Kagome quantum antiferromagnets in a magnetic field

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Numerical and analytical methods for strongly correlated systems

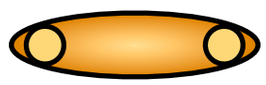
September 11th 2014

TP, and D. Poilblanc, arXiv:1406.7205 (2014)

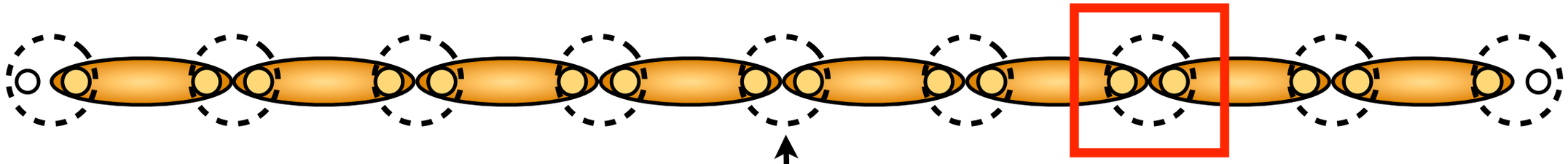
Outline

- AKLT S=2 state as a warm up
  - AKLT PEPS representation
  - iPEPS algorithm
  - Phase diagram
  - Nematic and supernematic phases
- Heisenberg S=1 phase diagram

AKLT 1D

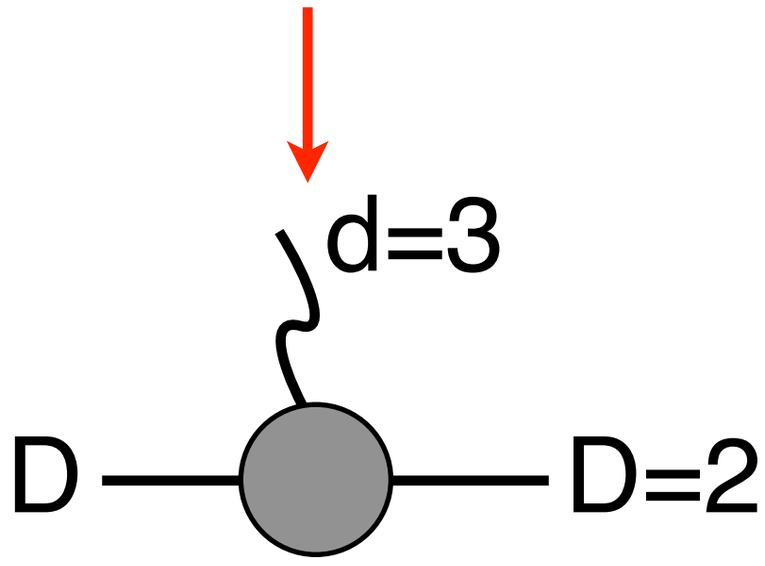
1 singlet on each bond  $\frac{|+-\rangle - |-+\rangle}{\sqrt{2}}$

symmetrization of the spin-1/2 on each site onto spin-1



$$H = \sum_{\langle ij \rangle} P_{ij}^{\mathbf{S}_i + \mathbf{S}_j = S_{max}}$$

$$S_{max} = 2$$

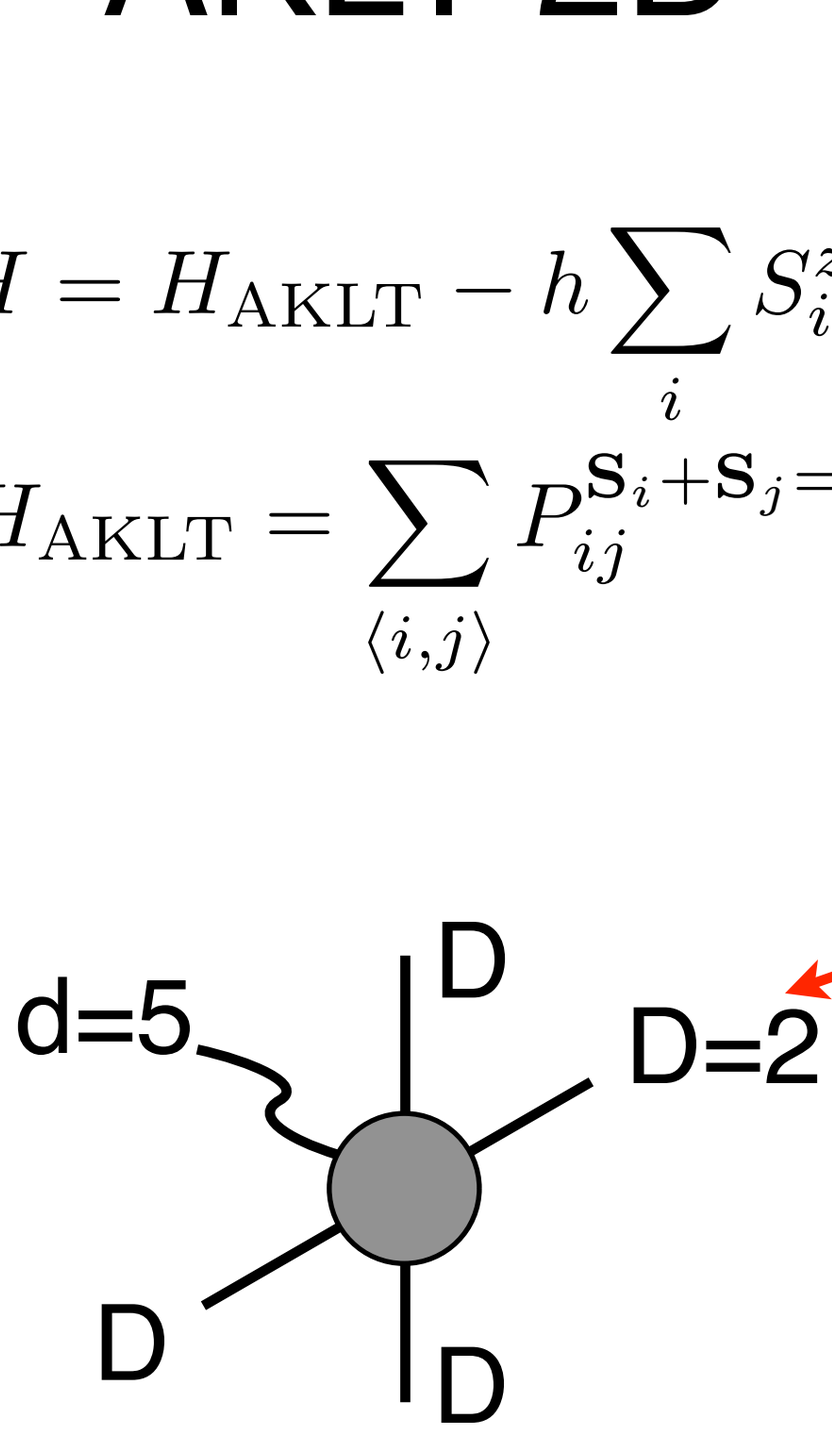


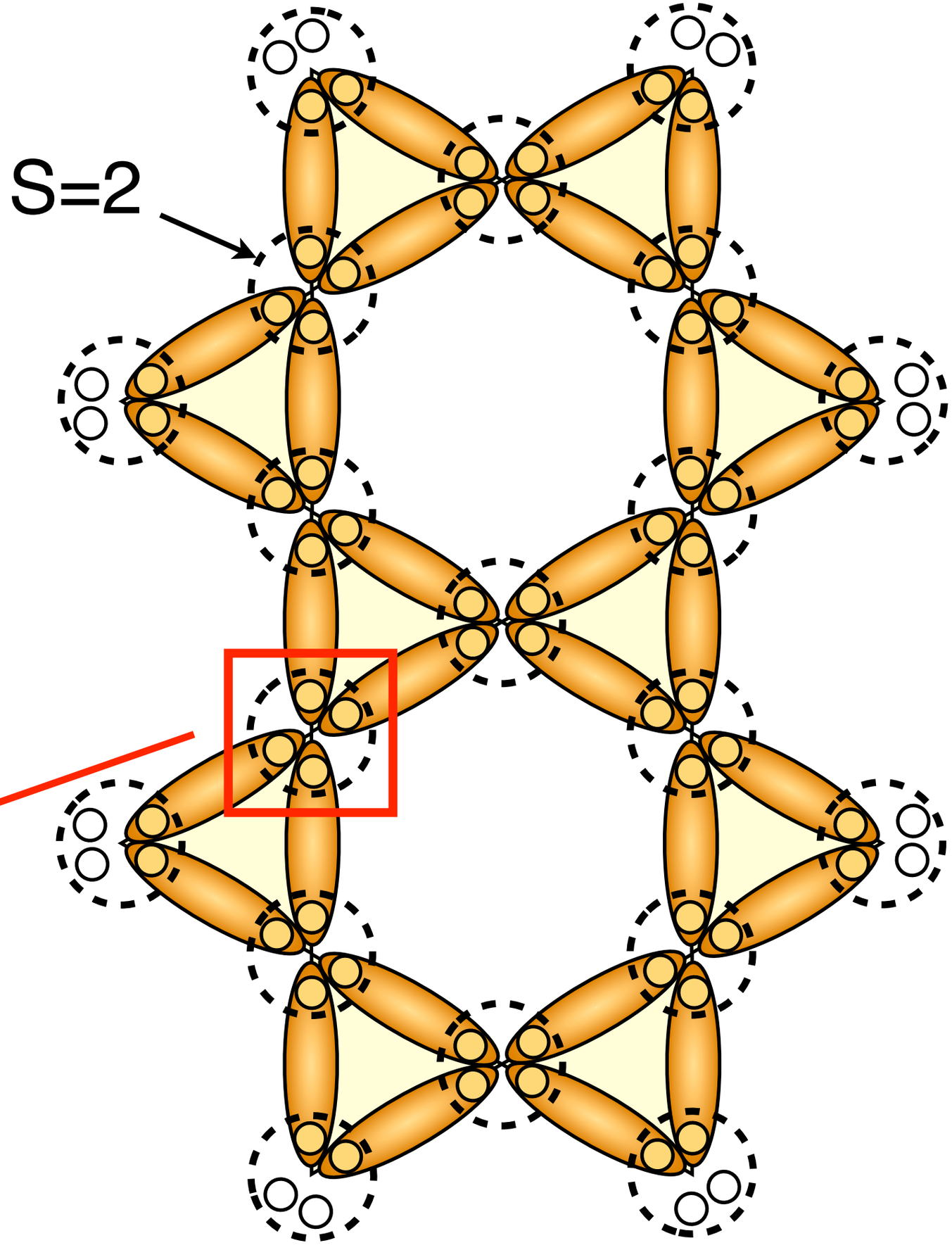
MPS representation

AKLT 2D

$$H = H_{\mathrm{AKLT}} - h \sum_i S_i^z$$

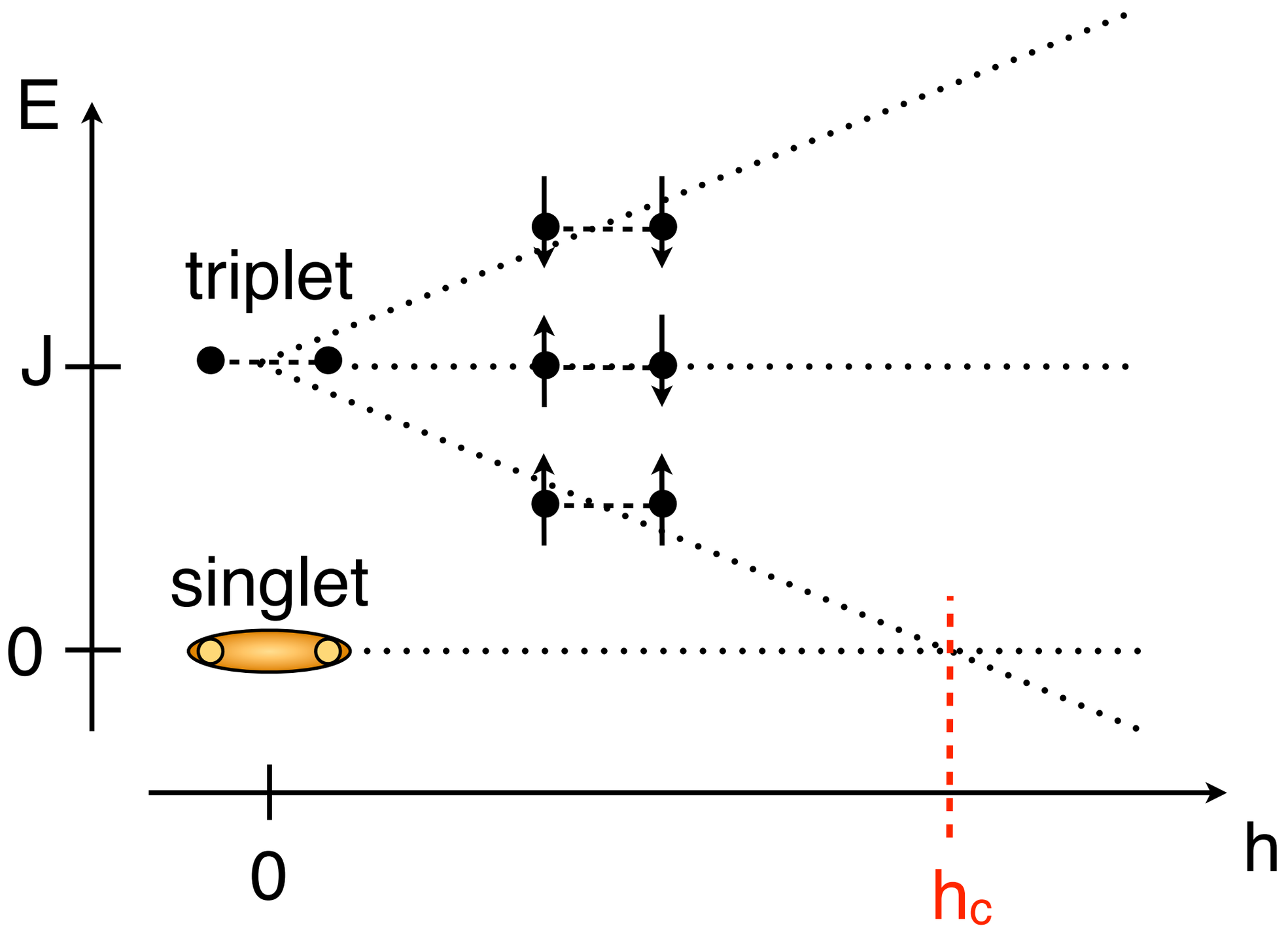
$$H_{\mathrm{AKLT}} = \sum_{\langle i,j \rangle} P_{ij}^{\mathbf{S}_i + \mathbf{S}_j = 4}$$





PEPS representation

Zeeman coupling : a simple example



What do we expect for a 2D system?

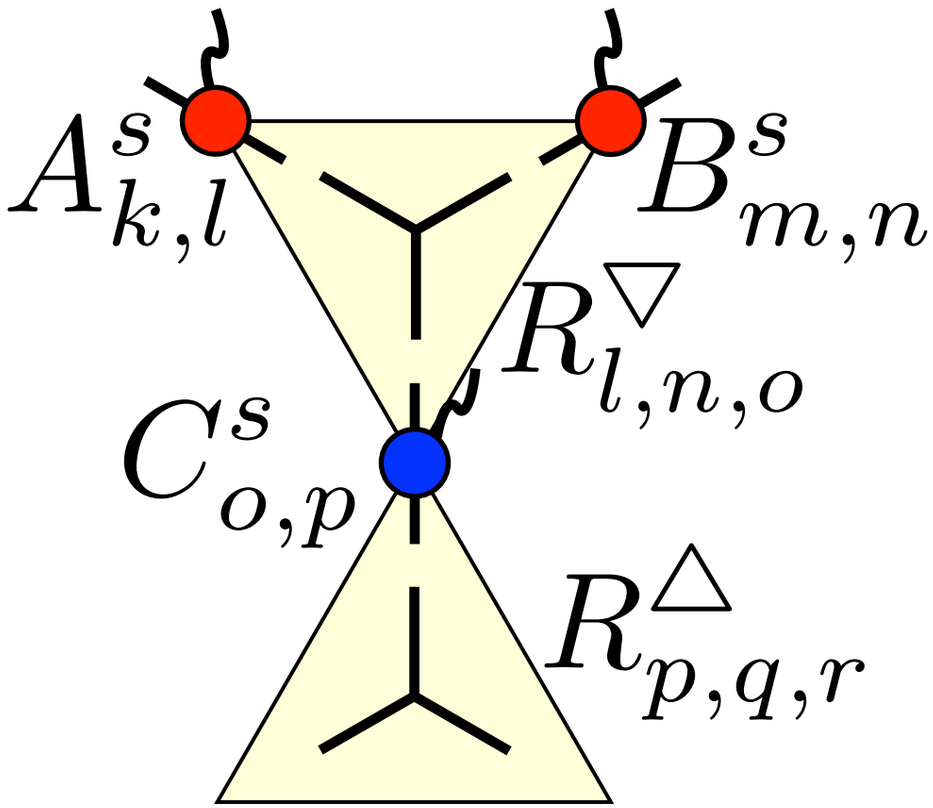
Exotic phases at $h > h_c$

- Superfluid
- Incompressible phase which breaks translation symmetry: triplet crystal

Thierry Giamarchi, *et al*, Nature Physics 4, 198 - 204 (2008)
Works of P. Corboz, F. Mila

New incompressible phase without translation symmetry breaking ? !

iPEPS algorithm



3 sites per unit cell:
translational invariance ansatz

Imaginary time evolution

$$|GS\rangle \lim_{\tau \to +\infty} e^{-\tau H} |\Psi_0\rangle$$

CTMRG
T. Nishino, K. Okunishi, J. Phys. Soc. Jpn. **65**, 891 (1996)
R. Orus, G. Vidal, Phys. Rev. B **80** 094403 (2009)
MPS-based approach => iTEBD
G. Vidal, Phys. Rev. Lett. **98**, 070201
R. Orus, G. Vidal, Phys. Rev. B **78**, 155117 (2008)
PEPS + simplex tensor
N. Schuh, D. Poilblanc, J. I. Cirac, D. Perez-Garcia Phys. Rev. B **86**, 115108 (2012)
Z. Y. Xie, J. Chen, J. F. Yu, X. Kong, B. Normand, T. Xiang Phys. Rev. X **4**, 011025 (2014)

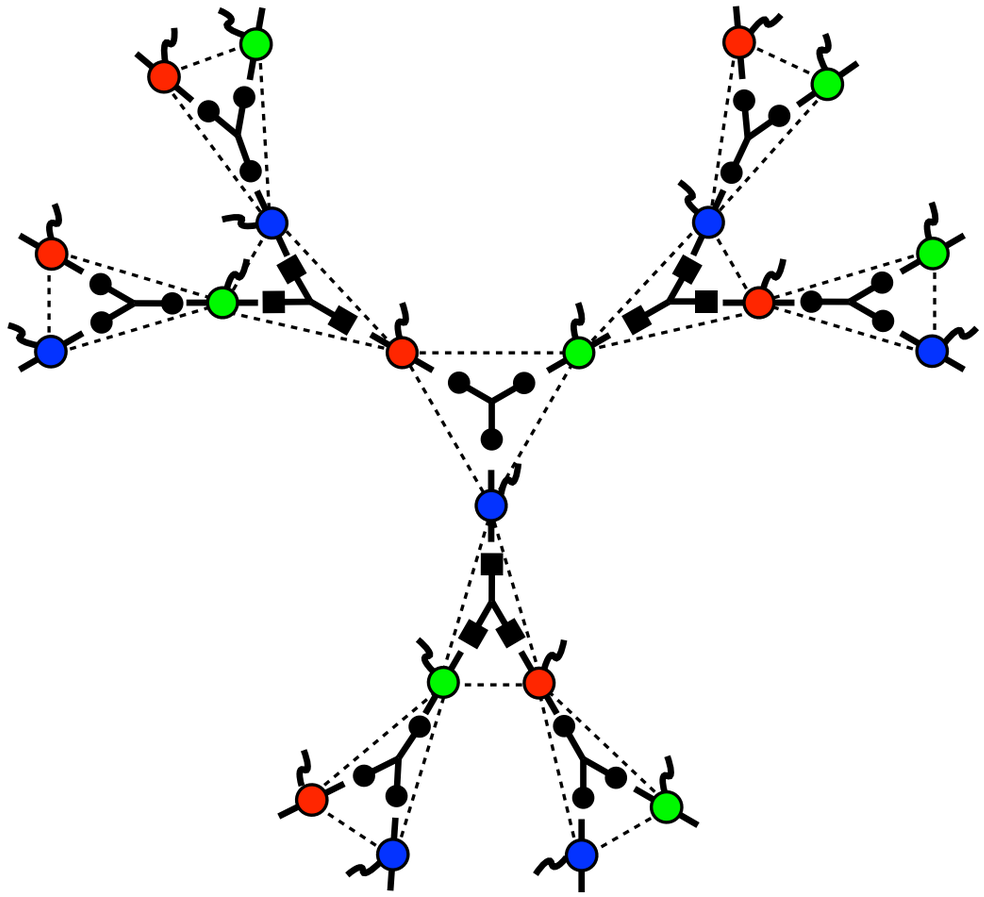
Simple Update

Faster than the Full Update
But less accurate

Good approximation for finite correlation length (gapped phase, far from critical point)

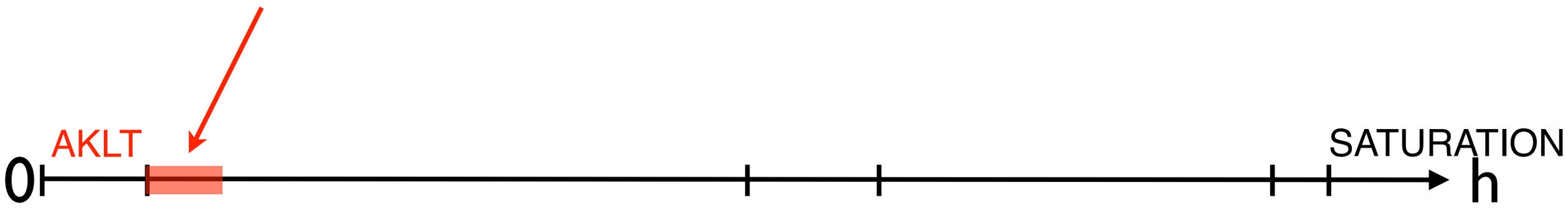
For S>1/2 and higher cluster, more stable

Otherwise, can exhibit instabilities



AKLT «plateau» phase

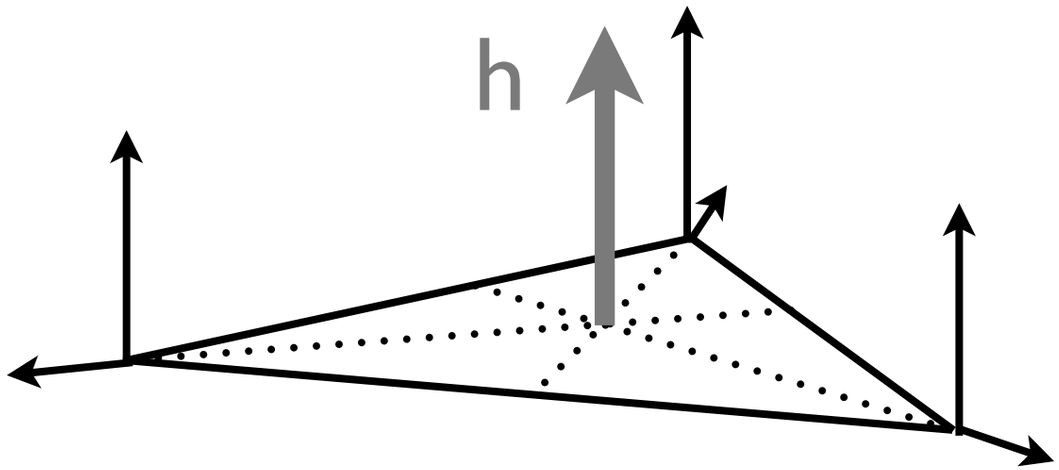
- Critical magnetic field -> minimum energy to break one singlet
- Spin gap $\Delta_S/S \sim 0.245$
- Magnetic field adds triplets to the system
- Bose-Einstein condensate of triplons



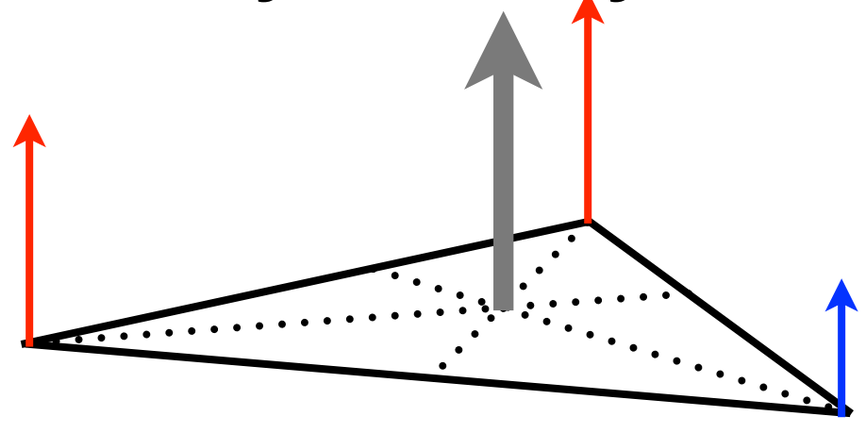
A. Garcia-Saez, Valentin Murg, T-C Wei, Phys. Rev. B 88, 245118 (2013)

What happens at $h > h_c$

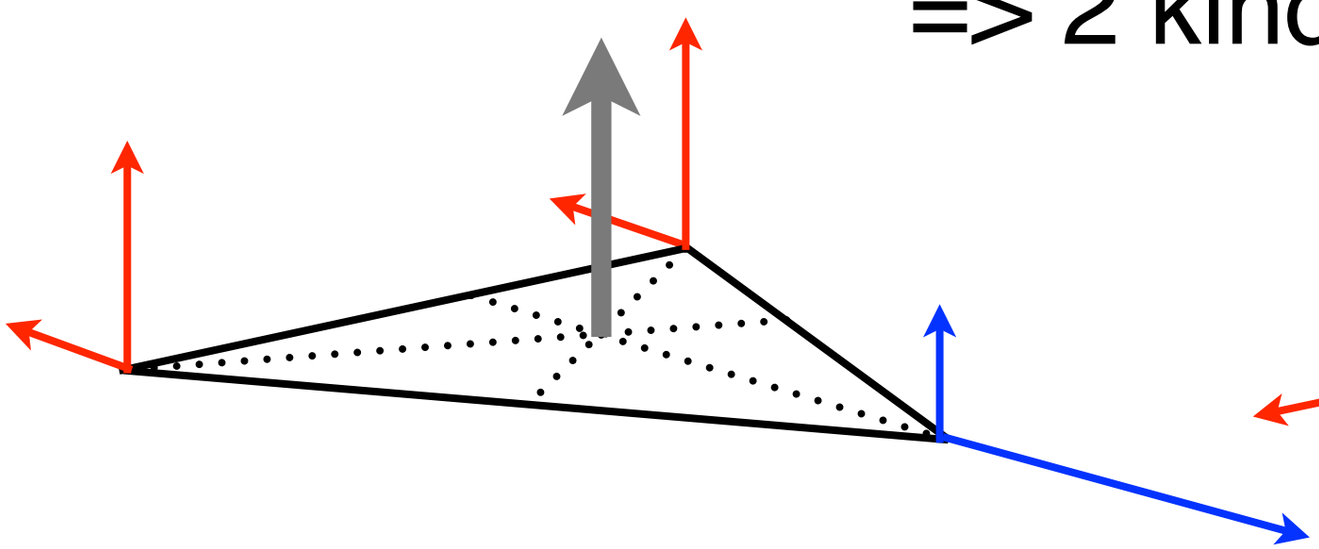
Superfluid
=> spin-U(1) broken

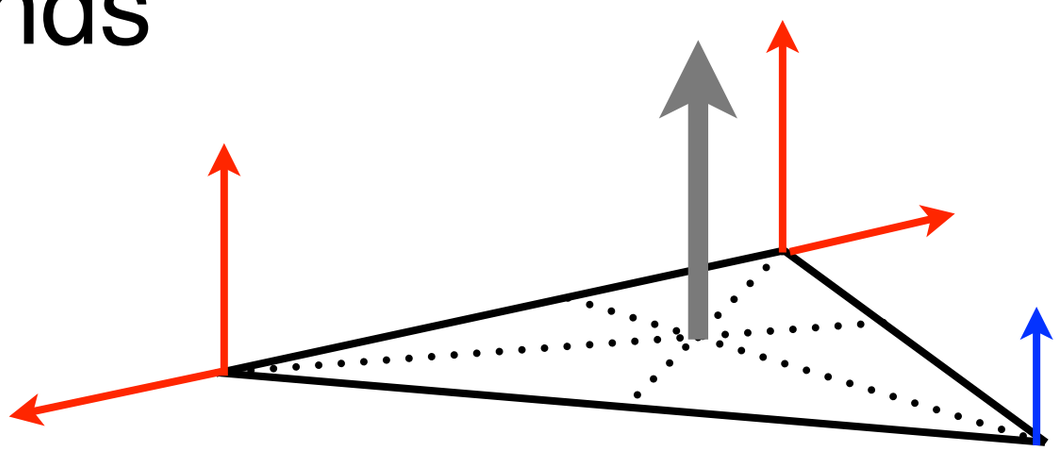


Nematic
=> C_3 symmetry broken

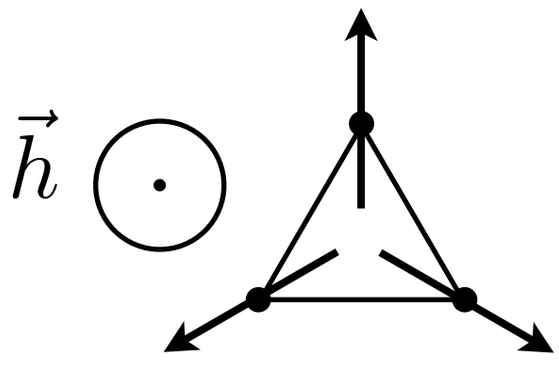


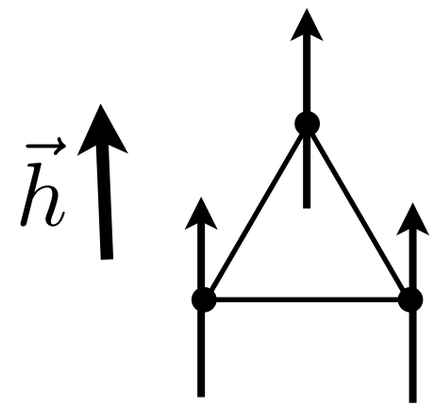
Supernematic = Superfluid + Nematic
=> 2 kinds





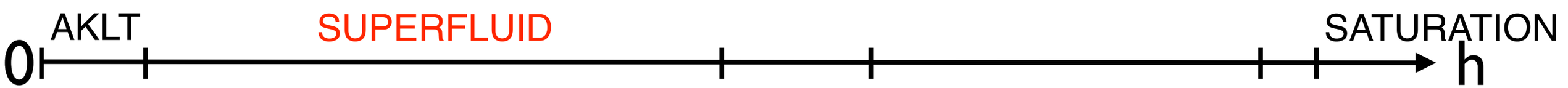
Superfluid phase





Compressible

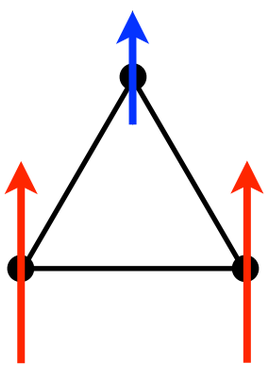
spin-U(1) symmetry broken



Magnetization plateau: Nematic phase

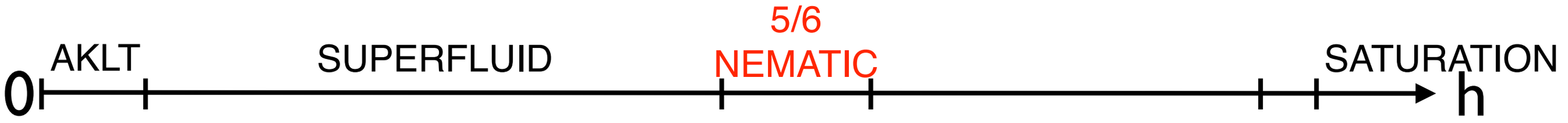
$$m_z = S^z / S^z_{max} = 5/6$$

$$m_\perp = 0$$

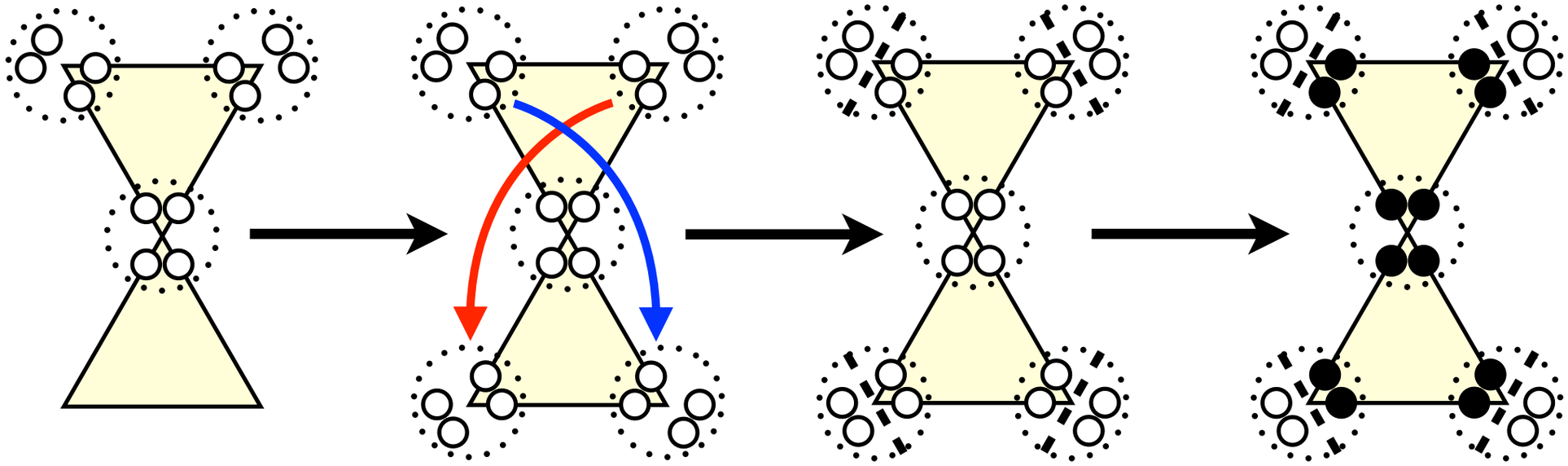


Incompressible phase

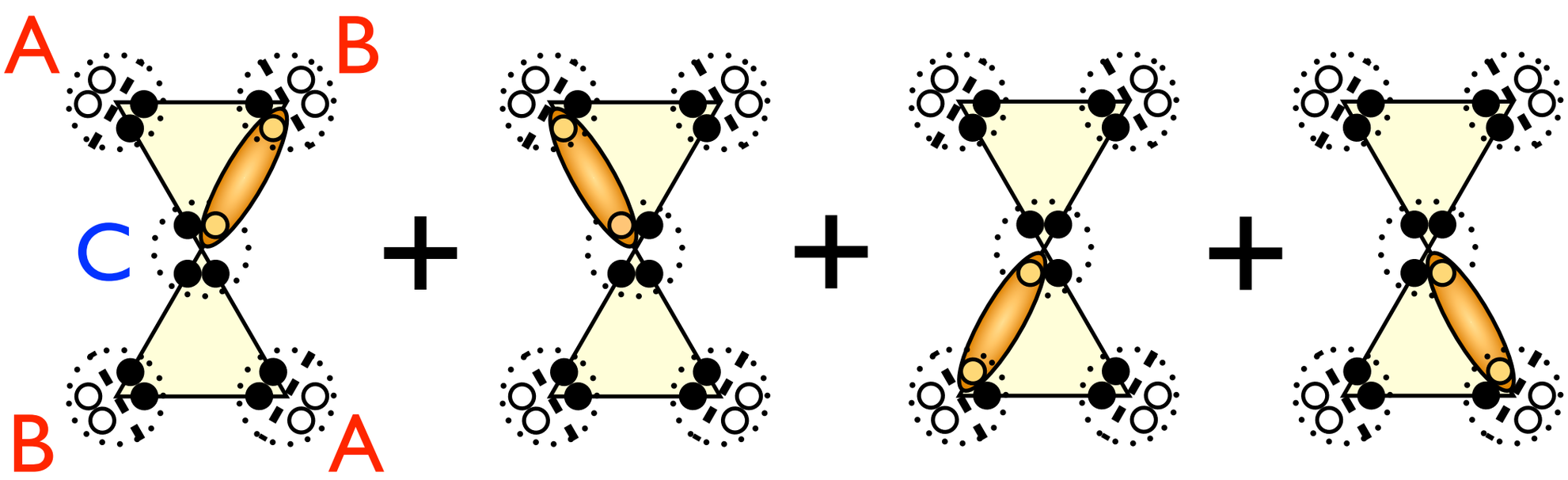
C_3 symmetry broken



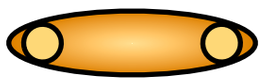
5/6 plateau: Nematic phase



5/6 plateau: Nematic phase



- $S_z = +1/2$



$$\frac{|+-\rangle - |-+\rangle}{\sqrt{2}}$$

$$\begin{aligned} m_z^C &= 0.67 \longrightarrow 0.76 \\ m_z^A = m_z^B &= 0.91 \longrightarrow 0.87 \\ e_0 &= -1.92 \longrightarrow -1.80 \end{aligned}$$

Hardcore singlets!

Optimized state

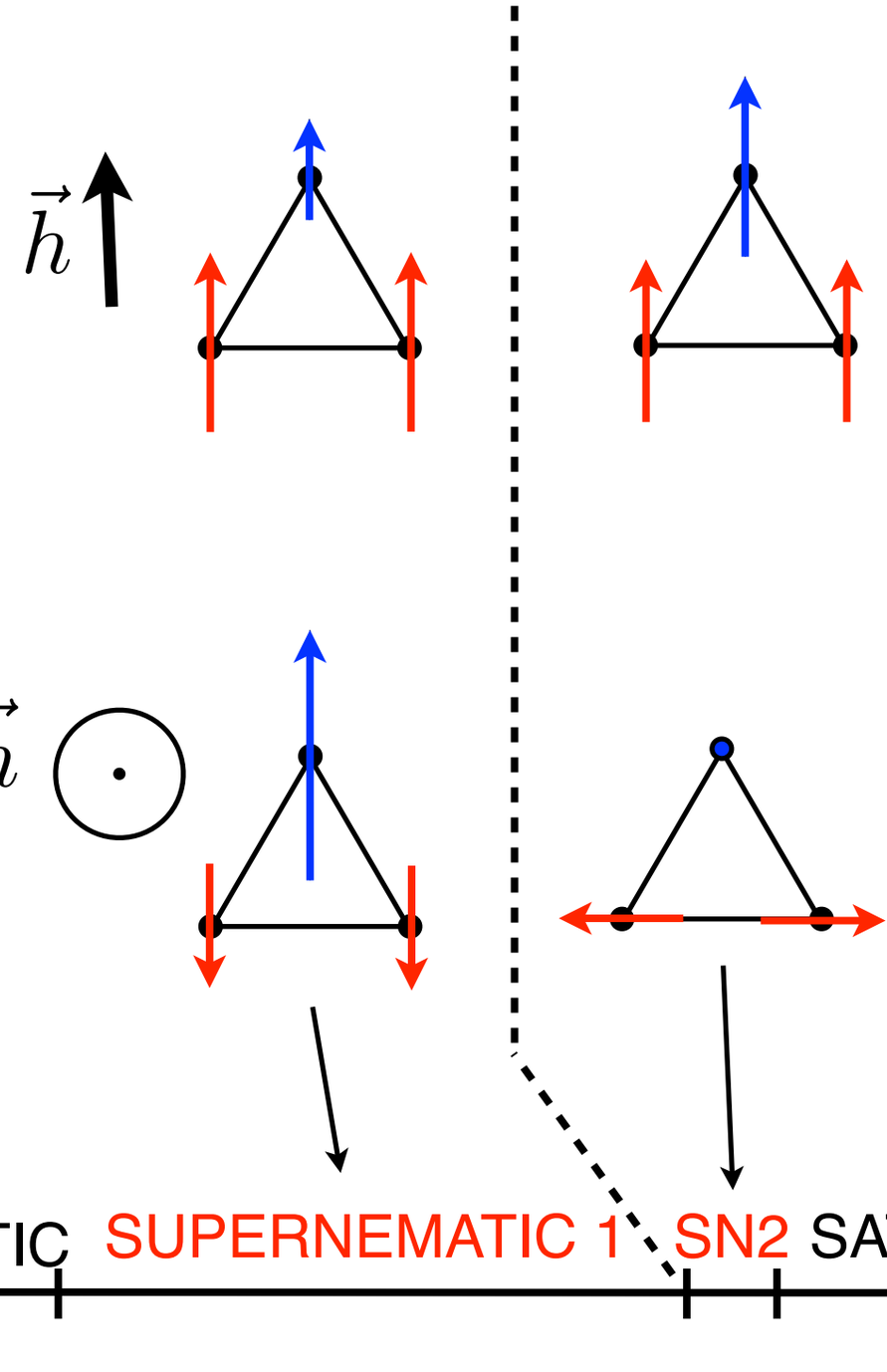
Supernematic phase

Nematic +
Superfluid

Compressible

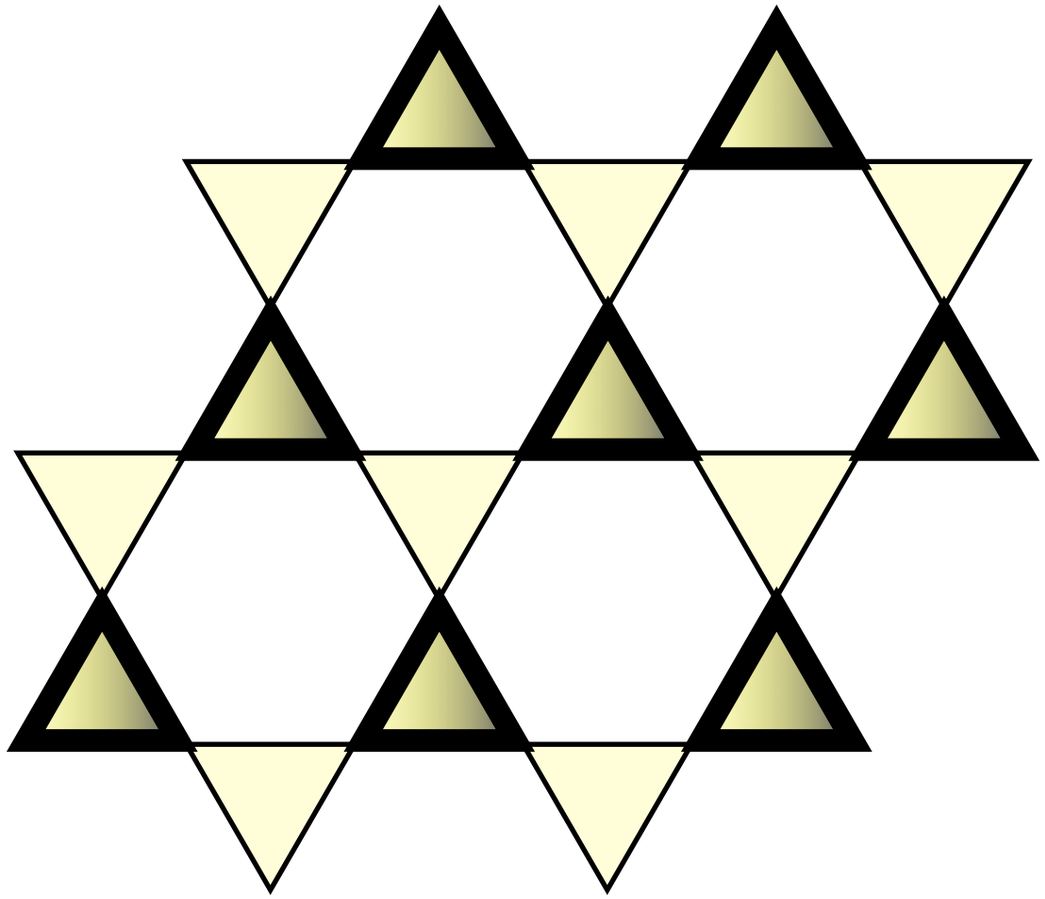
spin U(1) symmetry broken

C_3 symmetry broken



Heisenberg S=1 KAFM

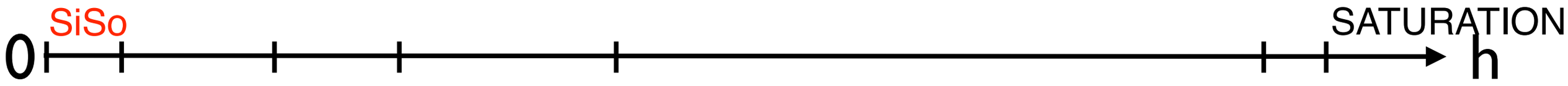
$$H = \sum_{\langle ij \rangle} \mathbf{S}_i . \mathbf{S}_j - h \sum_i S_i^z$$



h=0 Simplex Solid

C_2 symmetry is broken

$$\delta = 2 \left| \frac{E_\nabla - E_\triangle}{E_\nabla + E_\triangle} \right| \simeq 21\%$$



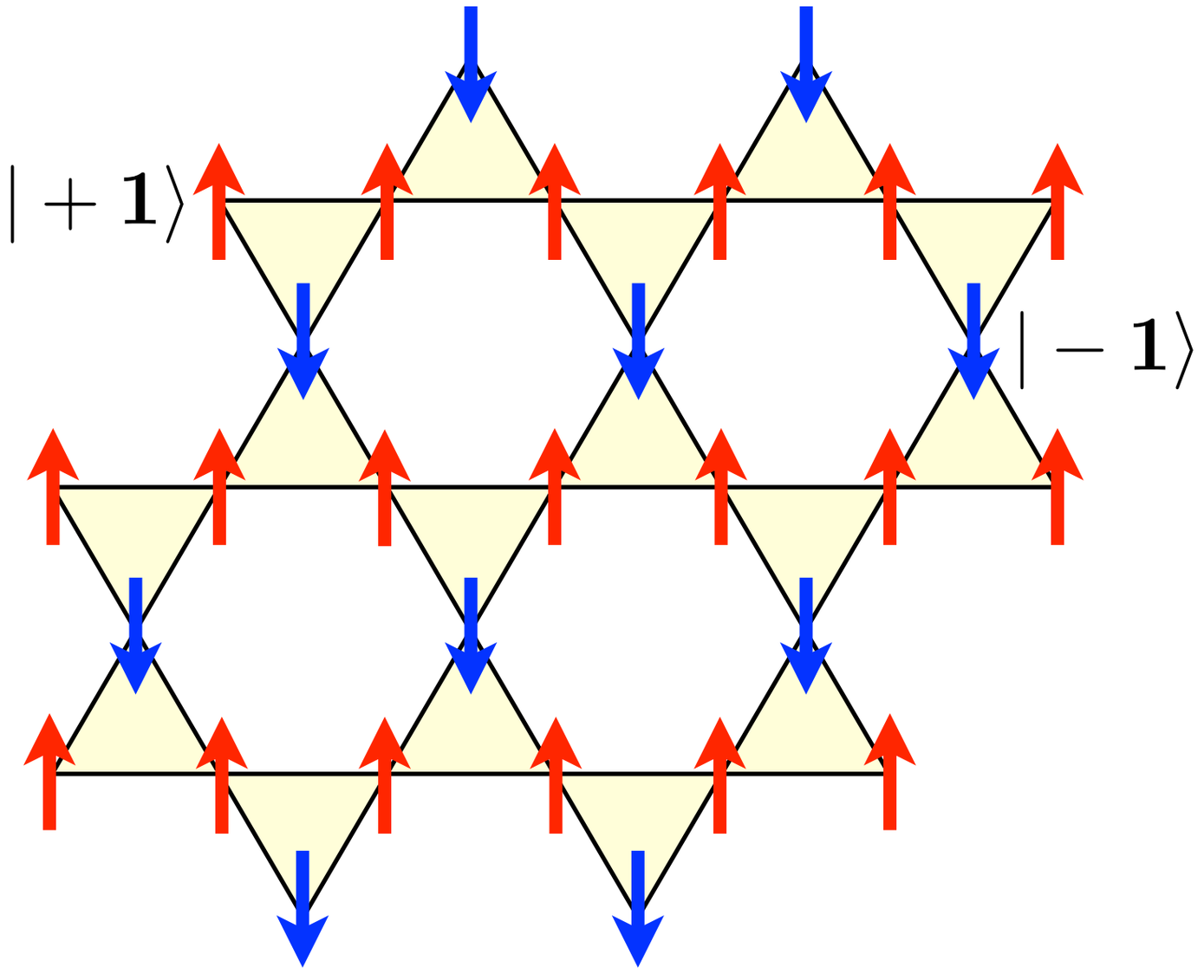
O. Götze, *et al.* Phys. Rev. B 84,224428 (2011)
H.J. Changlani and A. M. Läuchli, arXiv:1406.4767 (2014)
T. Liu, W. Li, A. Weichselbaum, J. von Delft, and G. Gu, arXiv:1406.5905 (2014)
TP, and D. Poilblanc, arXiv:1406.7205 (2014)

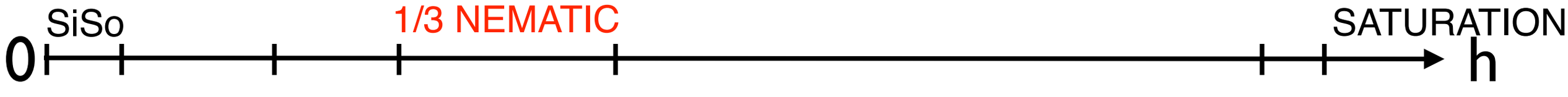
1/3 magnetization plateau : Nematic phase

$m_\perp = 0$

Incompressible phase

C_3 symmetry broken

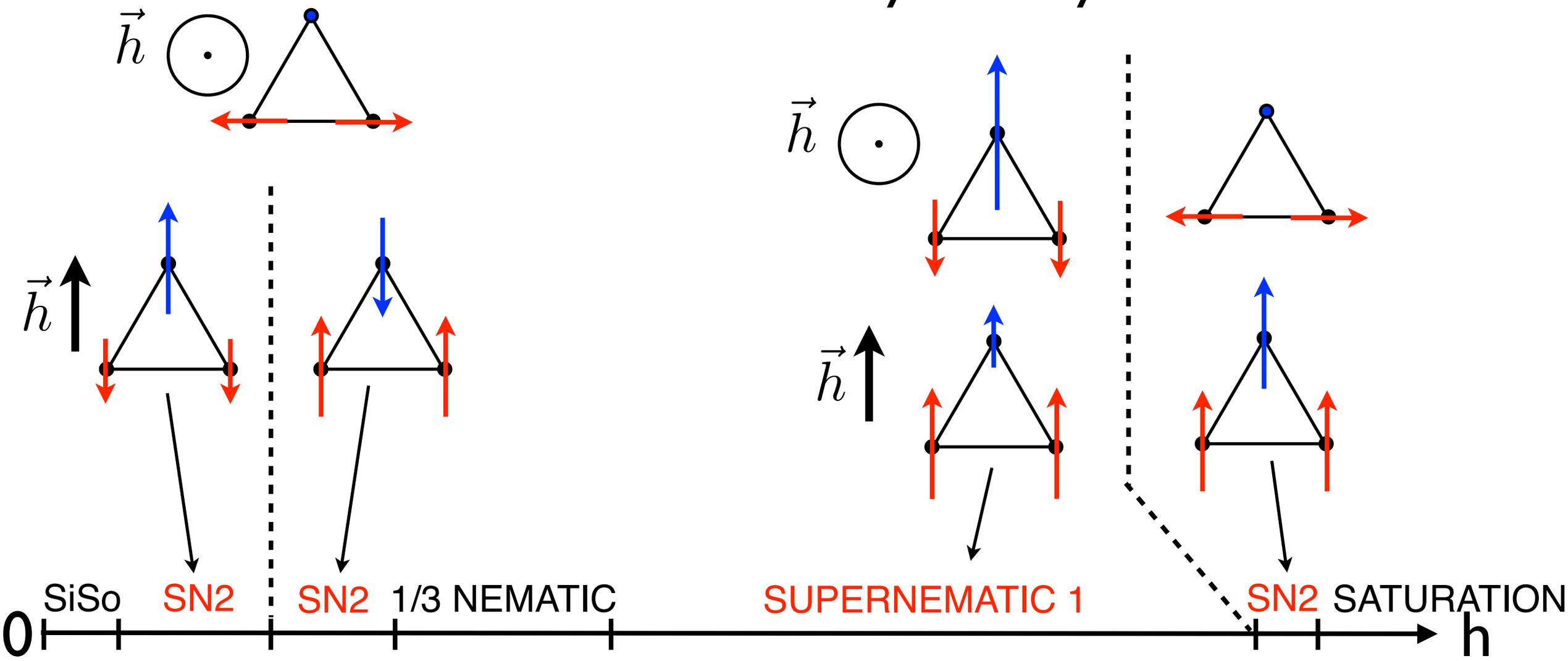




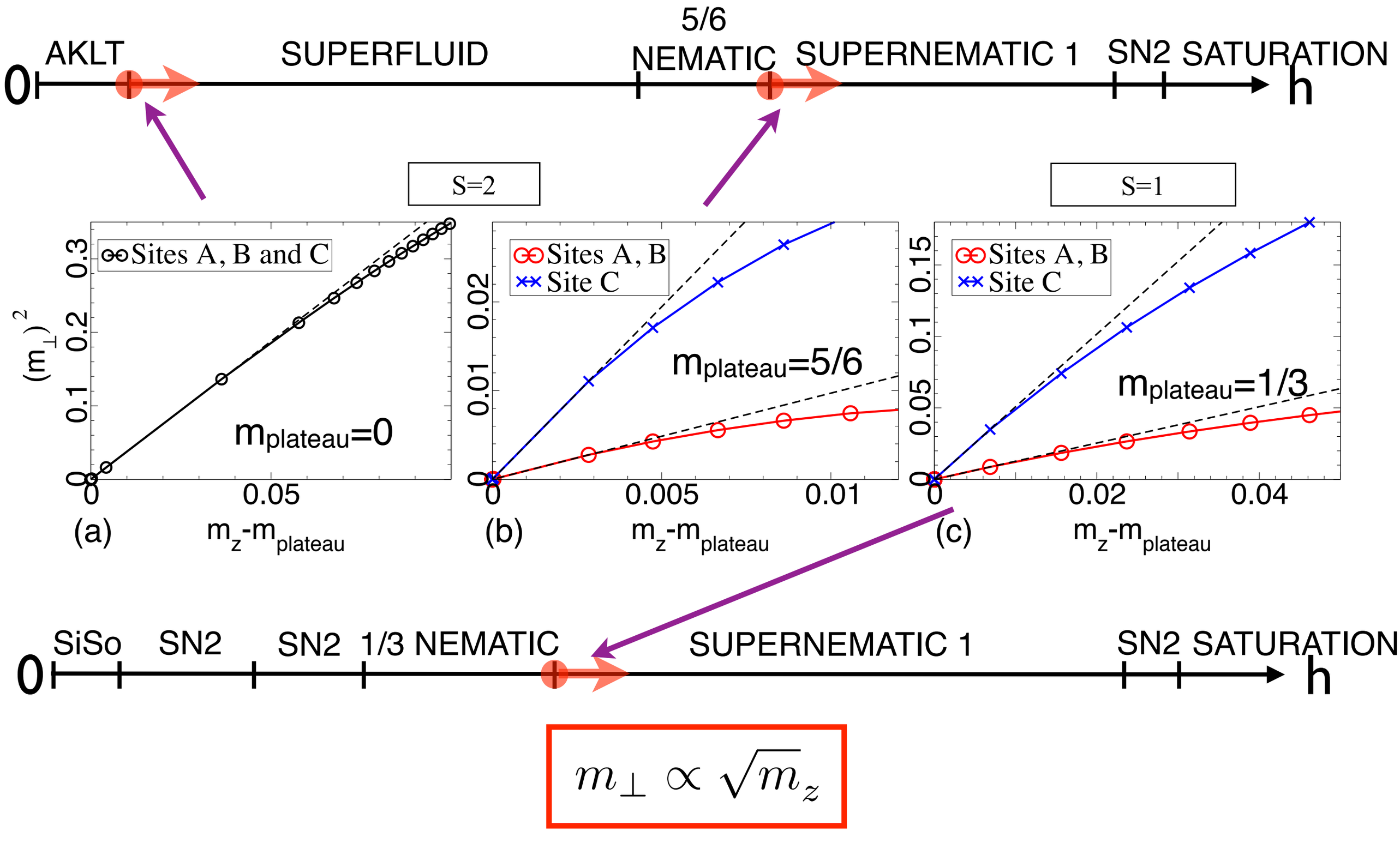
Supernematic phase

Nematic +
Superfluid

Compressible
spin U(1) symmetry broken
C_3 symmetry broken



Bose-Einstein condensate

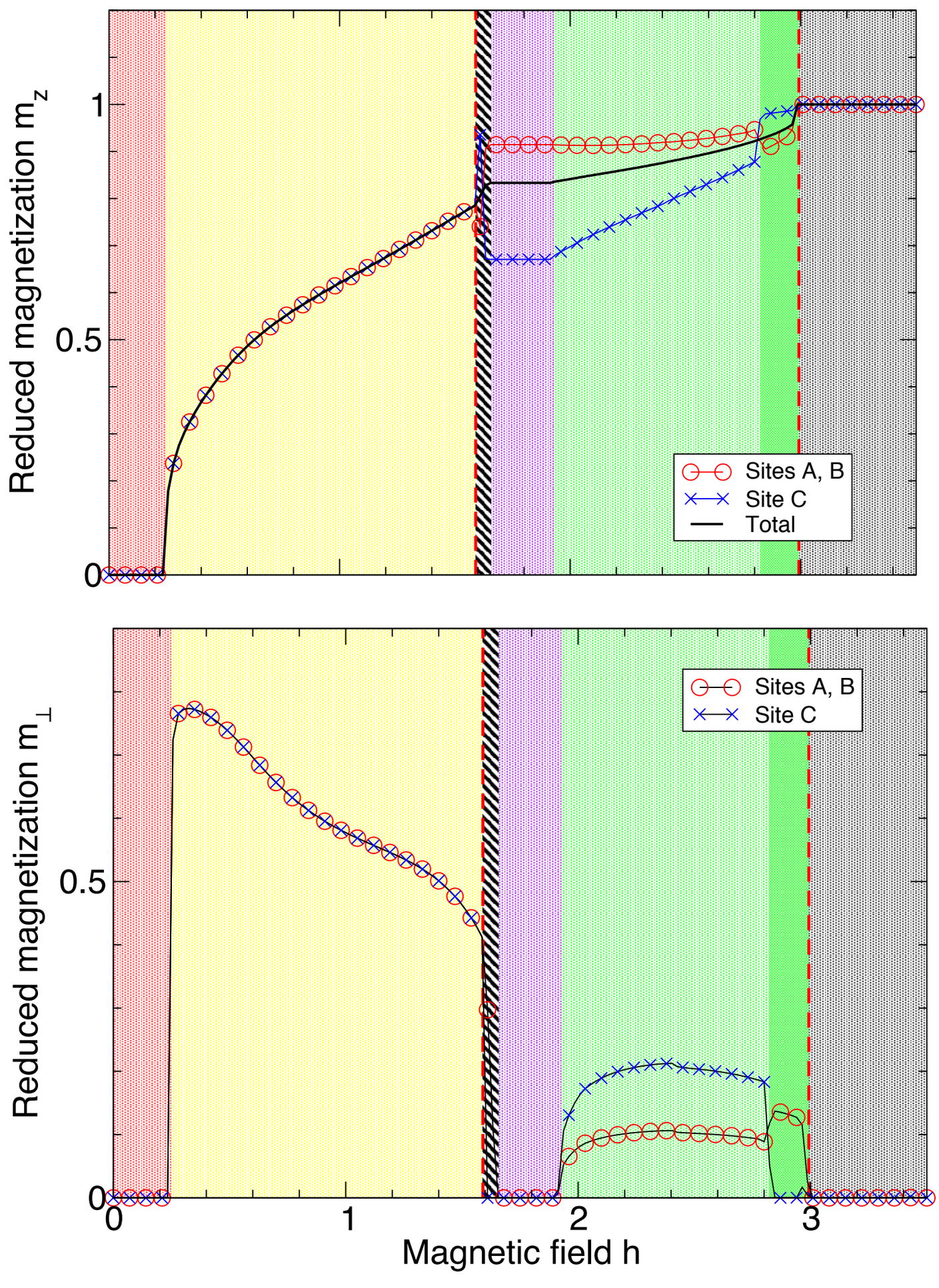


$$m_\perp \propto \sqrt{m_z}$$

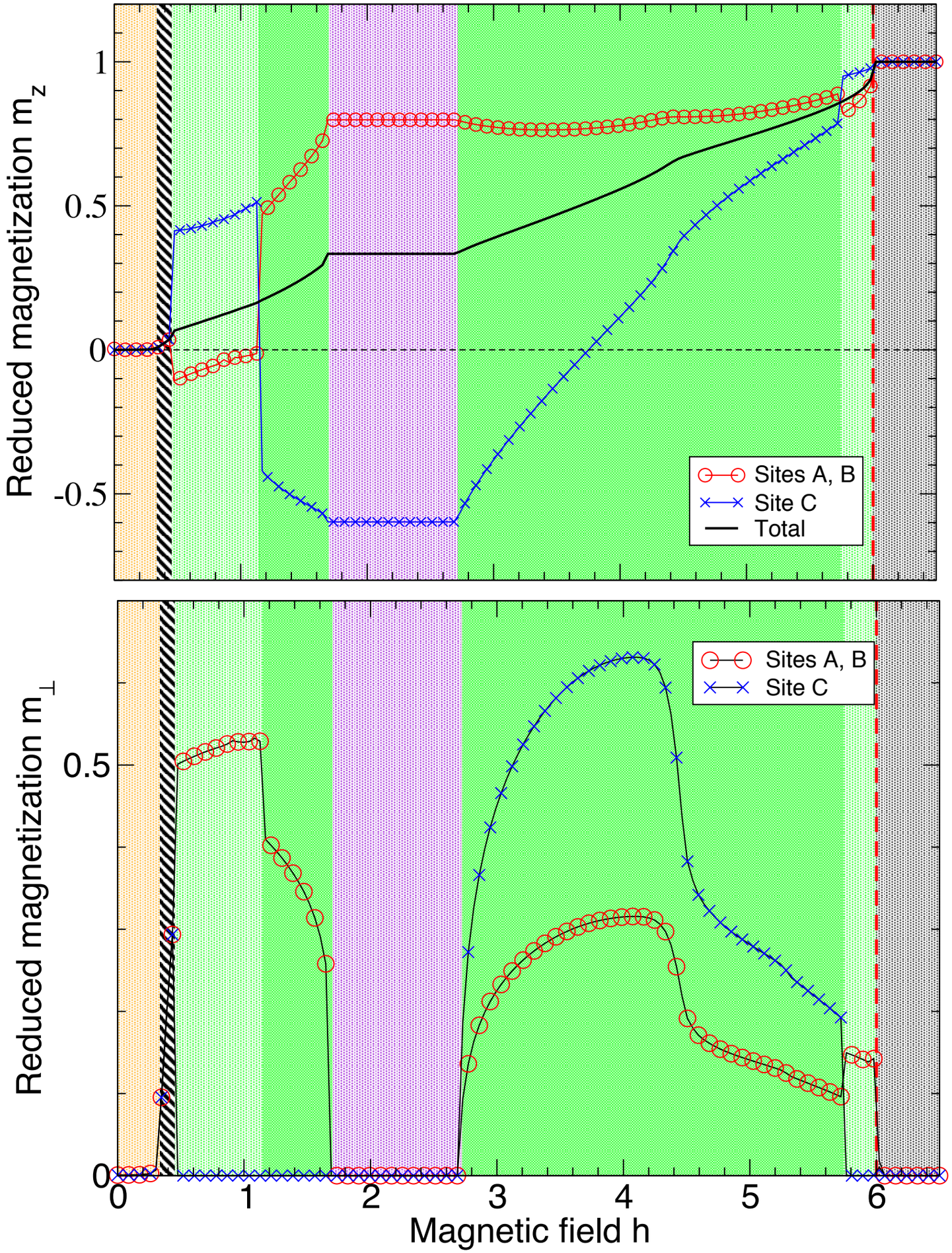
Summary & Outlook

- iPEPS simple update efficient
- S=1 Heisenberg GS gapped Simplex Solid
- Nematic and supernematic phases with frustration + magnetic field
- Larger unit cell?
- Full update?

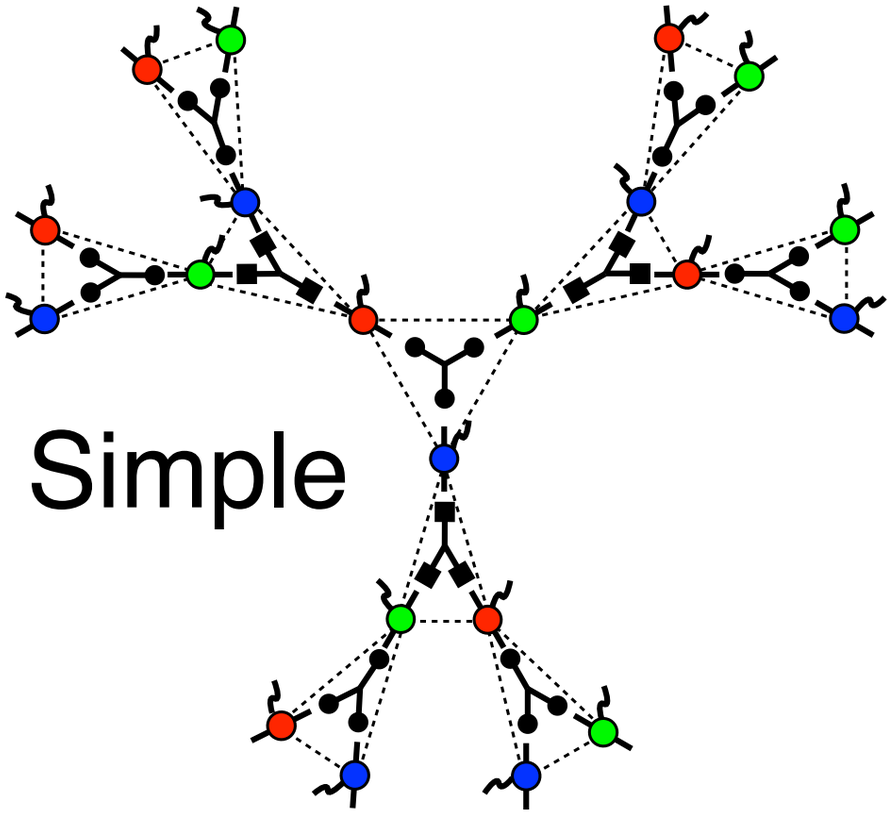
THANK YOU

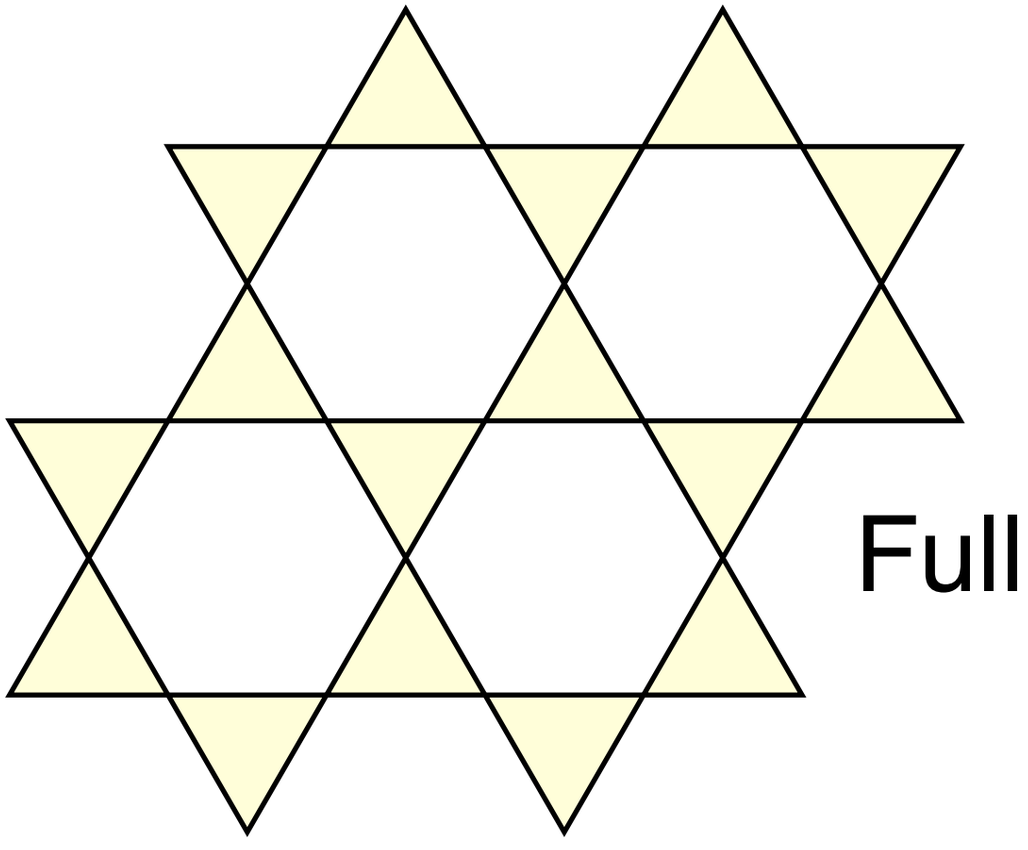

Reduced magnetization m_z
1
0.5
0
Sites A, B
Site C
Total
Reduced magnetization $m_\perp$
0.5
0
0
1
2
3
Magnetic field h

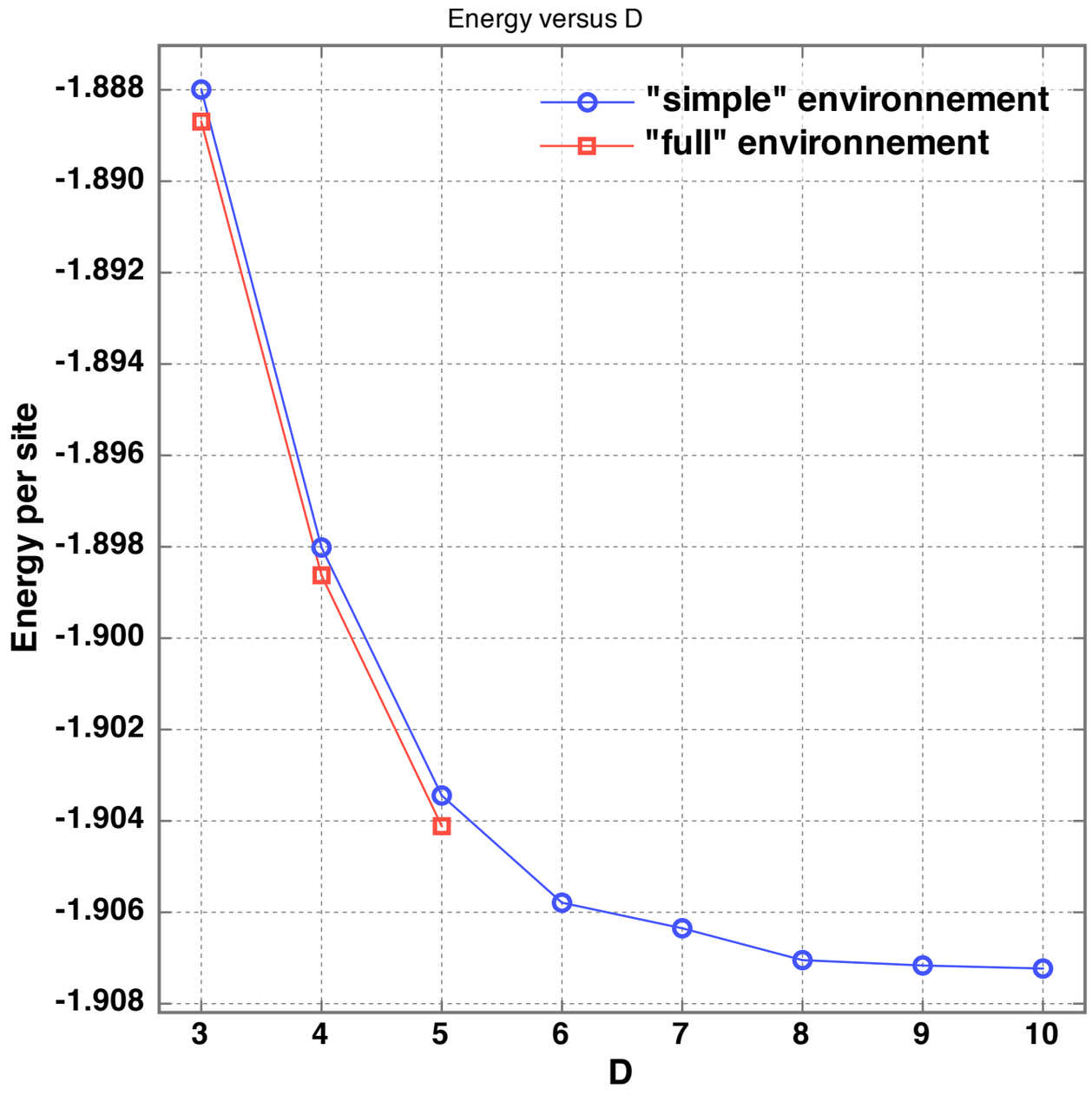
AKLT S=2



Heisenberg S=1


Simple


Full


Energy versus D
"simple" environnement
"full" environnement
Energy per site
-1.888
-1.890
-1.892
-1.894
-1.896
-1.898
-1.900
-1.902
-1.904
-1.906
-1.908
3
4
5
6
7
8
9
10
D

$$h = 2.6$$

$$m_z = 1/3$$