Experiments:
  Phase transition into a gapped phase around ~1.7 GPa



Waki, et al. J. Phys. Soc. Jpn. 76, 073710 (2007).
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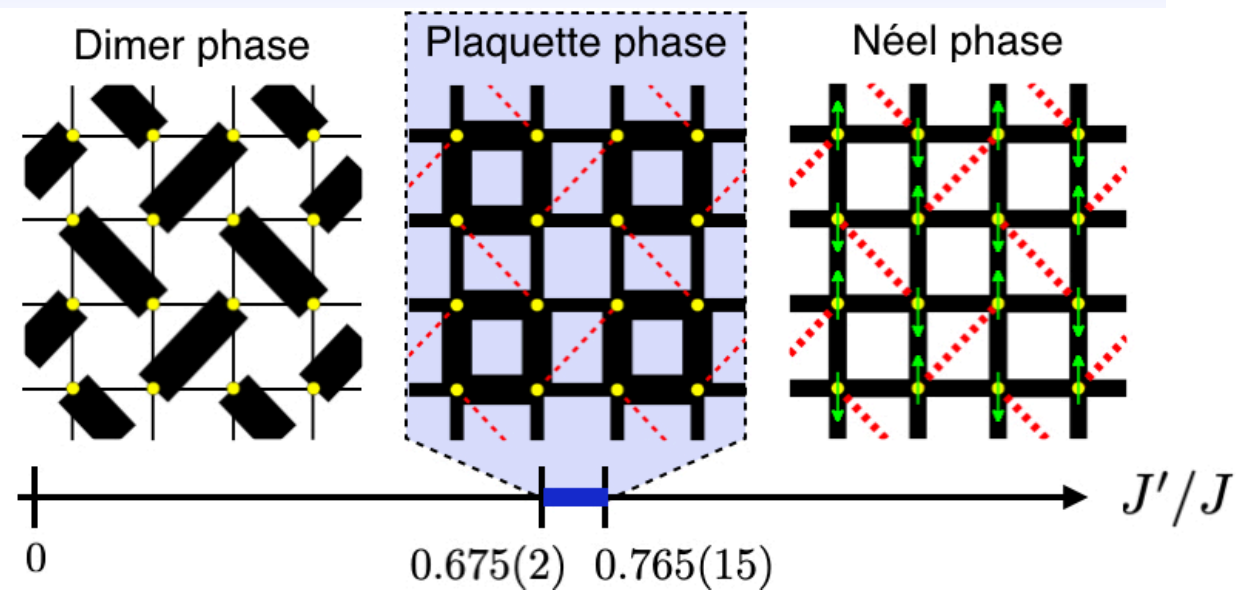
empty plaquette phase (EPP)



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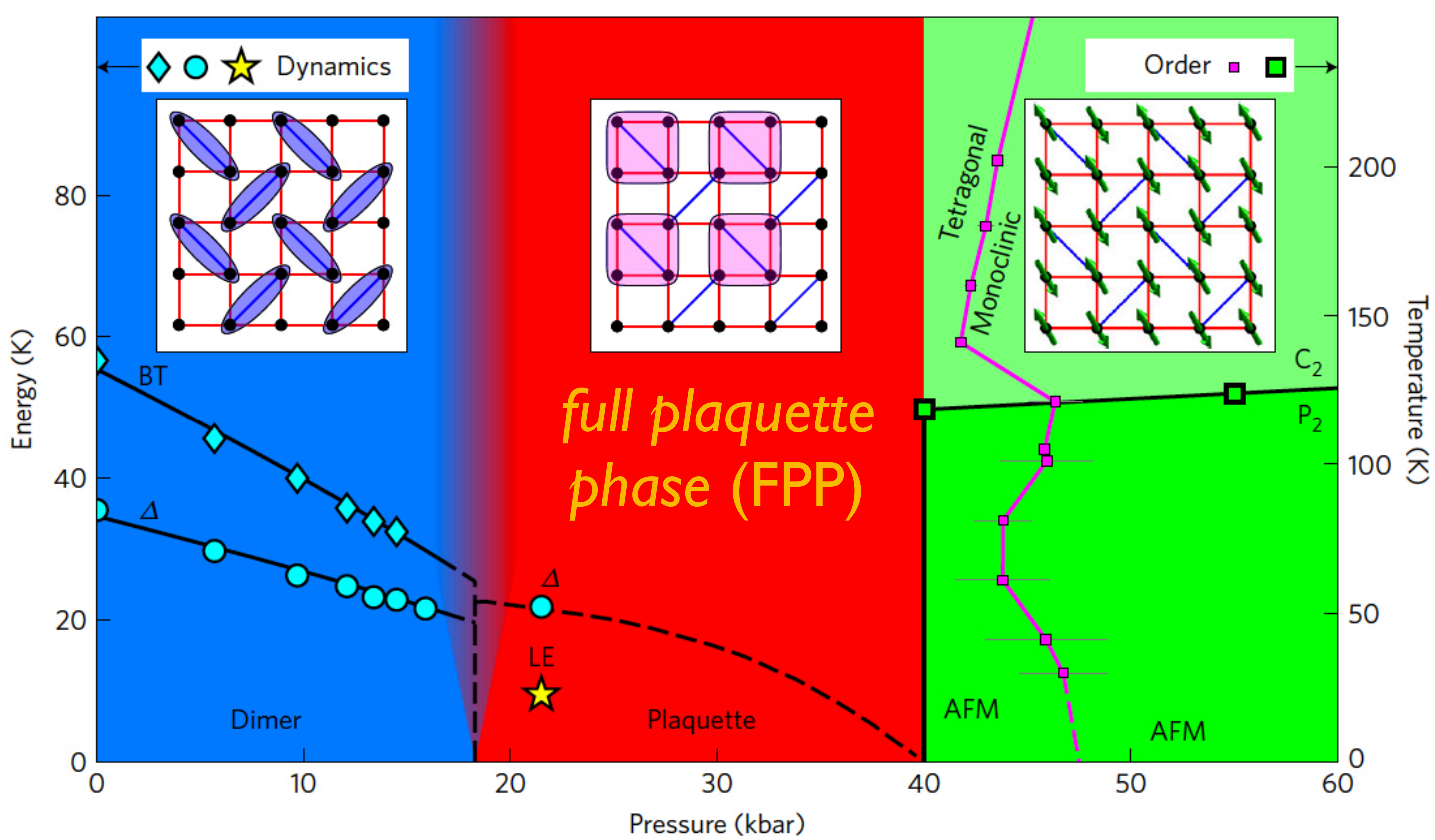

- However: data from inelastic neutron scattering experiments: *full plaquette phase* (FPP), not *empty plaquette phase* (EPP)

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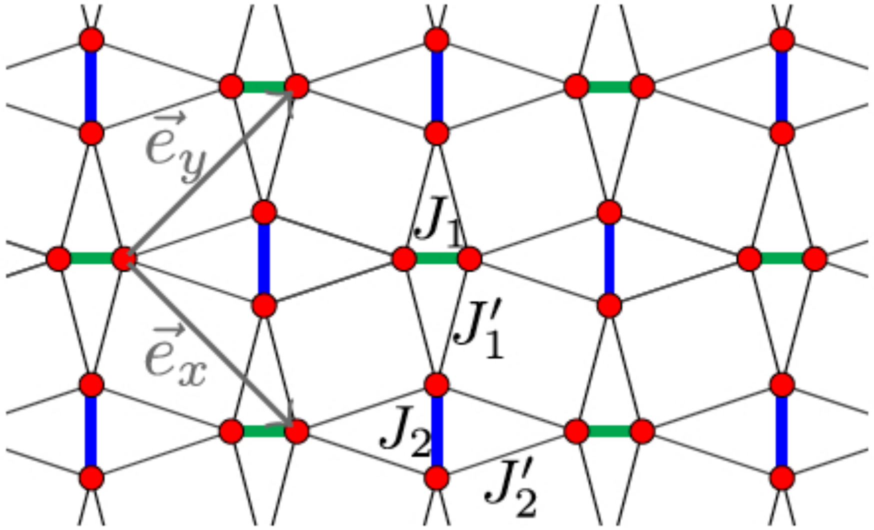
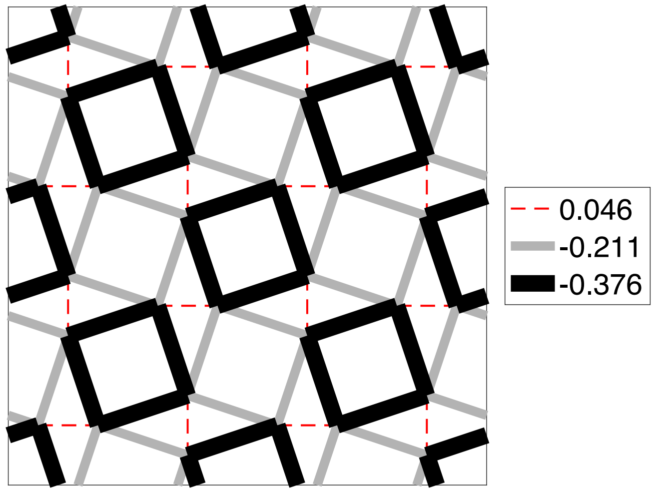
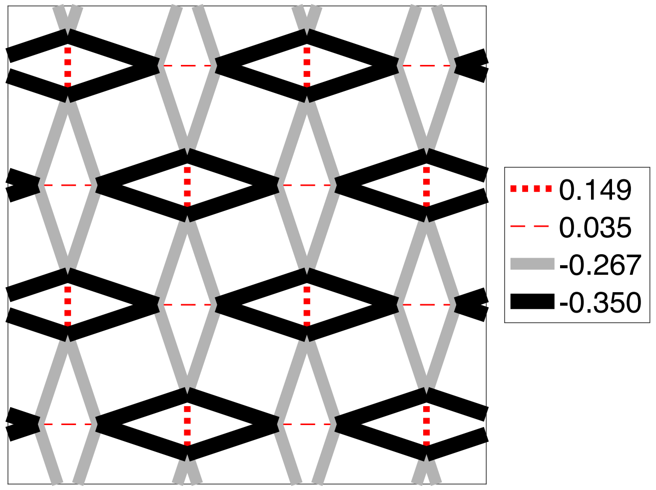
$SrCu_2(BO_3)_2$ under pressure

Boos, Crone, Niesen, PC, Schmidt & Mila, PRB 100 (2019)

- Distorted Shastry-Sutherland model: *competition between EPP and FPP phase*







EPP *vs* *FPP*

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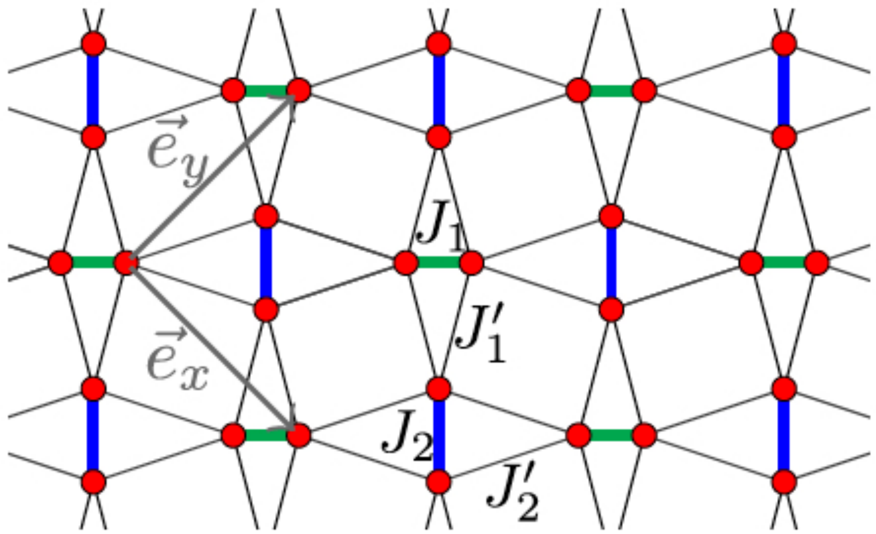

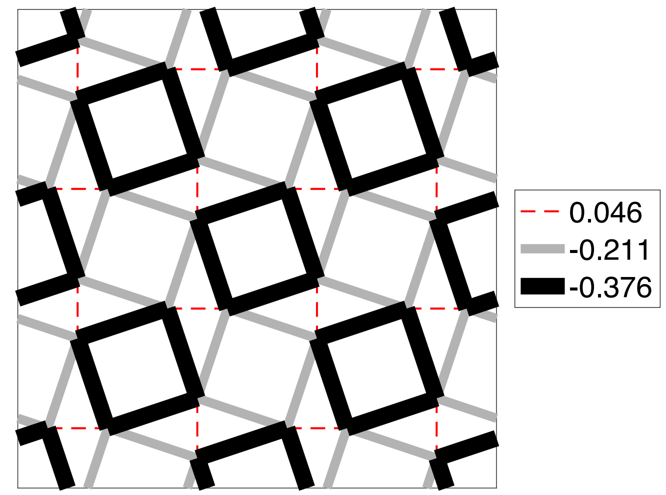

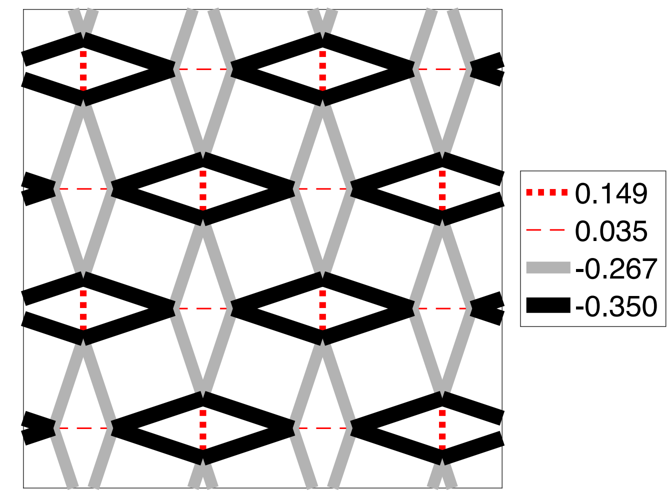

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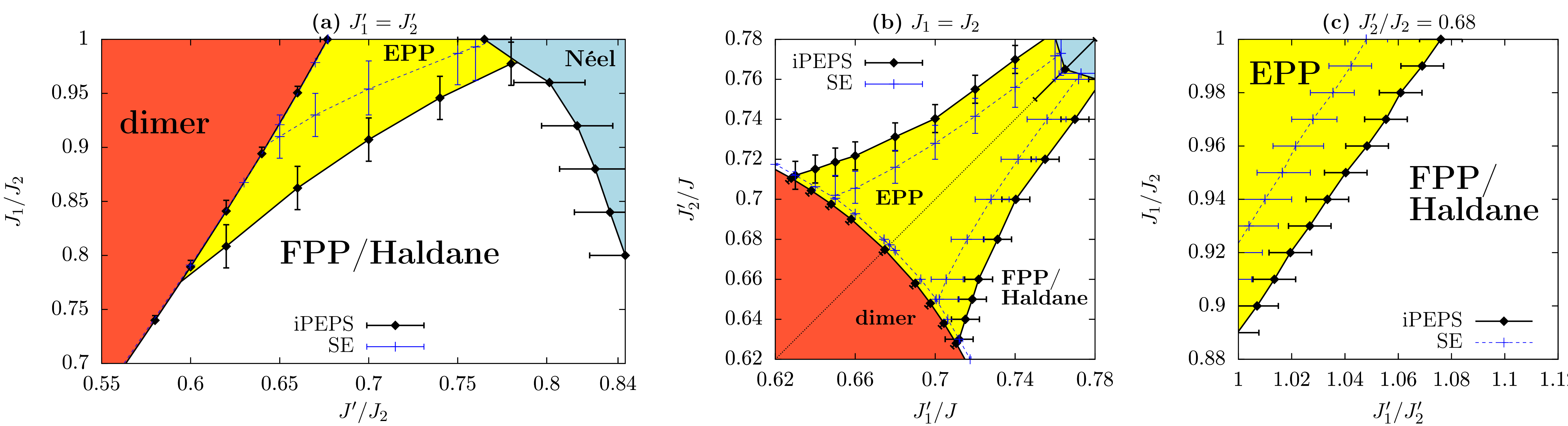

- Small deformation leads to FPP phase!

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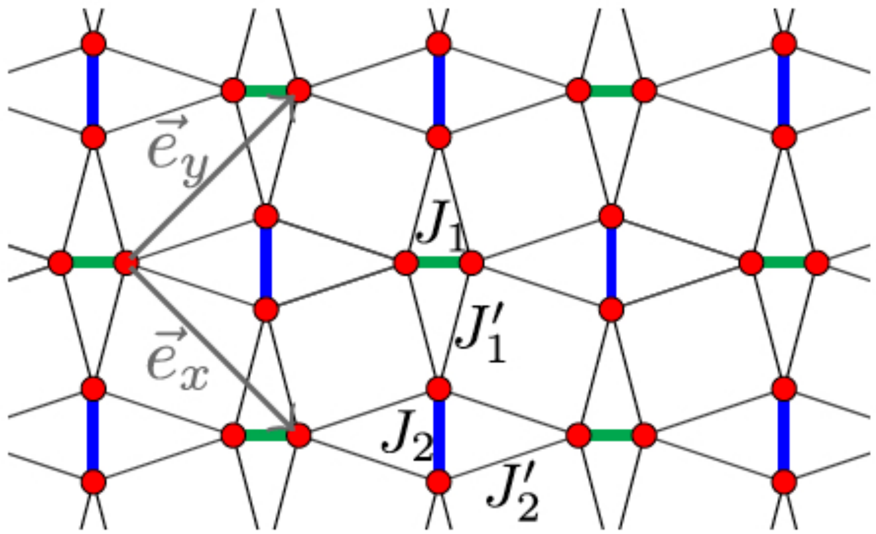

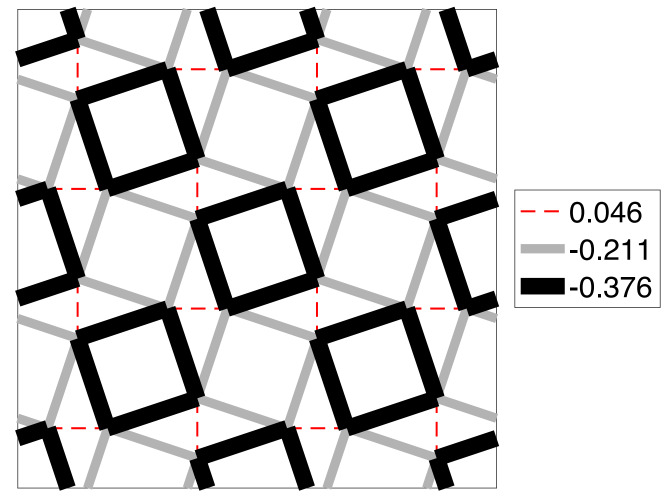

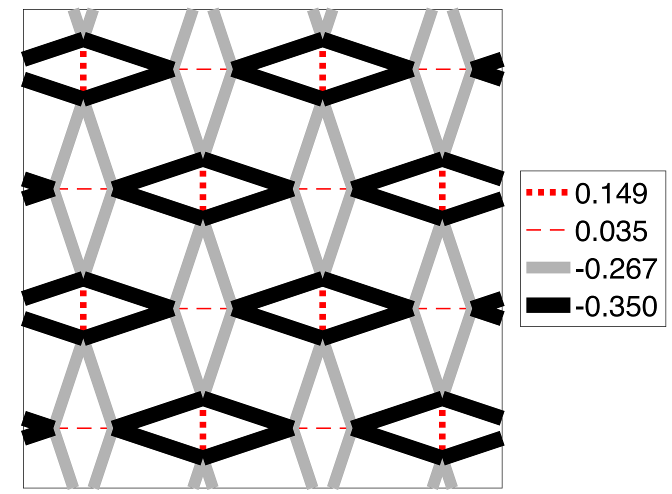

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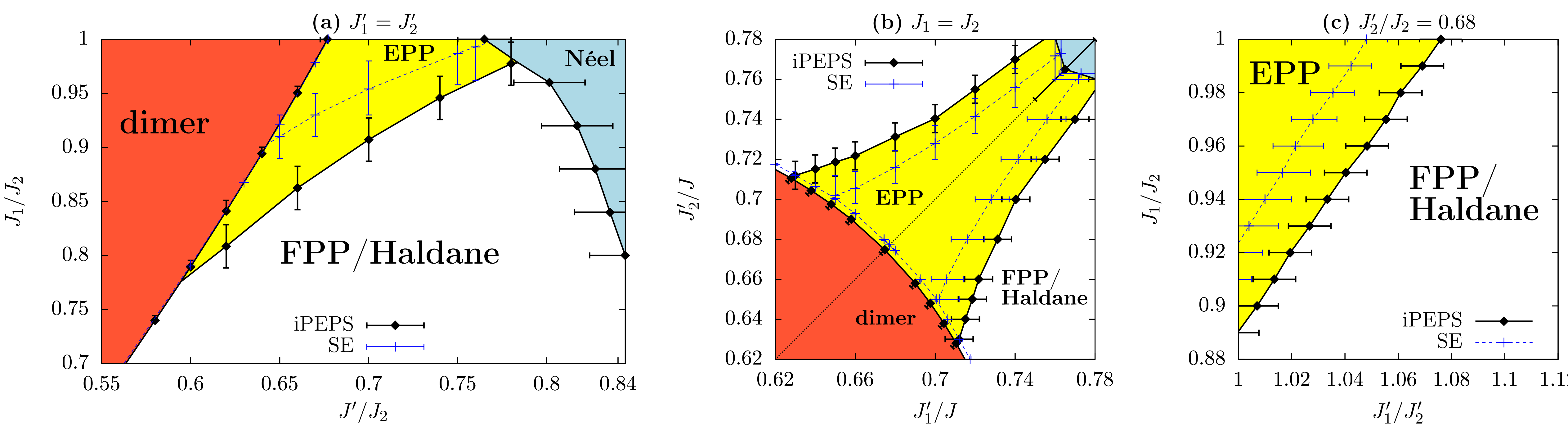

- Small deformation leads to FPP phase! *But precise model still unclear…*

Finite temperature simulations with iPEPS

- Methodological developments: P. Czarnik, J. Dziarmaga, PC, PRB 99 (2019)
  [see also Li et al. PRL 106 (2011); Czarnik et al. PRB 86 (2012); Xie et al., PRB 86 (2012); Czarnik & Dziarmaga PRB 90 (2014); PRB 92 (2015); Czarnik et al. PRB 94 (2016), Dai et al PRB 95 (2017); Kshetrimayum, Rizzi, Eisert, Orus, PRL 122 (2019)]

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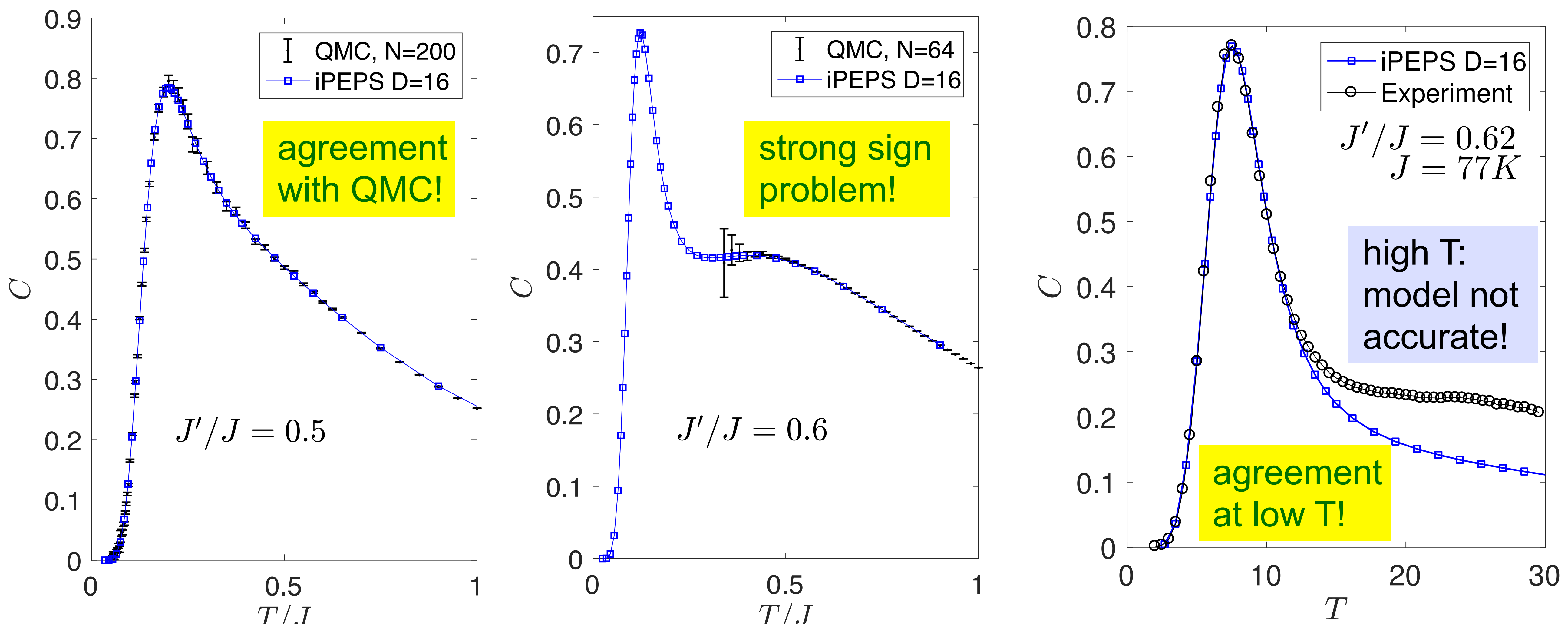

Miyahara & Ueda, cond-mat/0004260

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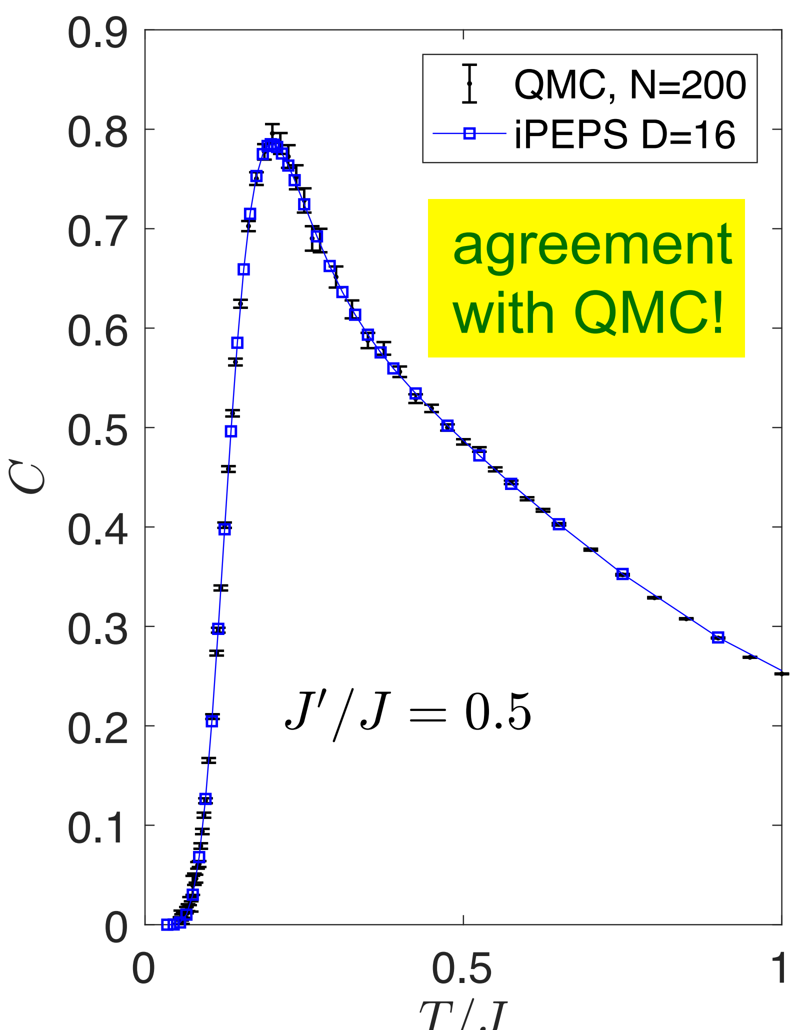
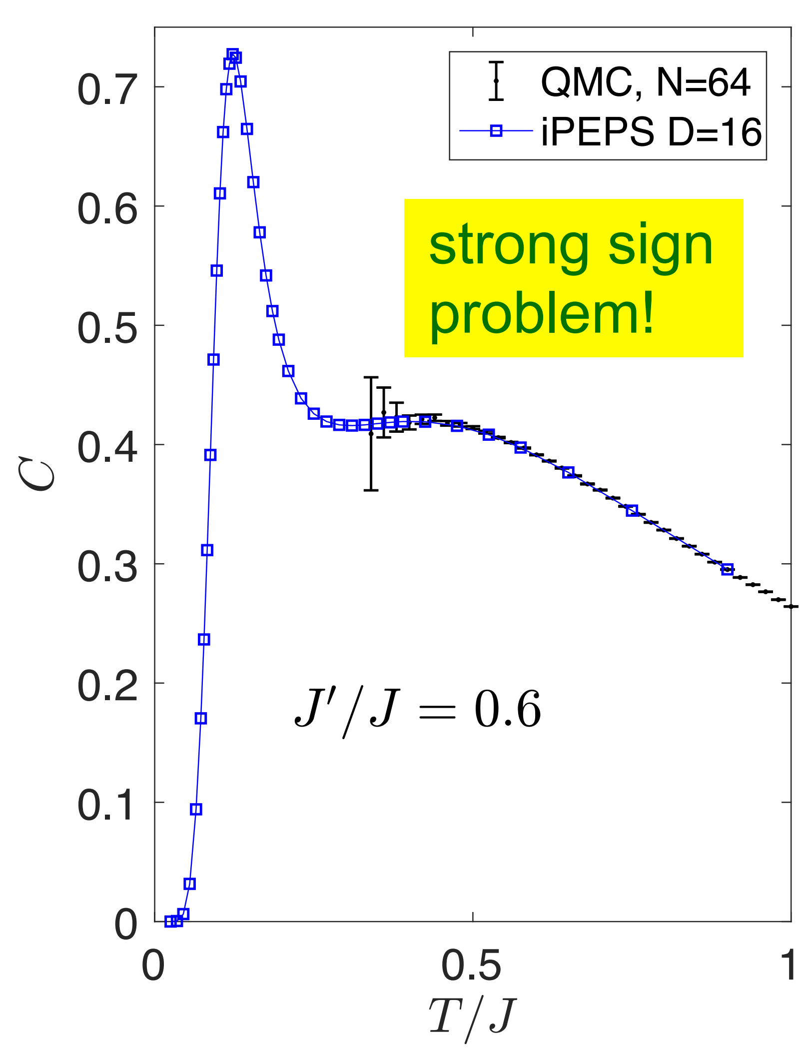
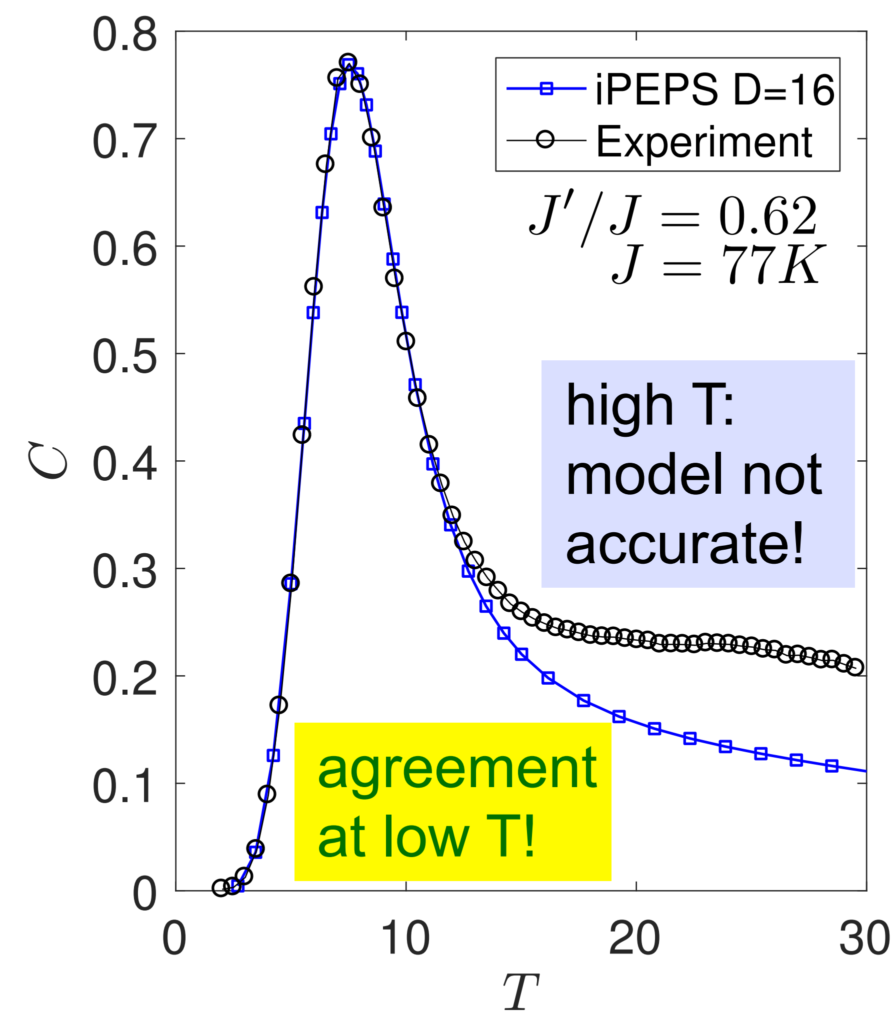






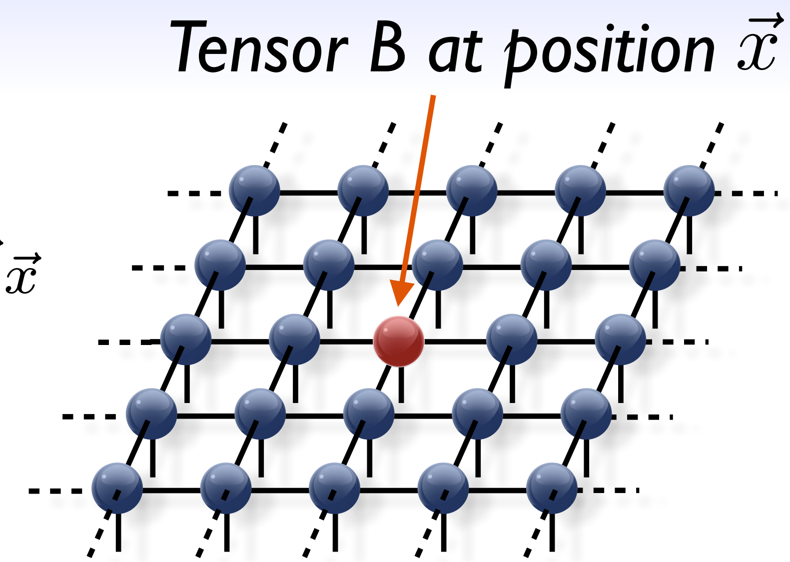
Miyahara & Ueda, cond-mat/0004260

Finite T study of SCBO under pressure (in progress)

iPEPS excitation ansatz

- Excitation on top of ground state with momentum k

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$



Haegeman, et al, PRB 85 (2012); Haegeman, et al, PRL 111 (2013).
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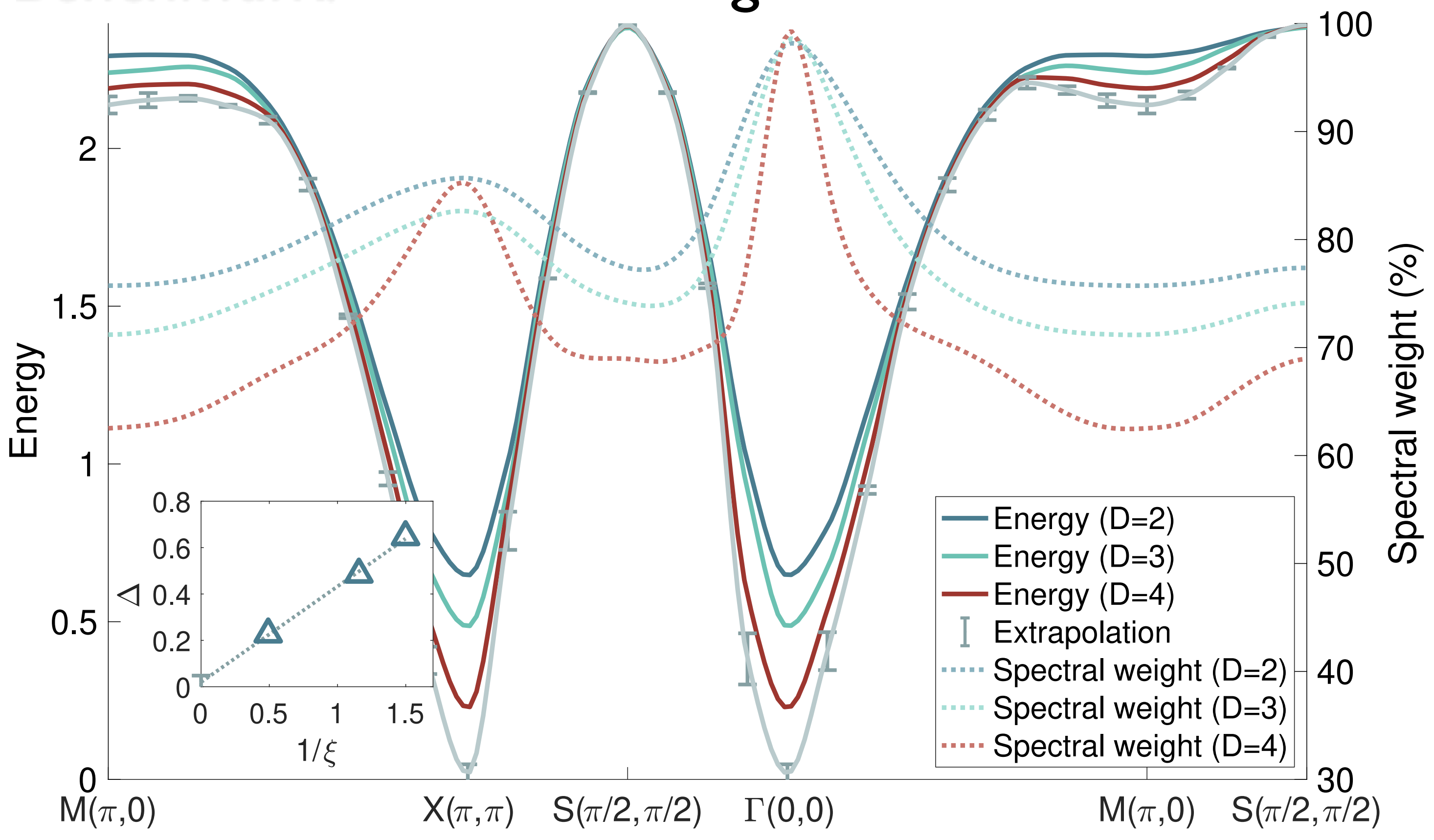

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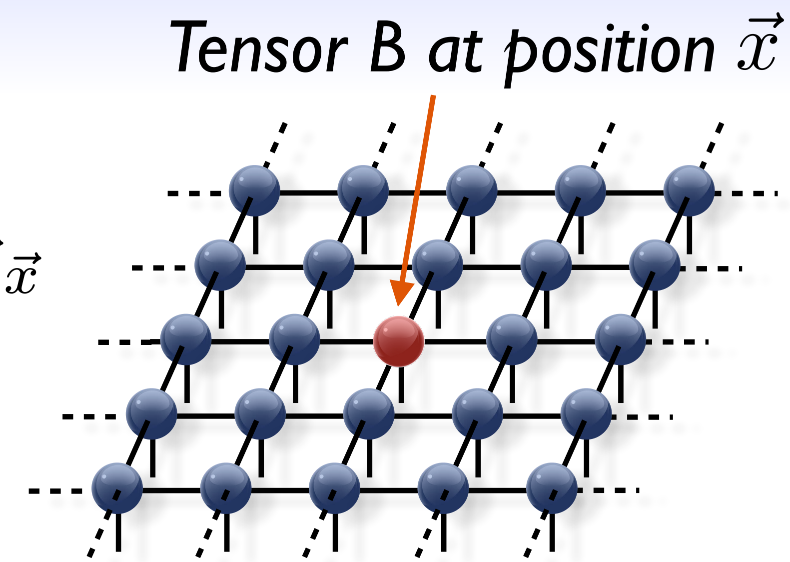

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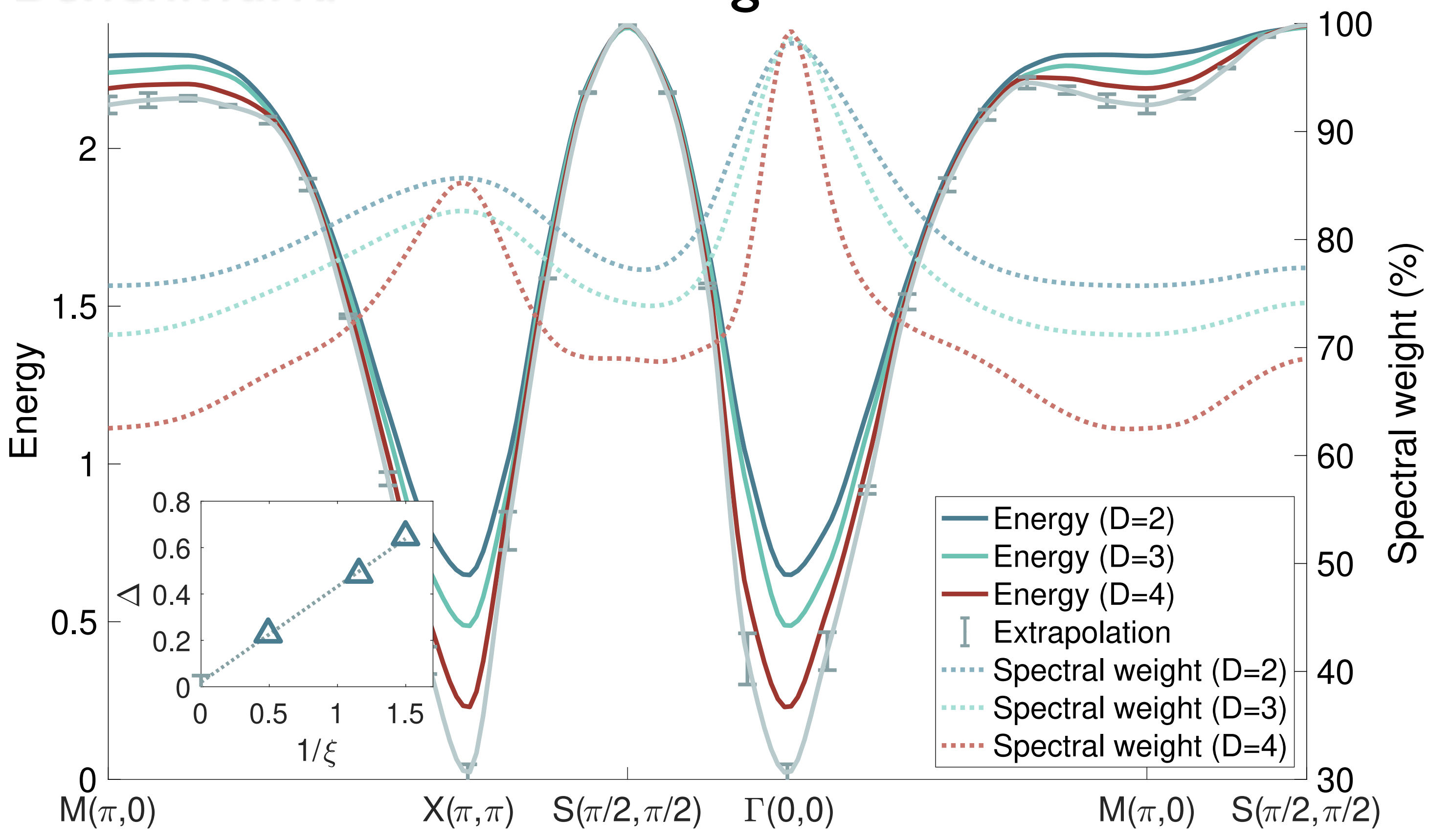

Study of excitations in EPP / FPP phase (work in progress)

Summary & outlook

✓ iPEPS: many new insights into the physics of $SrCu_2(BO_3)_2$

- ★ New understanding of the magnetization process at low magnetic fields
- ★ Supersolid phases at high magnetic fields
- ★ Nature of the new anomalies in the Mg-doped case
- ★ Competition of plaquette phases in the extended Shastry-Sutherland model

- Future/ongoing work:
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  - Study of excitations in EPP / FPP phase
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Thank you for your attention!

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F. Mila, S. Haravifard, S. Crone, I. Niesen, B. Ponsioen, Z. Shi, W. Steinhardt, D. Graf, F. Weickert, N. Harrison, M. Jaime, C. Marjerrison, H. A. Dabkowska, Y. H. Matsuda, N. Abe, S. Takeyama, H. Kageyama, A. Honecker, S. Manmana, G. Foltin, K. Schmidt, A. Wietek, S. Wessel, B. Normand

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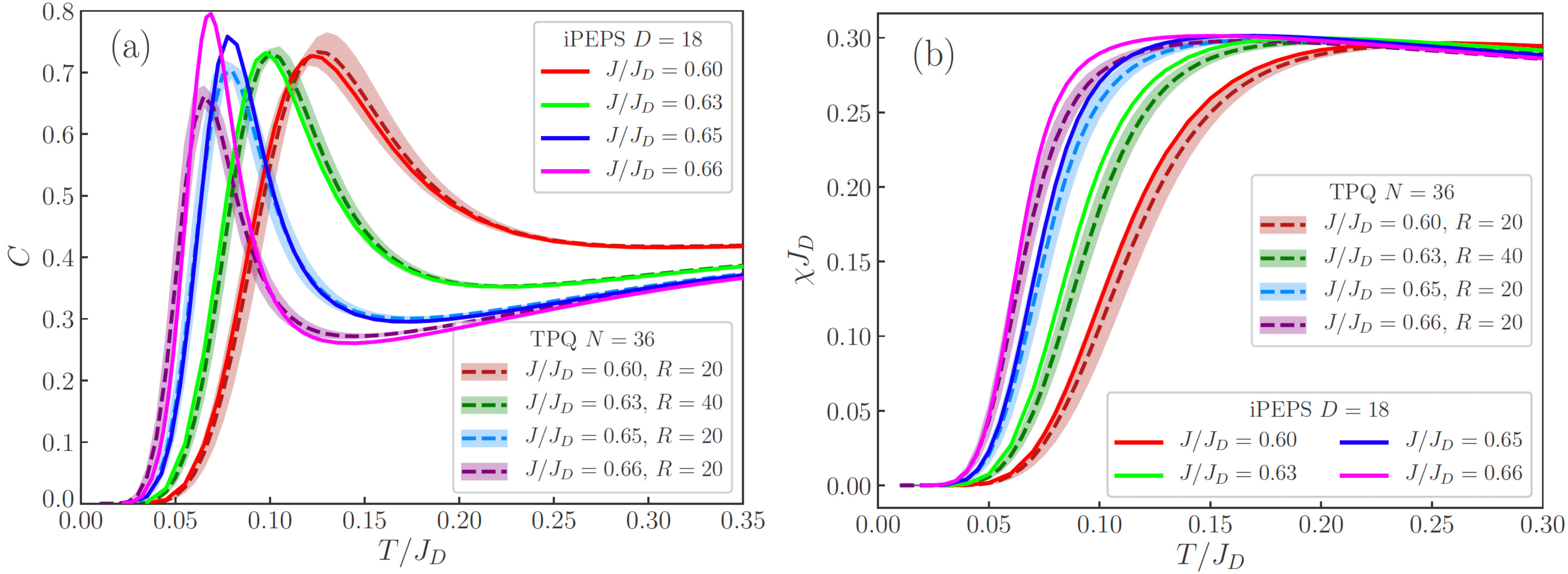
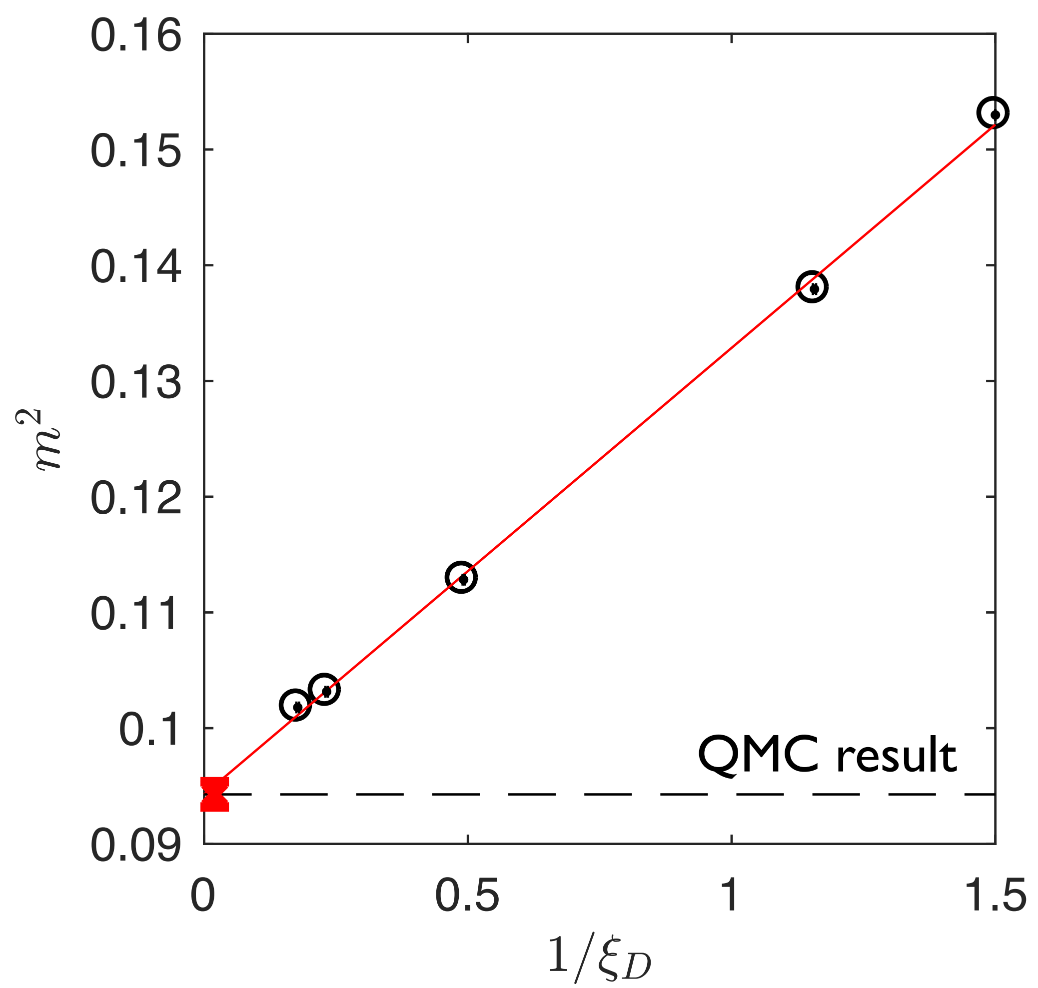


(a)
iPEPS $D = 18$
$J/J_D = 0.60$
$J/J_D = 0.63$
$J/J_D = 0.65$
$J/J_D = 0.66$
TPQ $N = 36$
$J/J_D = 0.60$, $R = 20$
$J/J_D = 0.63$, $R = 40$
$J/J_D = 0.65$, $R = 20$
$J/J_D = 0.66$, $R = 20$
C
T/J_D
(b)
χJ_D
T/J_D

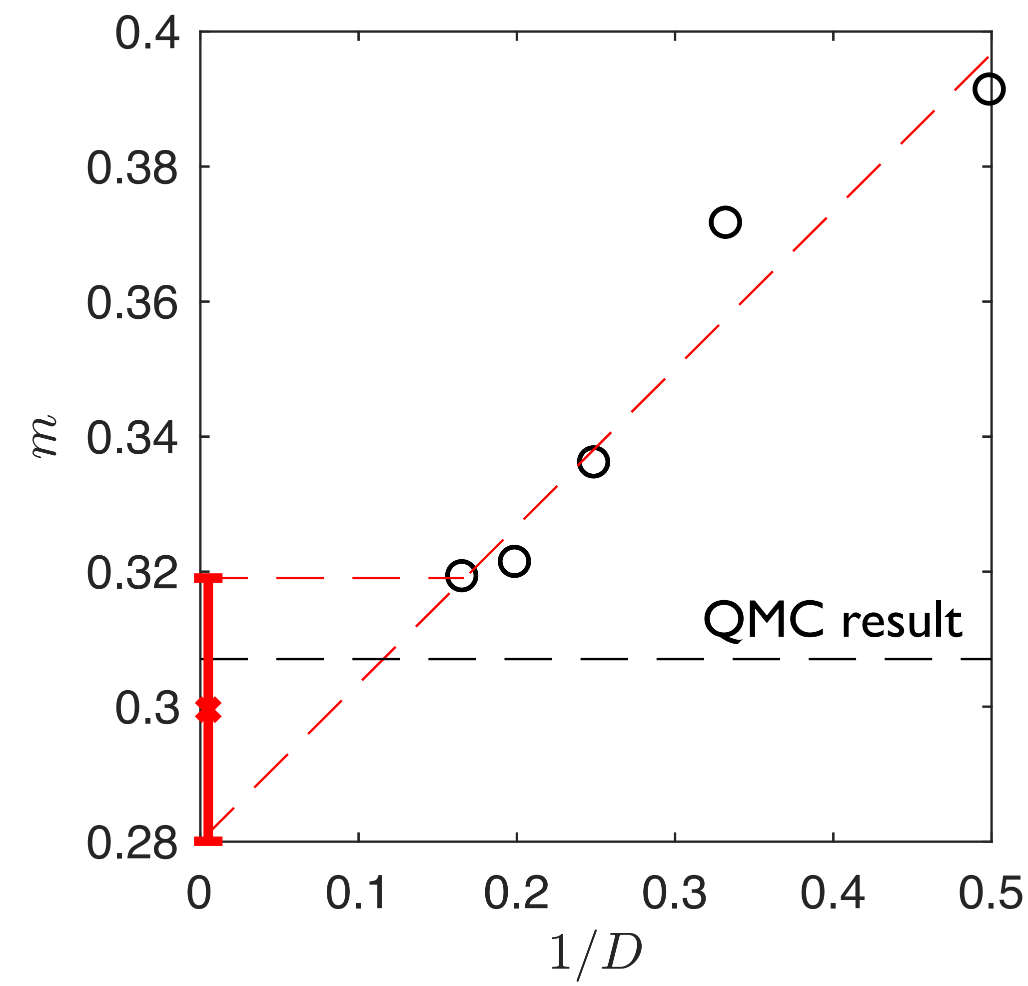
Extrapolation of order parameter: 2D Heisenberg model

- Use FCL scaling to extrapolate the order parameter in gapless system

Extrapolation in $1/\xi_D$



$1/D$ extrapolation



iPEPS: $m = 0.307 \pm 0.002$

QMC: $m = 0.30743(1)$

Sandvik & Evertz (2010)

Strong improvement compared to "naive" 1/D extrapolation!

Finite temperature simulations with iPEPS (J’/J=0.63)