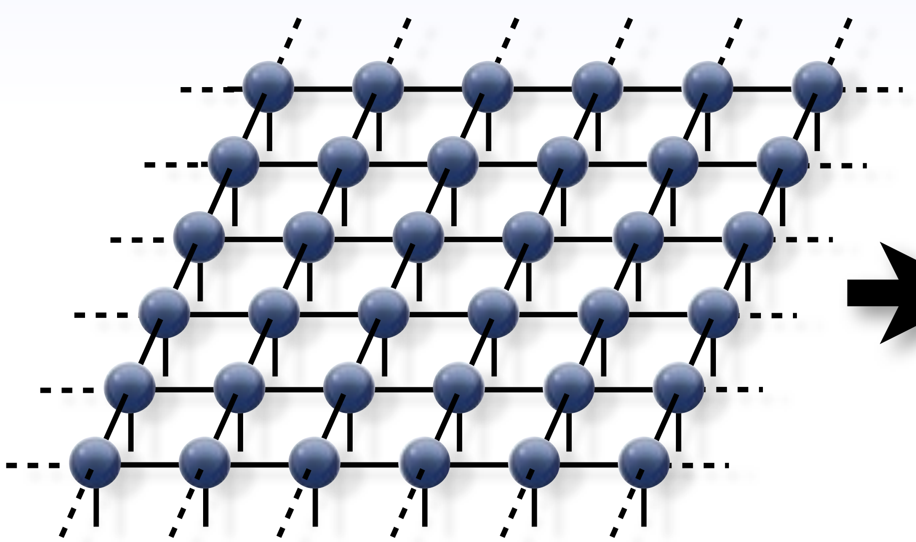
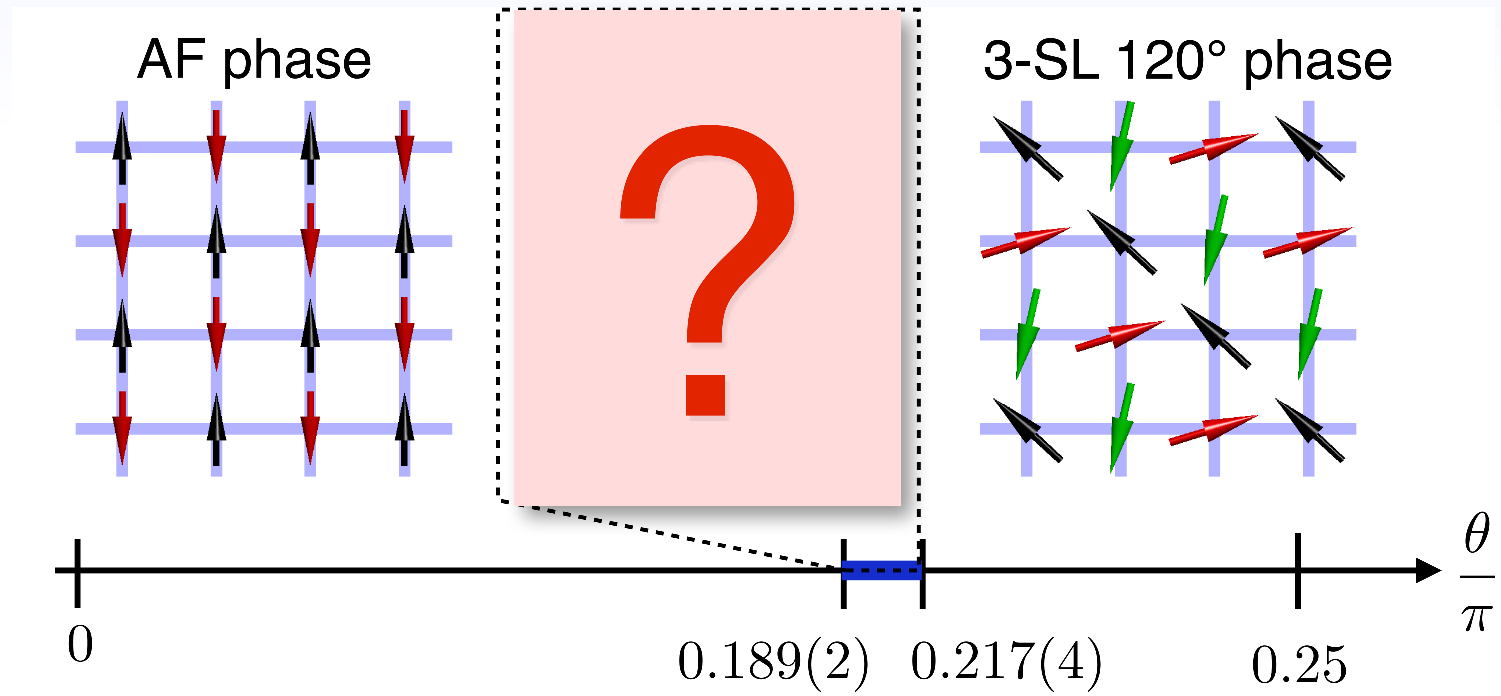
2D tensor network study of the S=1 bilinear-biquadratic Heisenberg model

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



iPEPS

2D tensor network ansatz



I. Niesen and P. Corboz, Phys. Rev. B 95, 180404 (2017)

I. Niesen and P. Corboz, SciPost Phys. 3, 030 (2017)

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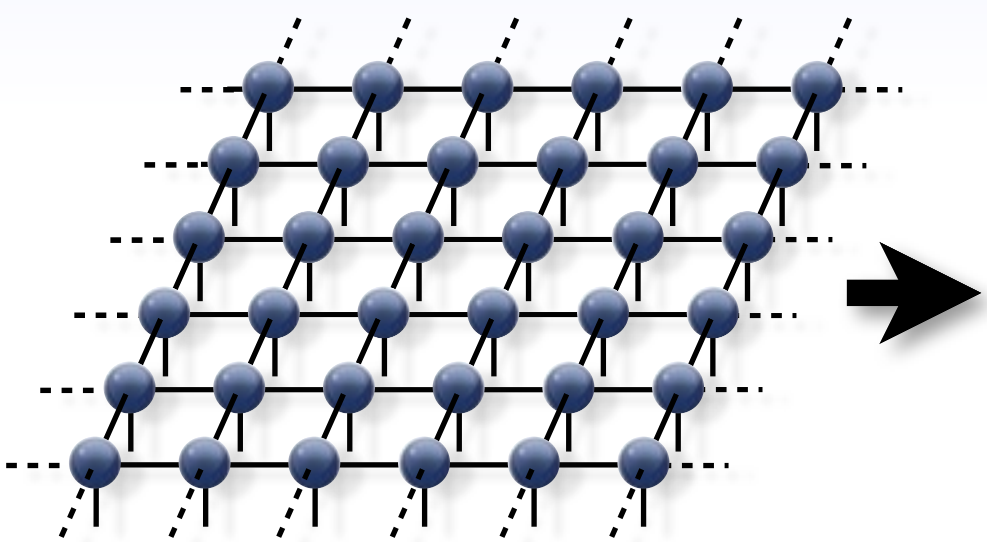
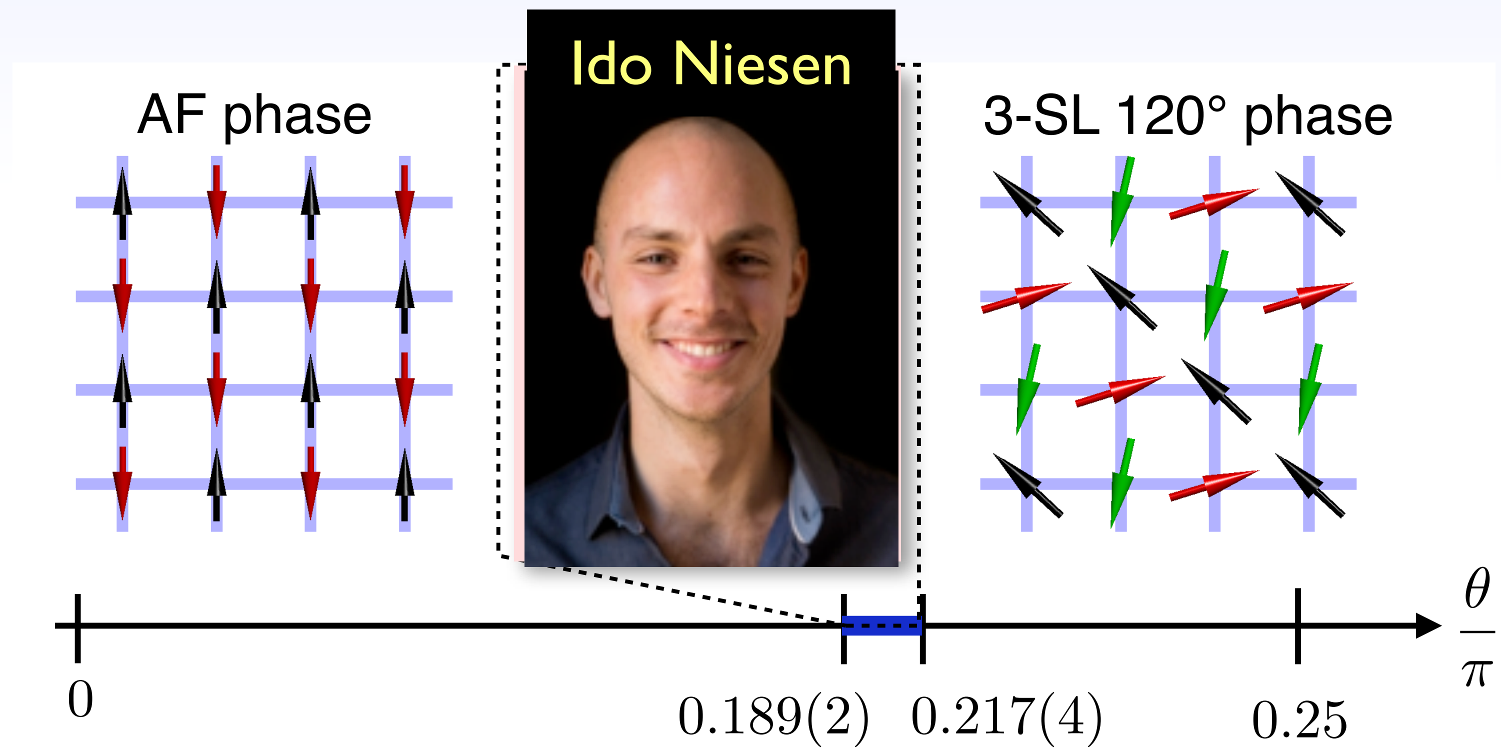


iPEPS

2D tensor network ansatz



I. Niesen and P. Corboz, Phys. Rev. B 95, 180404 (2017)

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Outline

- *Motivation*
  - ✦ SU(3) Heisenberg model & spin-nematic phases & benchmark problem
- *Method*
  - ✦ Introduction to tensor networks and iPEPS
  - ✦ Optimization
- *Results*
  - ✦ iPEPS results: 2 new phases
- *Conclusion*
- *Other recent work*
  - ✦ iPEPS vs iMPS on infinite cylinders

S=1 bilinear-biquadratic Heisenberg model on a square lattice

bilinear *biquadratic*

$$H = \sum_{\langle i,j \rangle} \cos(\theta)\, S_i \cdot S_j + \sin(\theta)\, (S_i \cdot S_j)^2$$

S=1 operators

SU(2) symmetry

- **Motivation I: SU(3) Heisenberg model** $(\theta = \pi/4)$

  Experiments on alkaline-earth atoms in optical lattices

- **Motivation II: Spin nematic phases**

  Unusual properties of $NiGa_2S_4$ / $Ba_3NiSb_2O_9$

- **Motivation III: Benchmark problem for iPEPS**

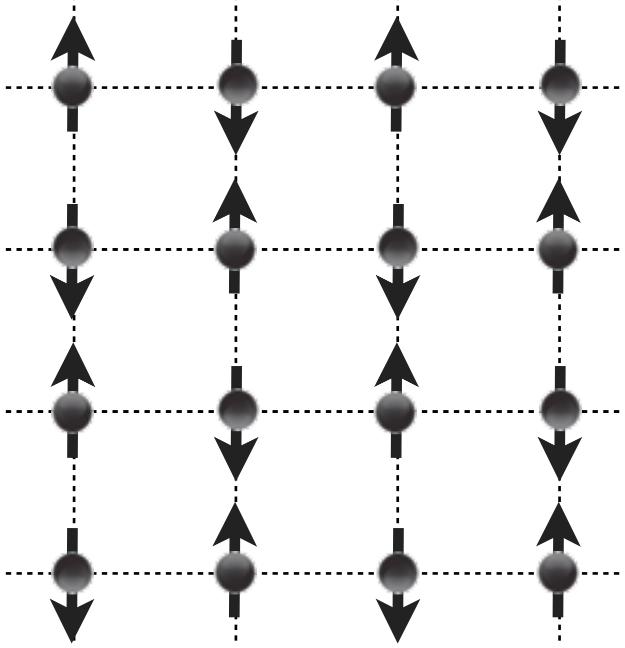
  Discover new phases?

Motivation I: SU(N) Heisenberg models

S=1/2 operators

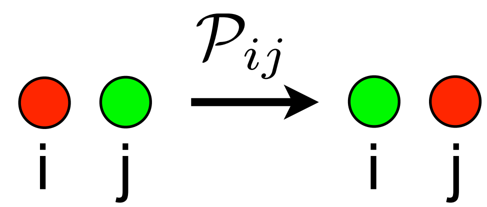
- N=2: $$H = \sum_{\langle i,j \rangle} S_i S_j$$

local basis states: $| \uparrow \rangle, \; | \downarrow \rangle$

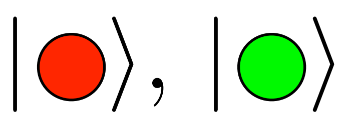


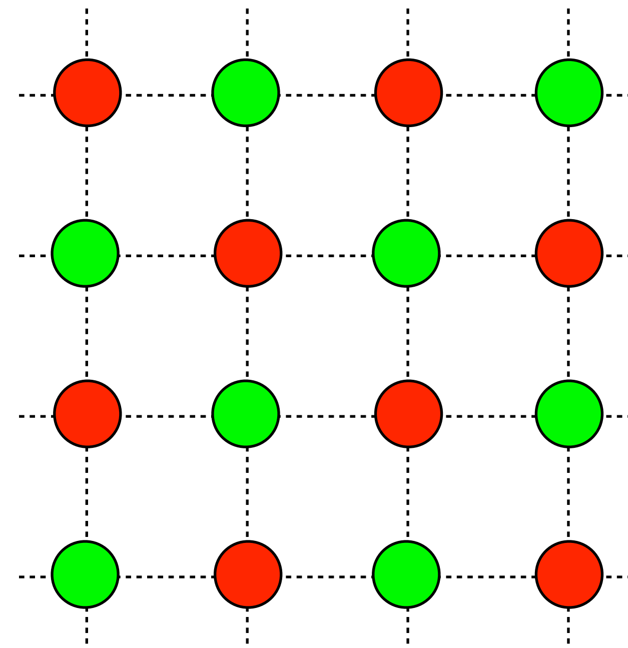
Néel order

Motivation I: SU(N) Heisenberg models

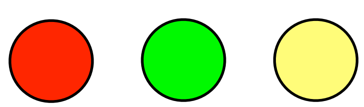


- N=2: $$H = \sum_{\langle i,j \rangle} P_{ij}$$

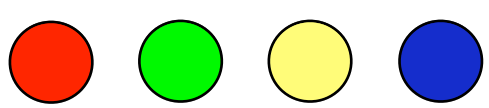
  local basis states: 



Néel order

- N=3 

Ground state??

- N=4 

nature physics

ARTICLES

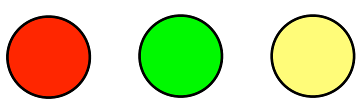
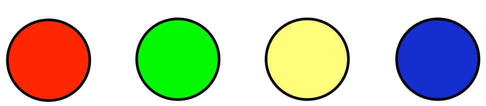
PUBLISHED ONLINE: 28 FEBRUARY 2010 | DOI: 10.1038/NPHYS1535

Two-orbital *SU*(*N*) magnetism with ultracold alkaline-earth atoms

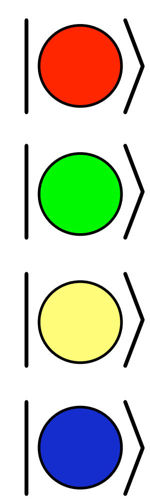
A. V. Gorshkov[1]*, M. Hermele[2], V. Gurarie[2], C. Xu[1], P. S. Julienne[3], J. Ye[4], P. Zoller[5,6], E. Demler[1,7], M. D. Lukin[1,7] and A. M. Rey[4]

Nuclear spin

$$^{87}Sr: \quad I = 9/2 \longrightarrow N_{max} = 2I + 1 = 10$$

- N=3 
- N=4 

$$|I_z = 3/2\rangle \leftrightarrow$$
$$|I_z = 1/2\rangle \leftrightarrow$$
$$|I_z = -1/2\rangle \leftrightarrow$$
$$|I_z = -3/2\rangle \leftrightarrow$$



Identify nuclear spin states with colors:

nature physics

ARTICLES

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Nuclear spin

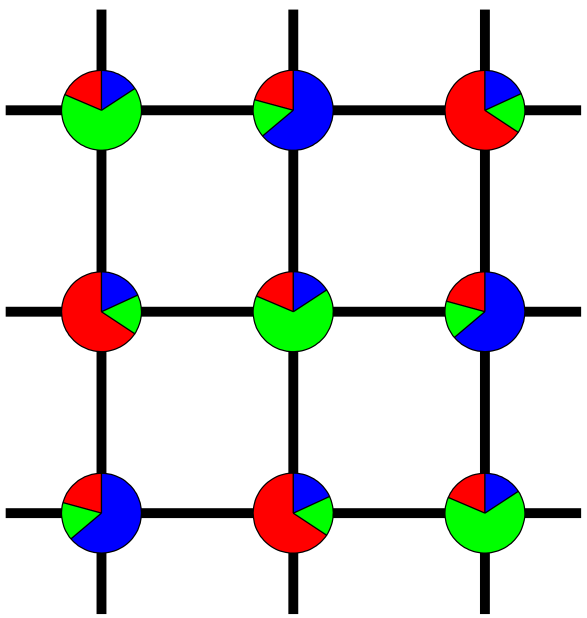
$$^{87}Sr: \quad I = 9/2 \quad \longrightarrow \quad N_{max} = 2I + 1 = 10$$

- N=3
- N=4

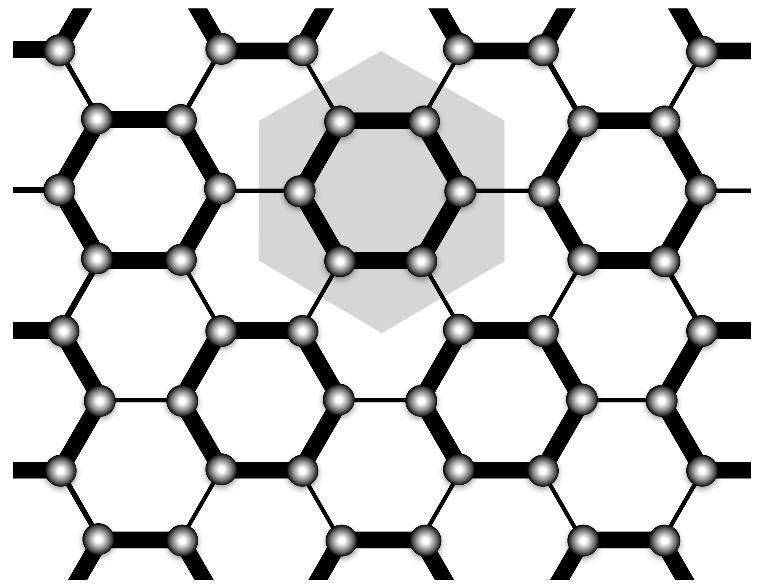
Cannot use QMC because of the **sign problem**!!!

SU(N) Heisenberg models

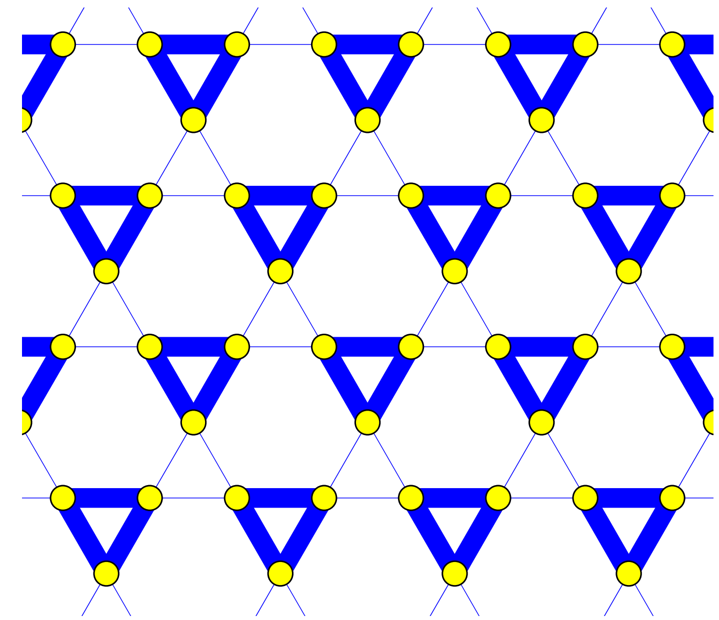
SU(3) square/triangular:
3-sublattice Néel order
Bauer, PC, et al., PRB **85** (2012)



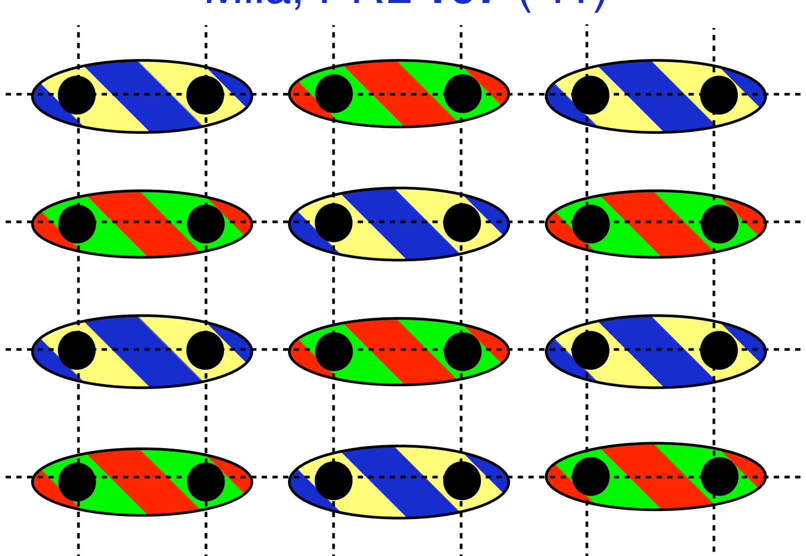
SU(3) honeycomb: *Plaquette state*
Zhao, Xu, Chen, Wei, Qin, Zhang, Xiang, PRB **85** (2012);
PC, Läuchli, Penc, Mila, PRB **87** (2013)



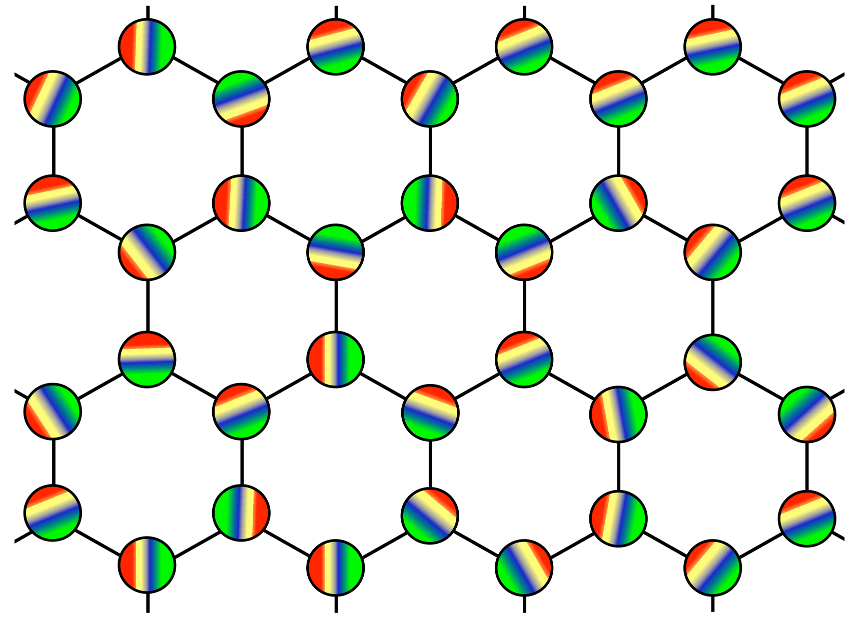
SU(3) kagome:
Simplex solid state
PC, Penc, Mila, Läuchli, PRB **86** (2012)



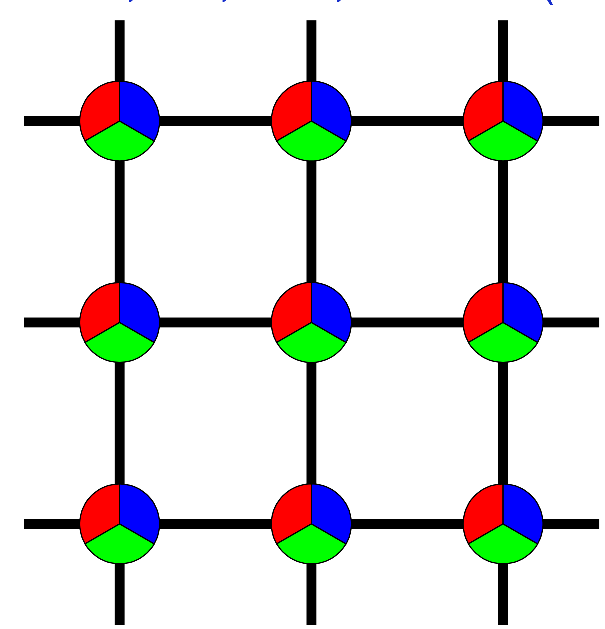
SU(4) square:
Dimer-Néel order
PC, Läuchli, Penc, Troyer, Mila, PRL **107** ('11)



SU(4) honeycomb:
spin-orbital (4-color) liquid
PC, Lajkó, Läuchli, Penc, Mila, PRX **2** ('12)

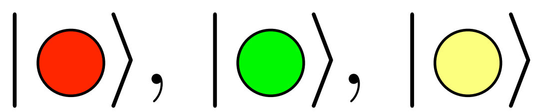


3-color quantum Potts:
superfluid phases
Messio, PC, Mila, PRB **88** (2013)

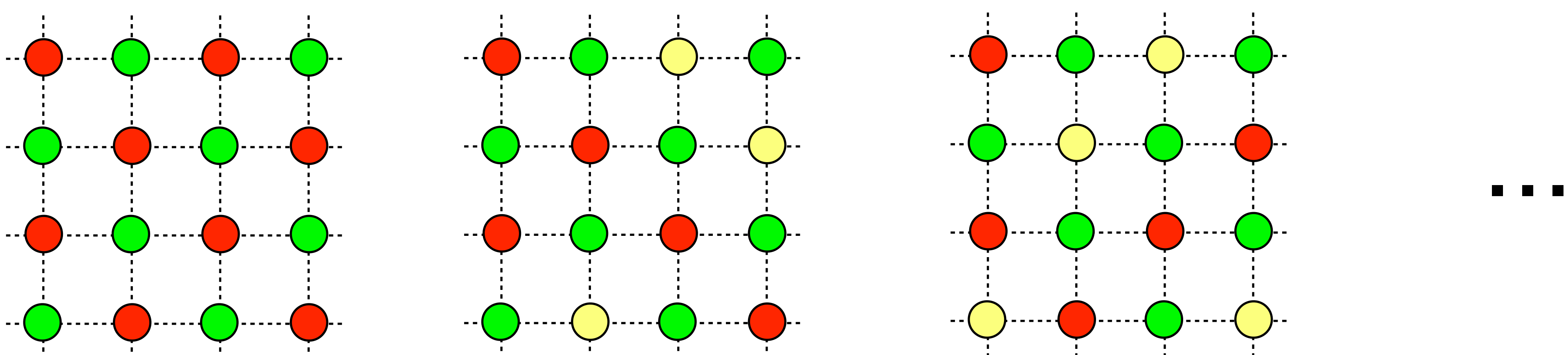


SU(3) Heisenberg model on the square lattice

- N=3: $H = \sum_{\langle i,j \rangle} P_{ij}$

  local basis states: 

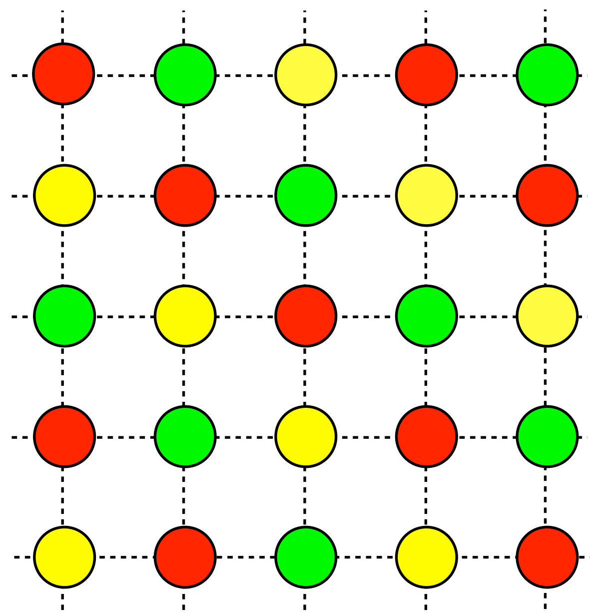
- Product state ansatz: different colors on neighboring sites



- Infinite classical ground state degeneracy!

SU(3) Heisenberg model on the square lattice

- Degeneracy lifted by quantum fluctuations:



3 sublattice
Néel order

- Exact diagonalization & linear flavor wave theory

T. A. Tóth, A. M. Läuchli, F. Mila & K. Penc, PRL 105 (2010)

- DMRG & iPEPS

Bauer, PC, Läuchli, Messio, Penc, Troyer & Mila, PRB 85 (2012)

Stability of 3-sublattice phase in an extended parameter space?

Stability of 3-sublattice phase away from SU(3) point?

$$H = \sum_{\langle i,j \rangle} \cos(\theta)\, S_i \cdot S_j + \sin(\theta)\, (S_i \cdot S_j)^2$$

$\theta = \pi/4$

SU(3) Heisenberg model

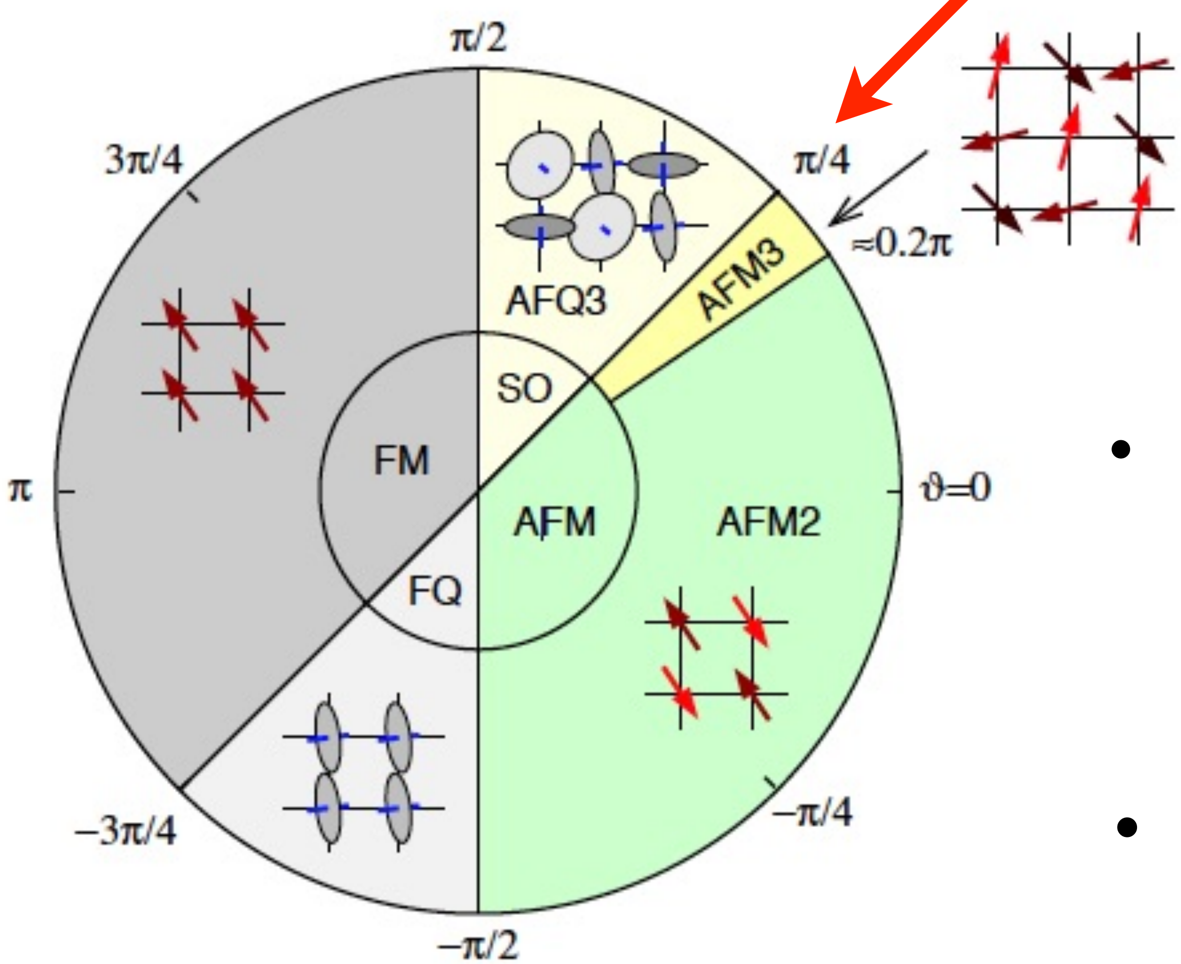


Figure from Tóth, et al. PRB 85 (2012)

- **ED + linear flavor wave theory:**
  3-sublattice state has finite extension
  Tóth, Läuchli, Mila & Penc, PRB 85 (2012)
- Compatible results: series expansion
  Oitmaa & Hamer, PRB 87 (2013)

➡ Can we reproduce this with systematic iPEPS simulations?

Motivation II: Spin nematic phases

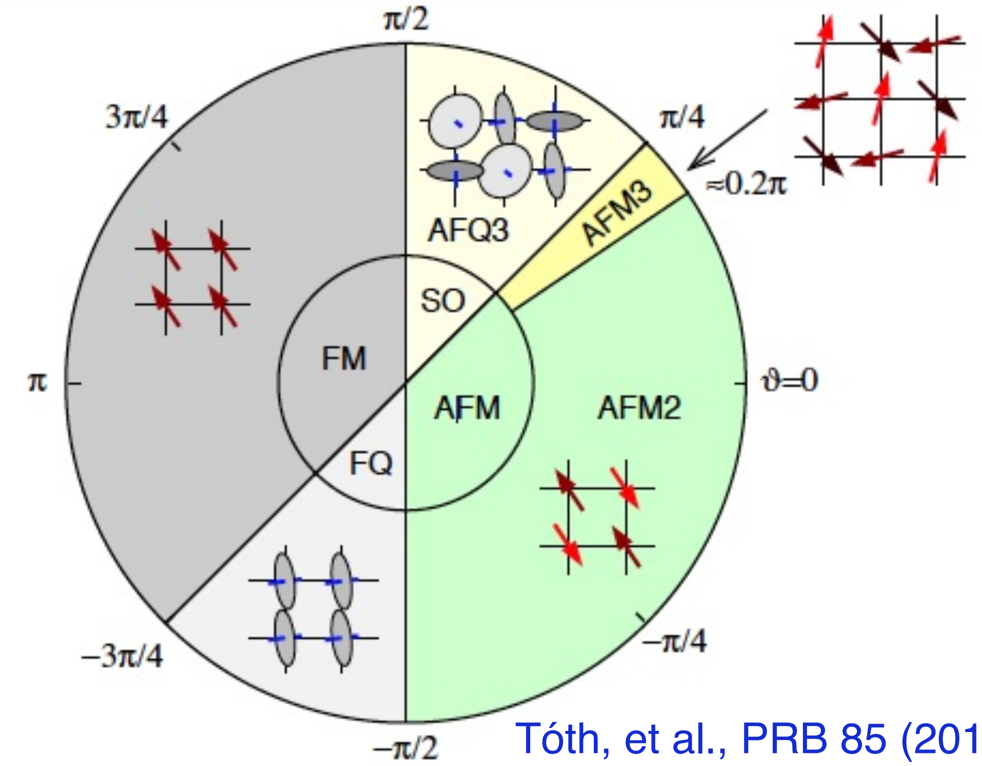
- Spin nematic phase:

  vanishing magnetic moment:

  $\langle S^x \rangle = \langle S^y \rangle = \langle S^z \rangle = 0$

  but still breaking SU(2) symmetry

  due to non-vanishing higher order moments.



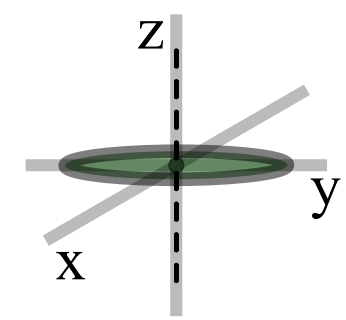
Tóth, et al., PRB 85 (2012)

- Example (S=1): $|0\rangle$

  vanishing magnetic moment, but

  $\langle (S^z)^2 \rangle = 0 \neq \langle (S^x)^2 \rangle = \langle (S^y)^2 \rangle = 1$

  ➡ Anisotropic spin fluctuations breaking SU(2) symmetry



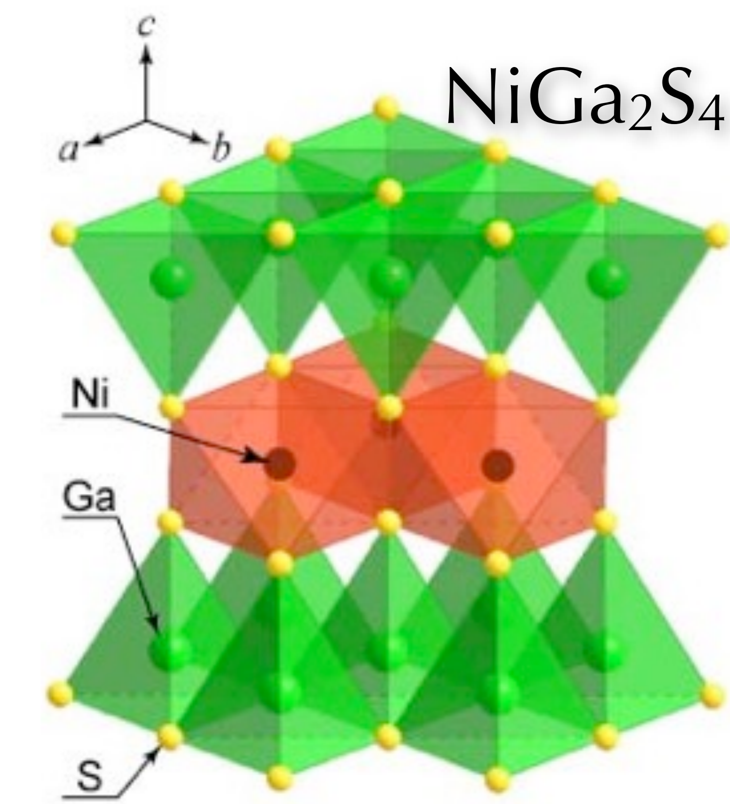
- Possible realization: $NiGa_2S_4$

  Tsunetsugu & Arikawa, J. Phys. Soc. Jap. 75 (2006)

  Tsunetsugu & Arikawa, J. Phys. Cond. Mat. 19 (2007)

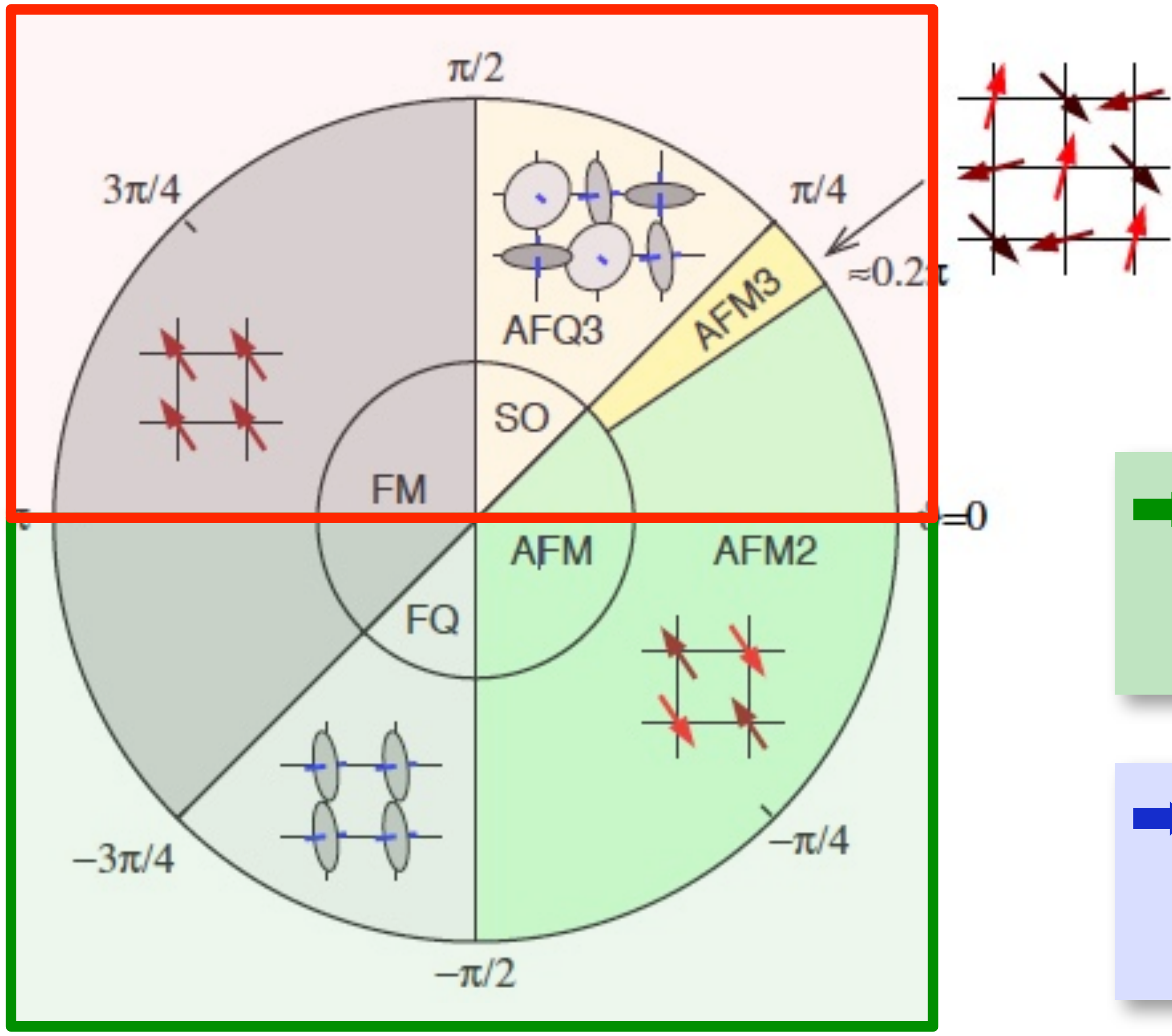
  Läuchli, Mila & Penc, PRL 97 (2006)

  Bhattacharjee, Shenoy & Senthil, PRB 74 (2006)



Nakatsuji et al., *Science* **309** (2005)

Motivation III: benchmark problem for iPEPS



- **Negative sign problem**
  controlled, systematic study
  has been lacking

➡ Obtain accurate estimate of the phase boundaries with iPEPS!

➡ turned out to be more complicated but also much richer than expected!

- Accessible by QMC:

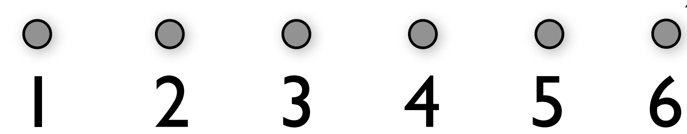
K. Harada and N. Kawashima, J. Phys. Soc. Jpn. 70 (2001)

K. Harada and N. Kawashima, PRB 65(5), 052403 (2002)

Introduction to iPEPS

Tensor network ansatz for a wave function

Lattice:



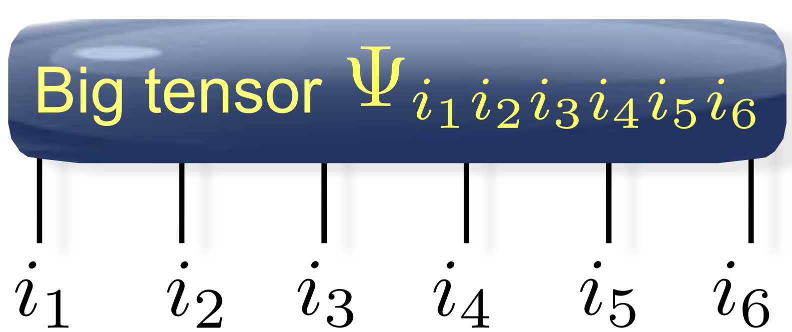
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

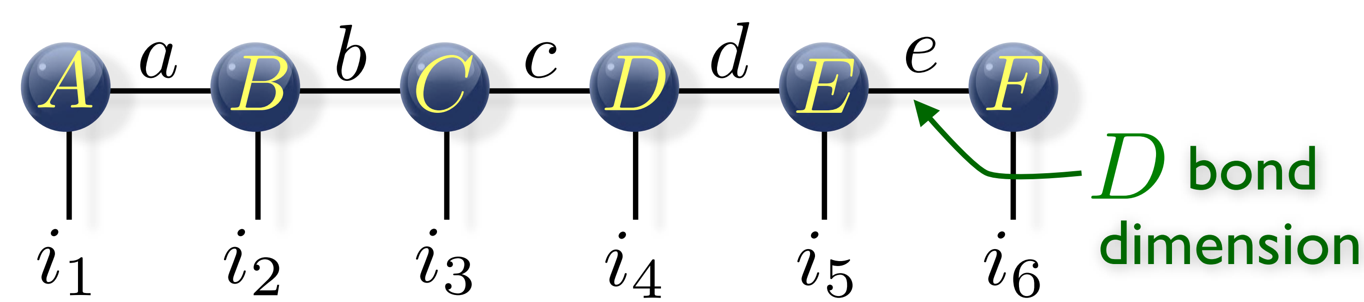
2^6 coefficients

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

Tensor/multidimensional array



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

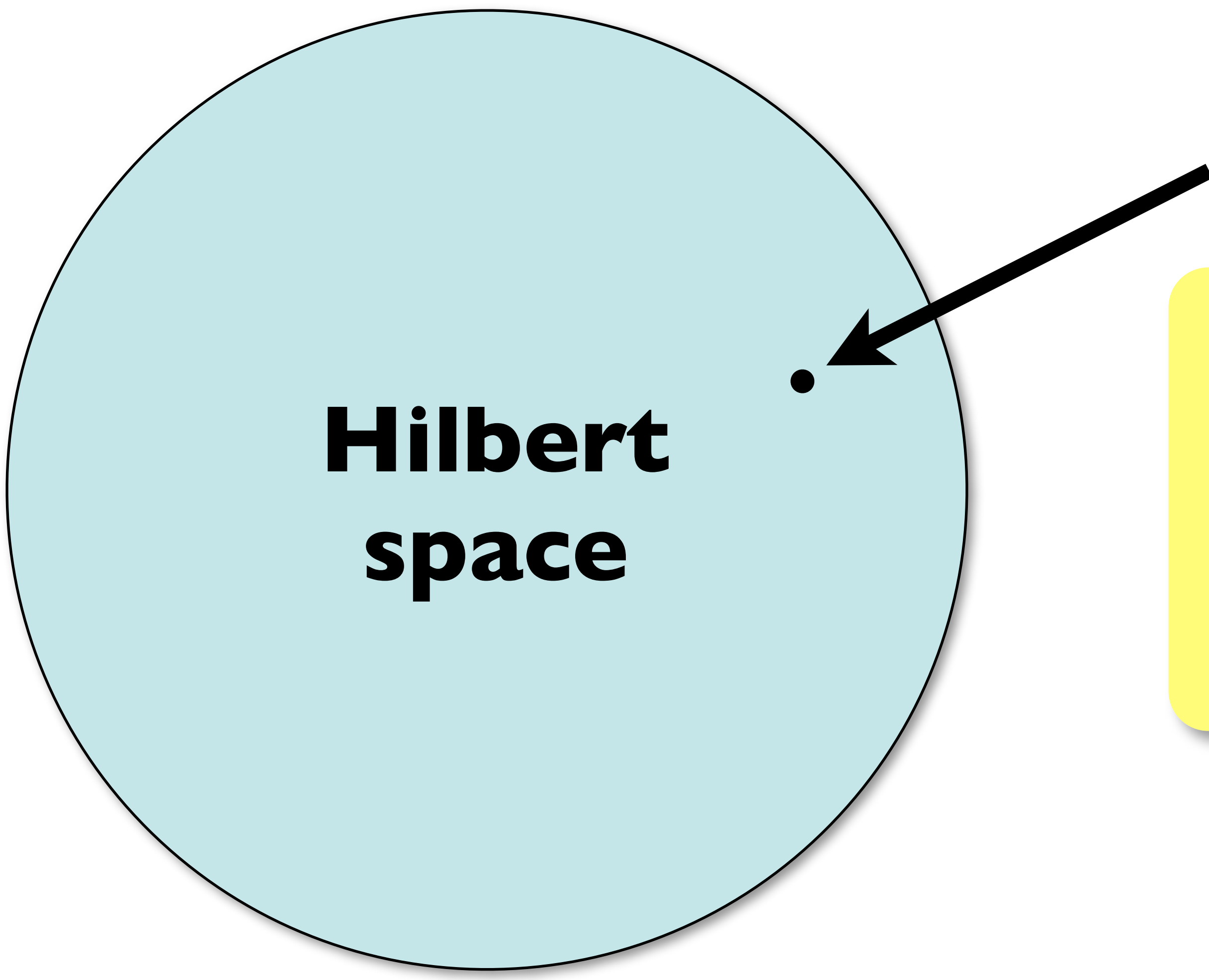


$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

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

Efficient representation!

"Corner" of the Hilbert space

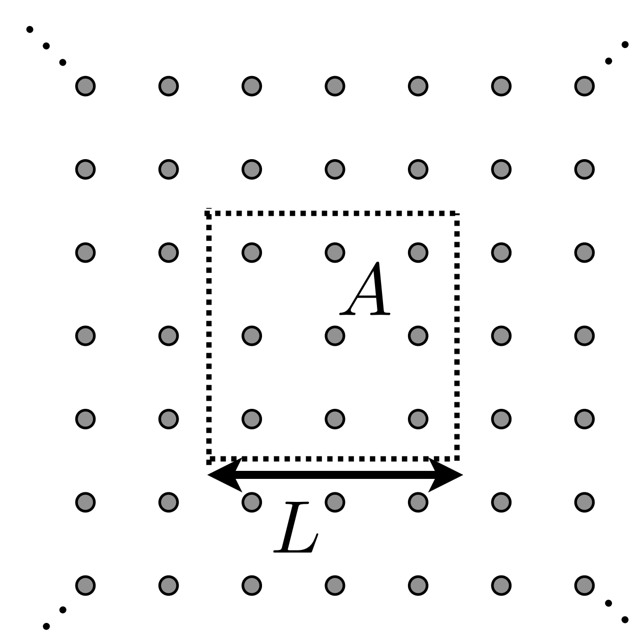


Ground states (local H)

★ GS of local H's are less entangled than a random state in the Hilbert space

★ *Area law of the entanglement entropy*

$$S(L) \sim L^{d-1}$$

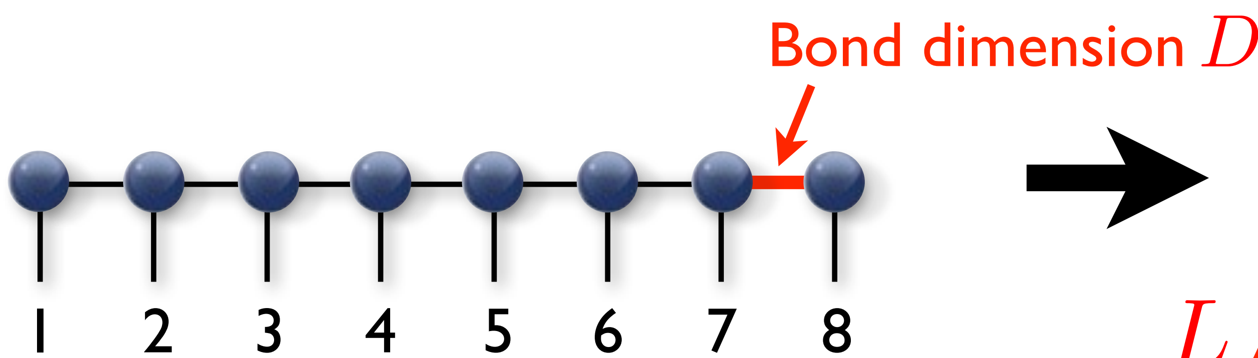


MPS & PEPS

1D

MPS

Matrix-product state
(underlying ansatz of DMRG)



Physical indices (lattices sites)

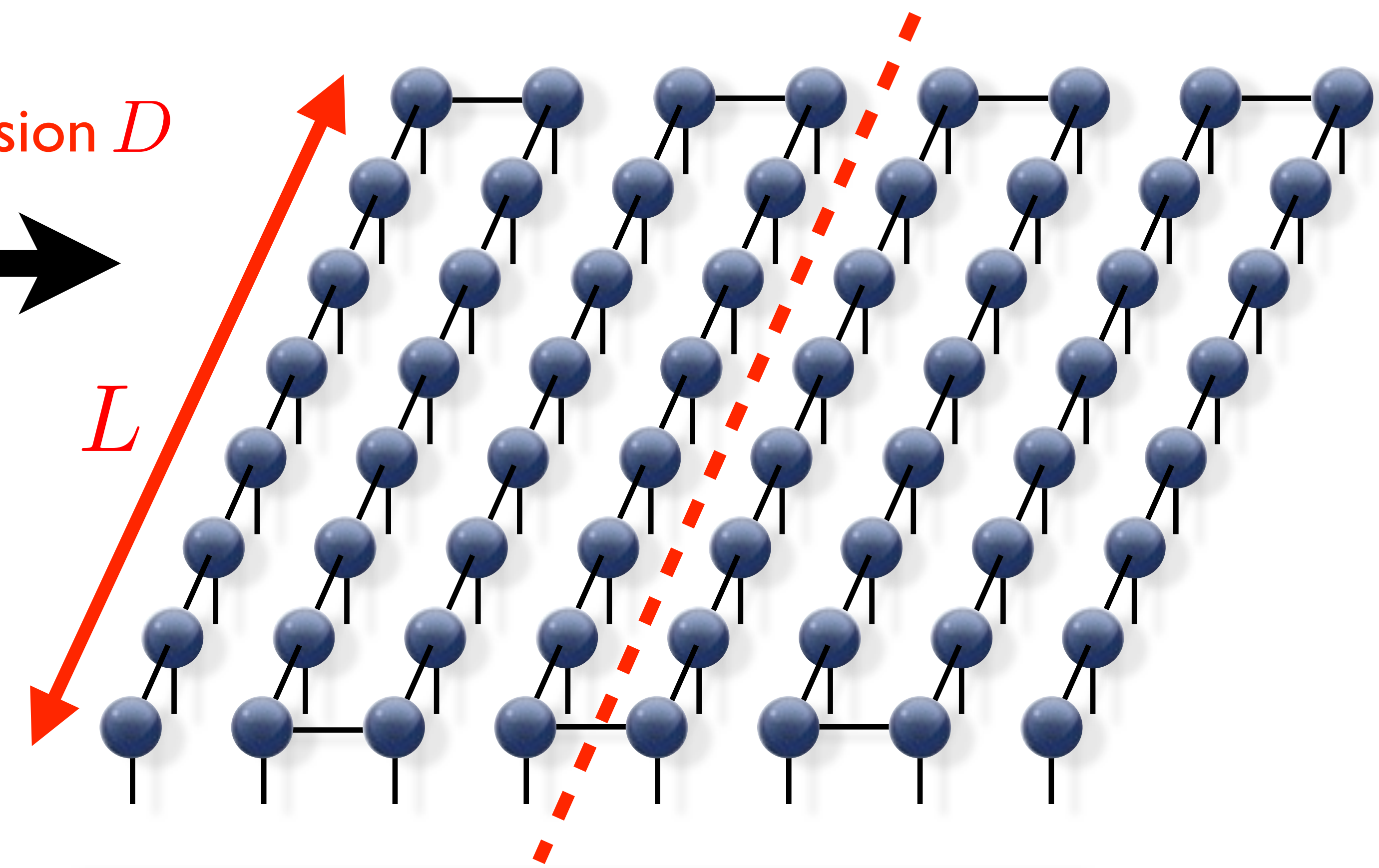
S. R. White, PRL 69, 2863 (1992)

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

Östlund, Rommer, PRL 75, 3537 (1995)

2D

Snake MPS



Computational cost:

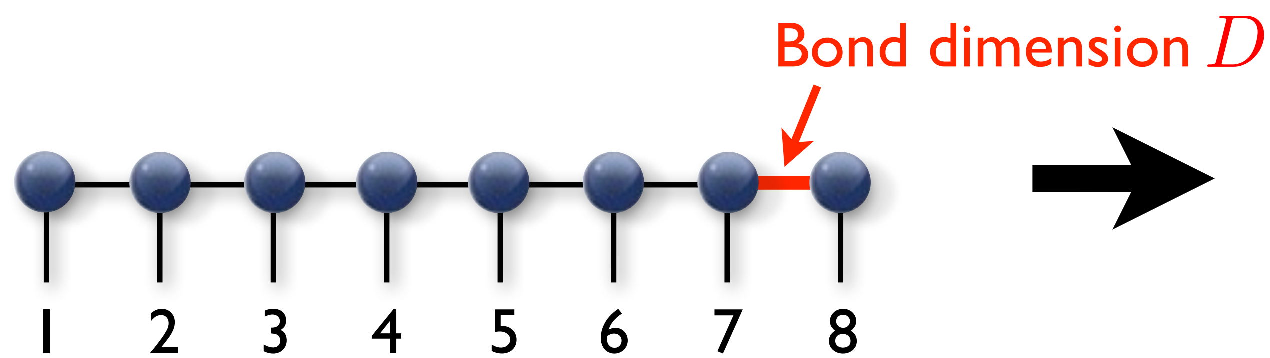
$$\propto \exp(L)$$

MPS & PEPS

1D

MPS

Matrix-product state
(underlying ansatz of DMRG)

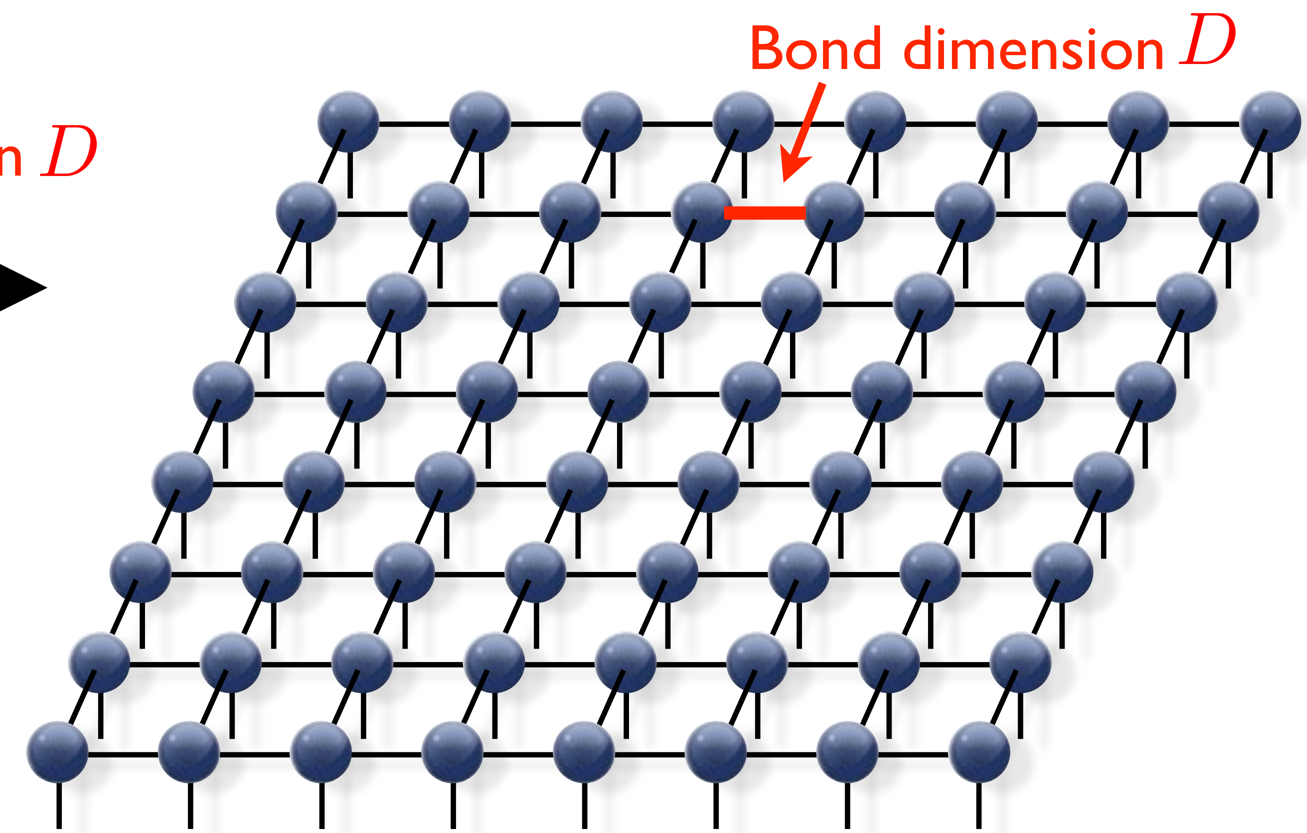


Physical indices (lattices sites)

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



Computational cost:

$$\propto poly(L, D)$$

and Gendiar,

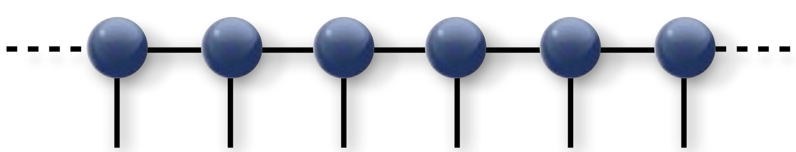
-mat/0401115

Infinite PEPS (iPEPS)

1D

iMPS

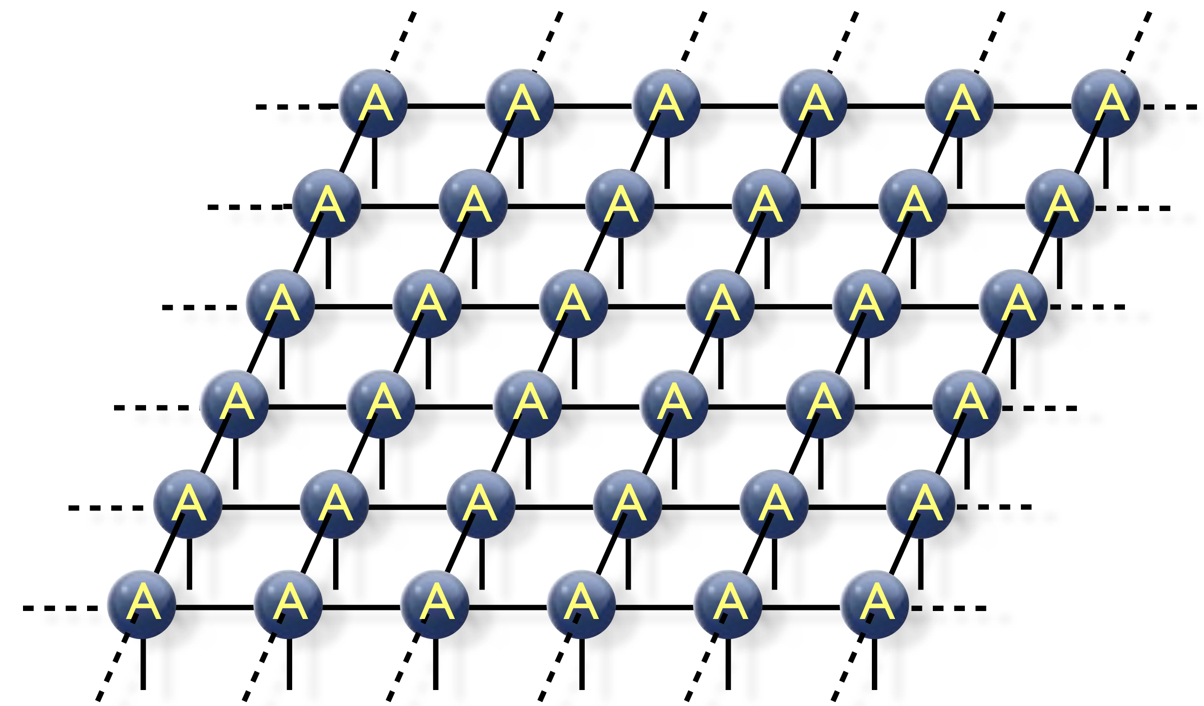
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

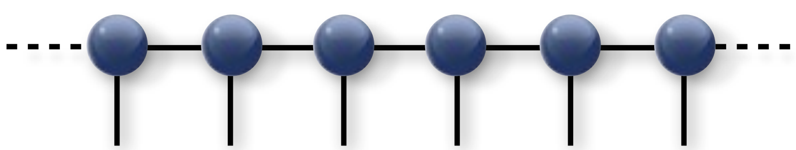
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

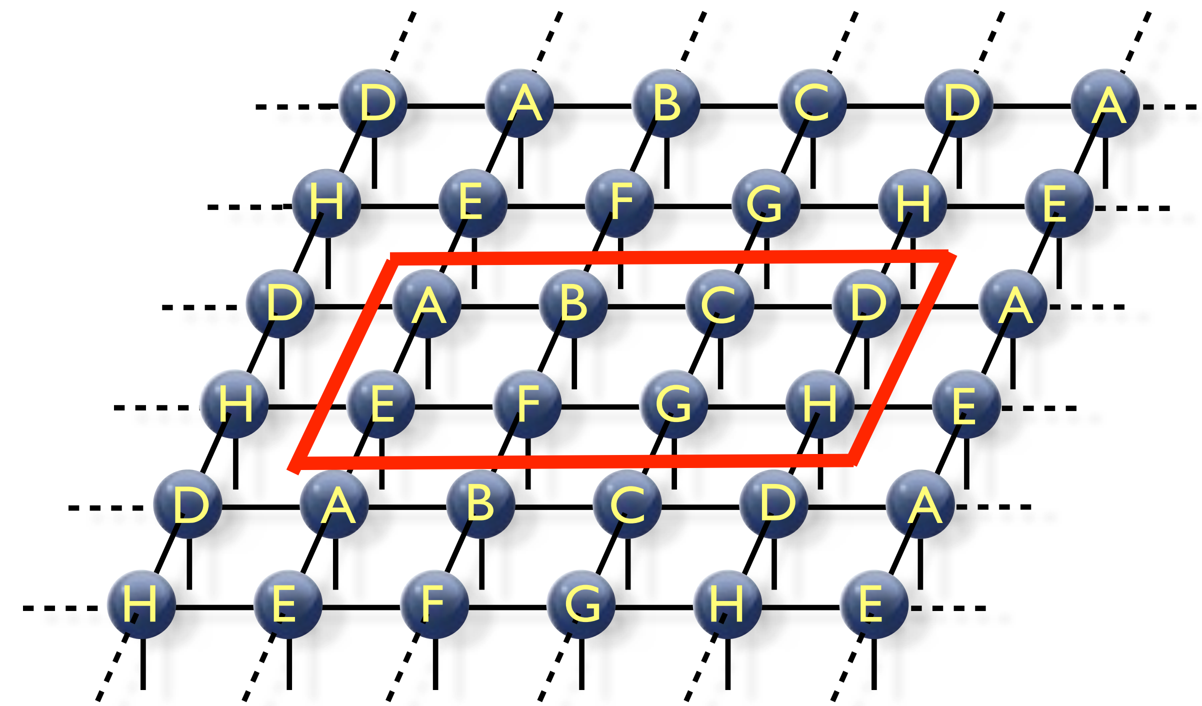
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors

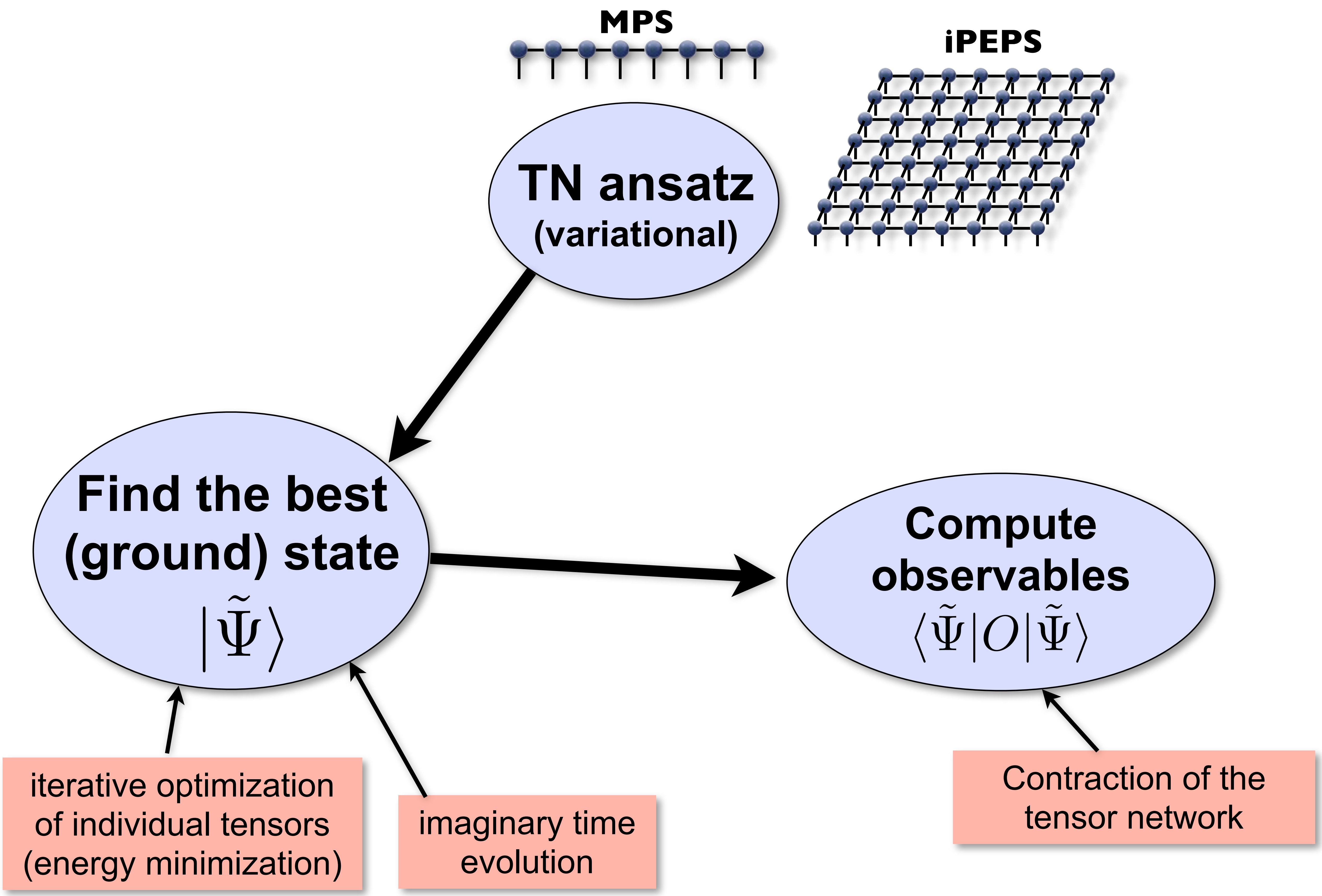


here: 4x2 unit cell

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

- ★ Run simulations with different unit cell sizes
- ★ Systematically compare variational energies

Overview: Tensor network algorithms (ground state)

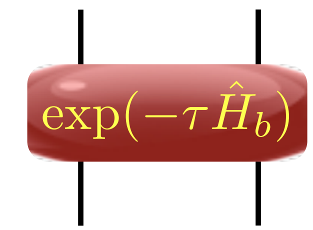


Optimization via imaginary time evolution

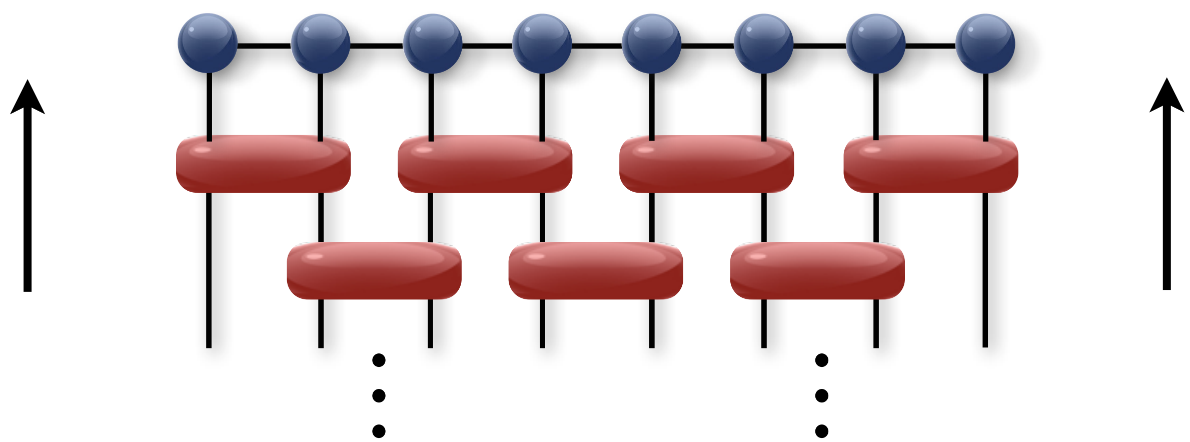
- Idea: $\exp(-\beta\hat{H})|\Psi_i\rangle \xrightarrow{\beta\to\infty} |\Psi_{GS}\rangle$

Trotter-Suzuki decomposition:

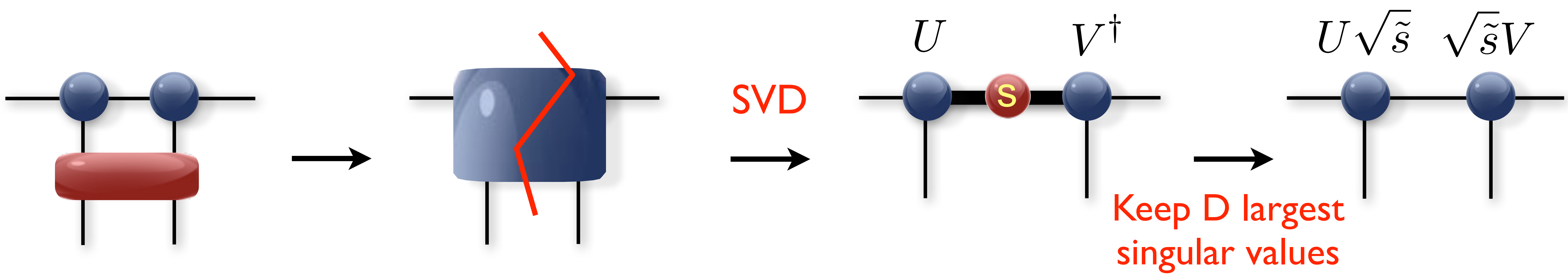
$$\exp(-\beta\hat{H}) = \exp(-\beta\sum_b \hat{H}_b) = \left(\exp(-\tau\sum_b \hat{H}_b)\right)^n \approx \left(\prod_b \exp(-\tau\hat{H}_b)\right)^n, \quad \tau = \beta/n$$



- 1D:



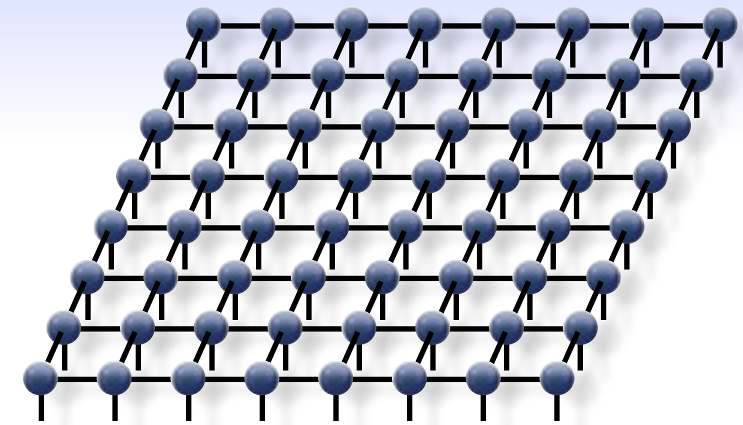
- At each step: apply a two-site operator to a bond and truncate bond back to *D*

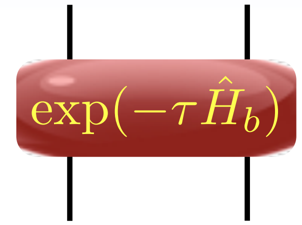


Time **E**volving **B**lock **D**ecimation (TEBD) algorithm

Note: MPS needs to be in canonical form

Optimization via imaginary time evolution



- **2D: same idea:** apply  to a bond and truncate bond back to *D*

- **However**, SVD update is not optimal (because of loops in PEPS)!

simple update (SVD)

Jiang et al, PRL 101 (2008)

★ "local" update like in TEBD

★ Cheap, but not optimal (e.g. overestimates magnetization in S=1/2 Heisenberg model)

★ reasonable energy estimates

full update

Jordan et al, PRL 101 (2008)

★ Take the full wave function into account for truncation

★ optimal, but computationally more expensive

★ Fast-full update [Phien et al, PRB 92 (2015)]

Overview: iPEPS simulations

- interacting spinless fermions
  - honeycomb & square lattice
- t-J model & Hubbard model
  - square lattice
- SU(N) Heisenberg models
  - N=3 square, triangular, kagome & honeycomb lattice
  - N=4 square, honeycomb & checkerboard lattice
  - N=5 square lattice
  - N=6 honeycomb lattice
- frustrated spin systems
  - Shastry-Sutherland model
  - Heisenberg model on kagome lattice
  - Bilinear-biquadratic S=1 Heisenberg model
  - Kitaev-Heisenberg model
  - J1-J2 Heisenberg model
- and many more...

iPEPS is a very **competitive** variational method!

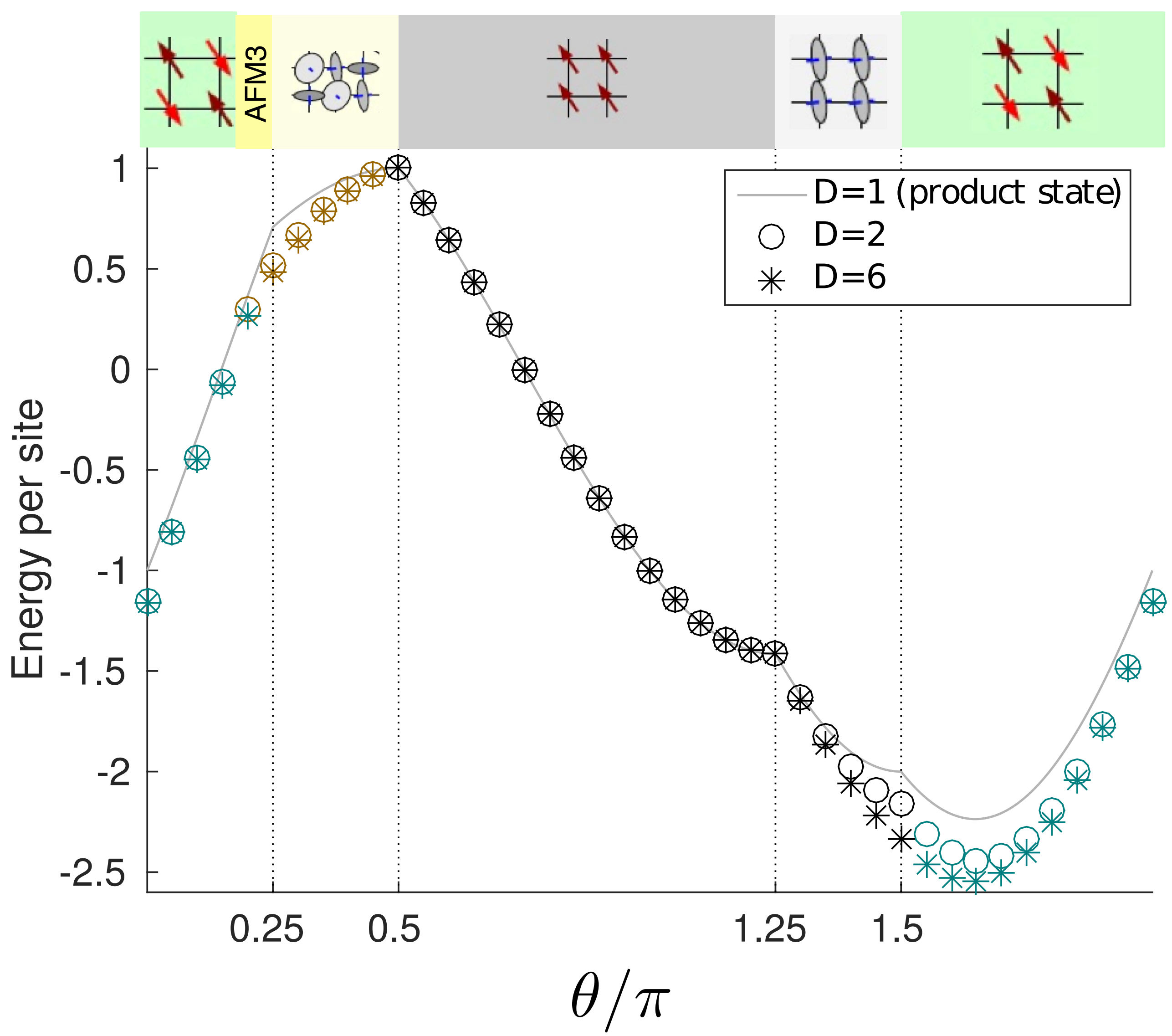
Find new physics thanks to (largely) unbiased simulations

Results:

S=1 bilinear-biquadratic Heisenberg model

Low-D iPEPS (simple update) results

$$H = \sum_{\langle i,j \rangle} \cos(\theta)\, S_i \cdot S_j + \sin(\theta)\, (S_i \cdot S_j)^2$$



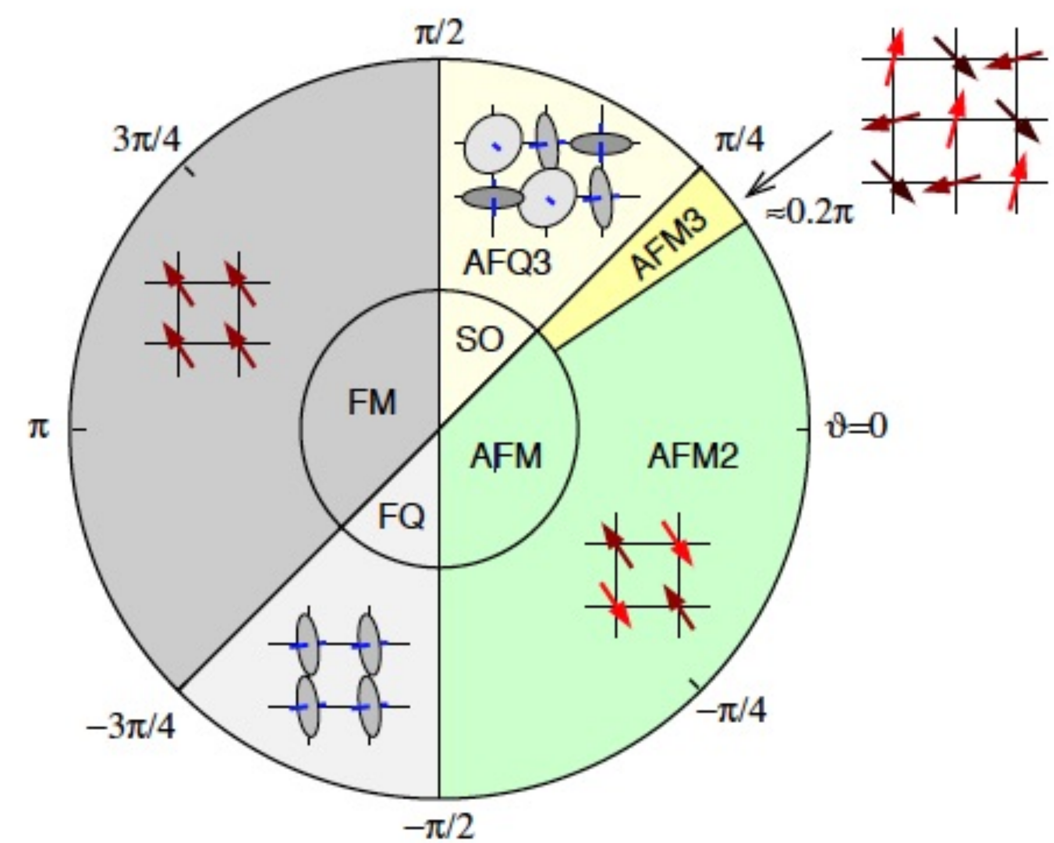


Figure from Tóth, et al. PRB 85 (2012)

- Simple update results reproduces previous phase diagram!

Low-D simple update result

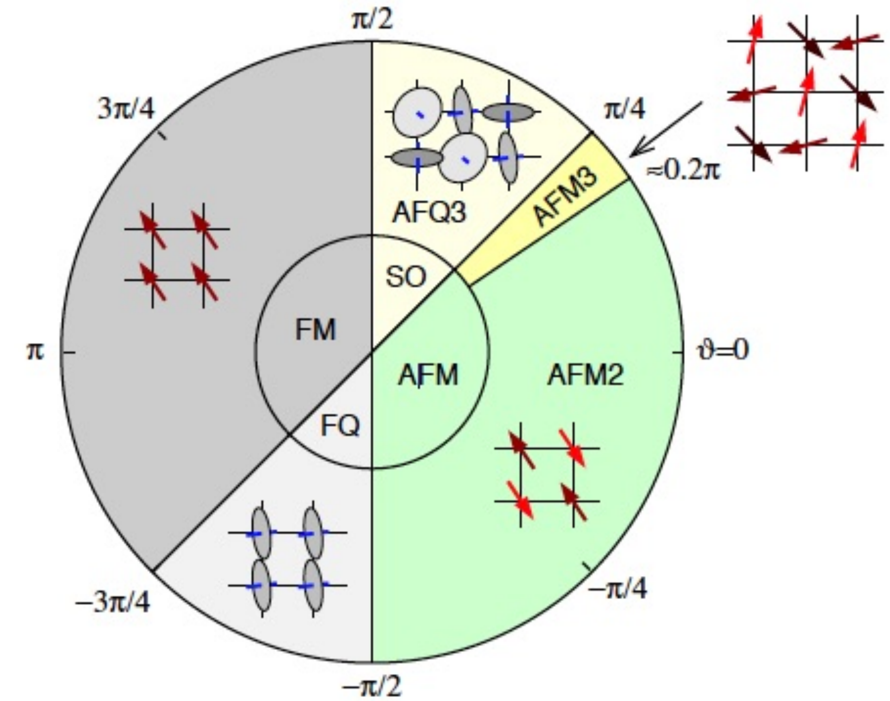
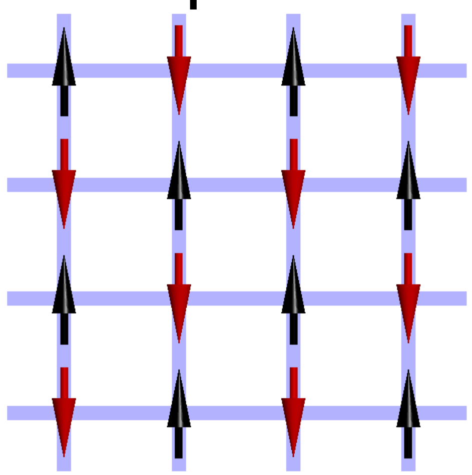


Figure from Tóth, et al. PRB 85 (2012)

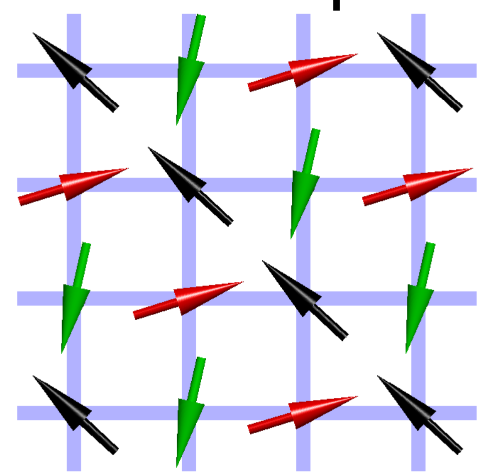
2-sublattice iPEPS:

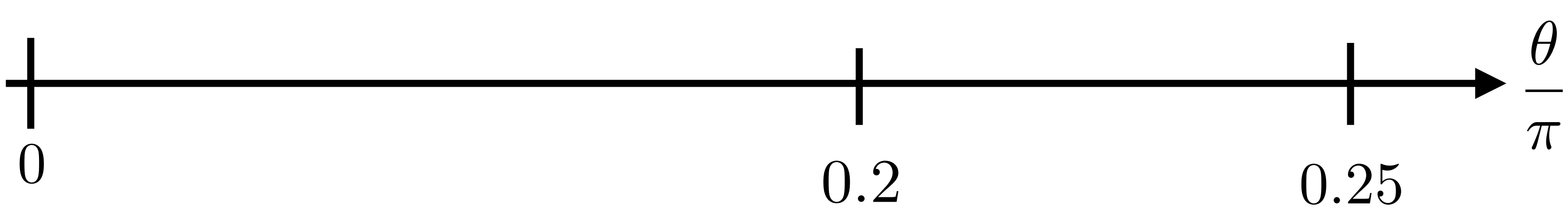
AF phase



3-sublattice iPEPS:

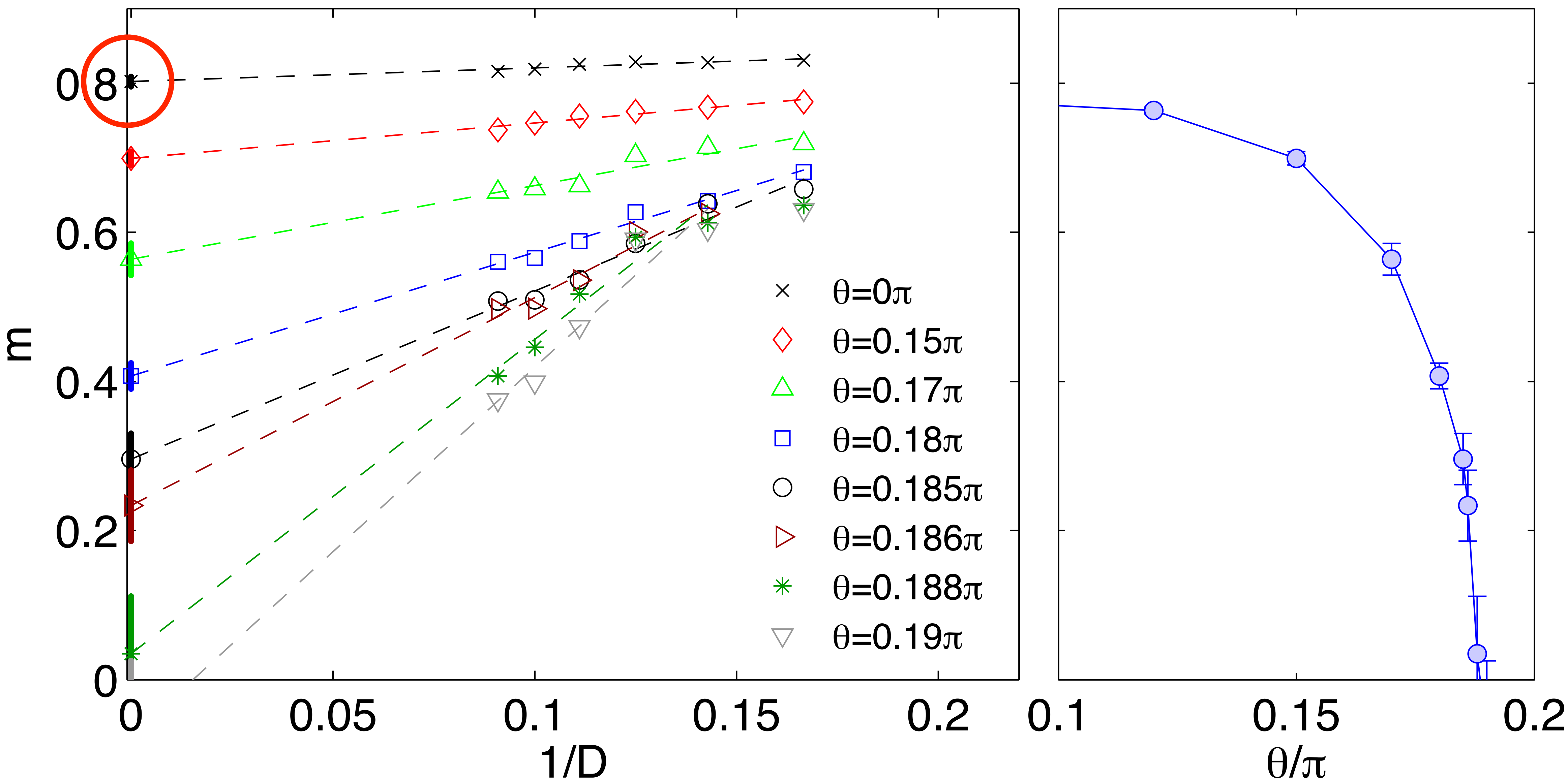
3-SL 120° phase





- Simple update result: transition around $\theta/\pi \approx 0.2 \ldots 0.21$
  in agreement with previous studies

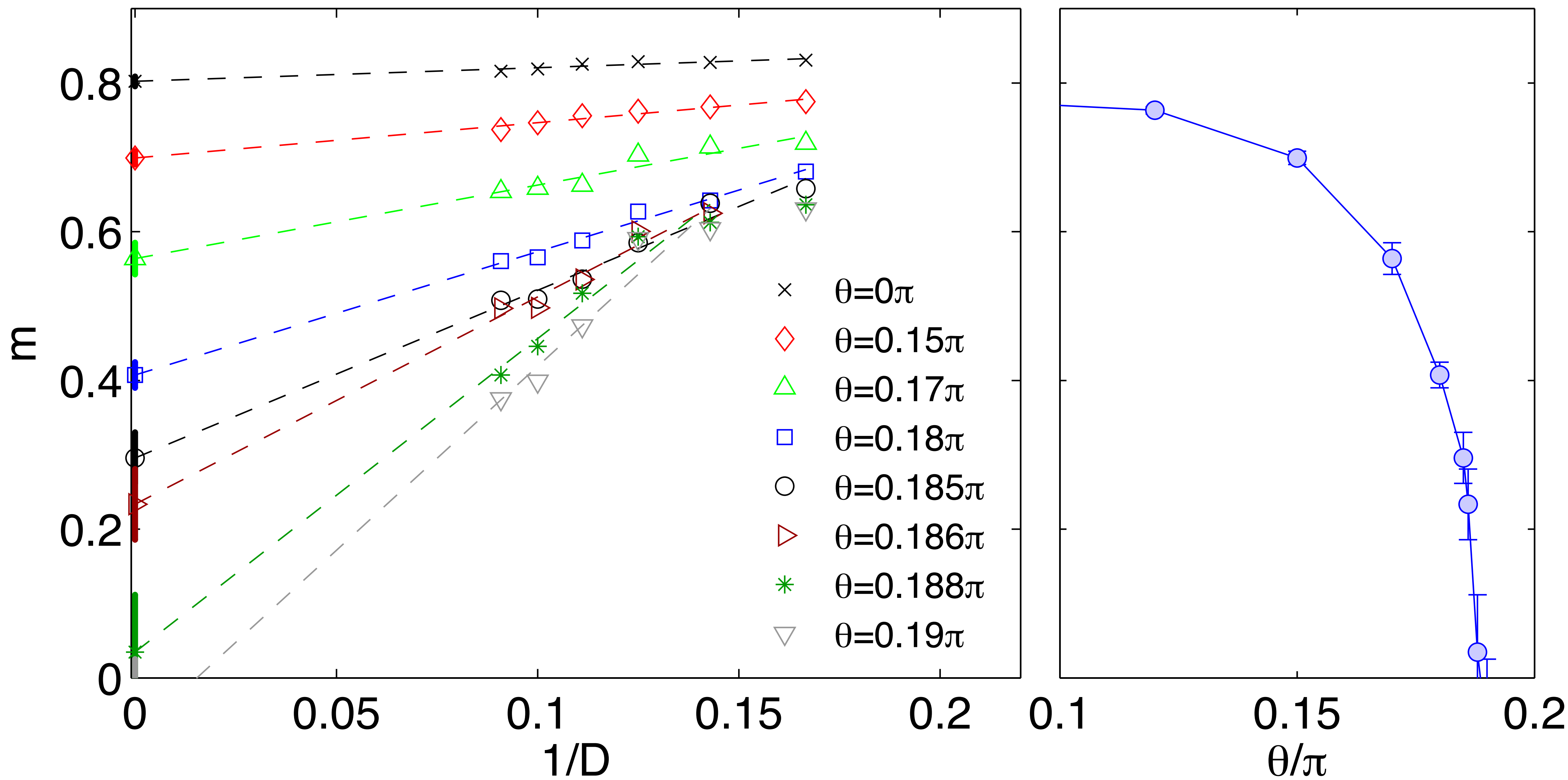
Accurate full update simulations



Heisenberg point ($\theta = 0$): QMC: m=0.805(2)
iPEPS: m=0.802(7)

Matsumoto et al. PRB 65 (2001)

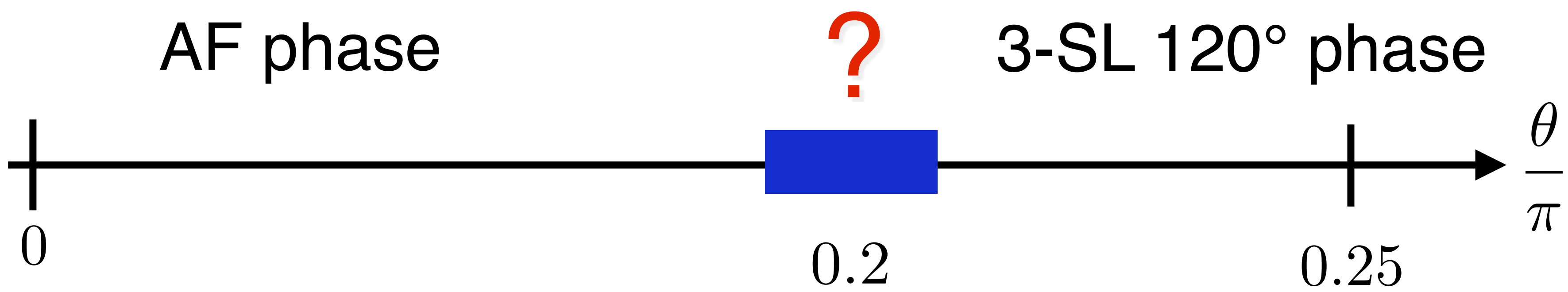
Accurate full update simulations



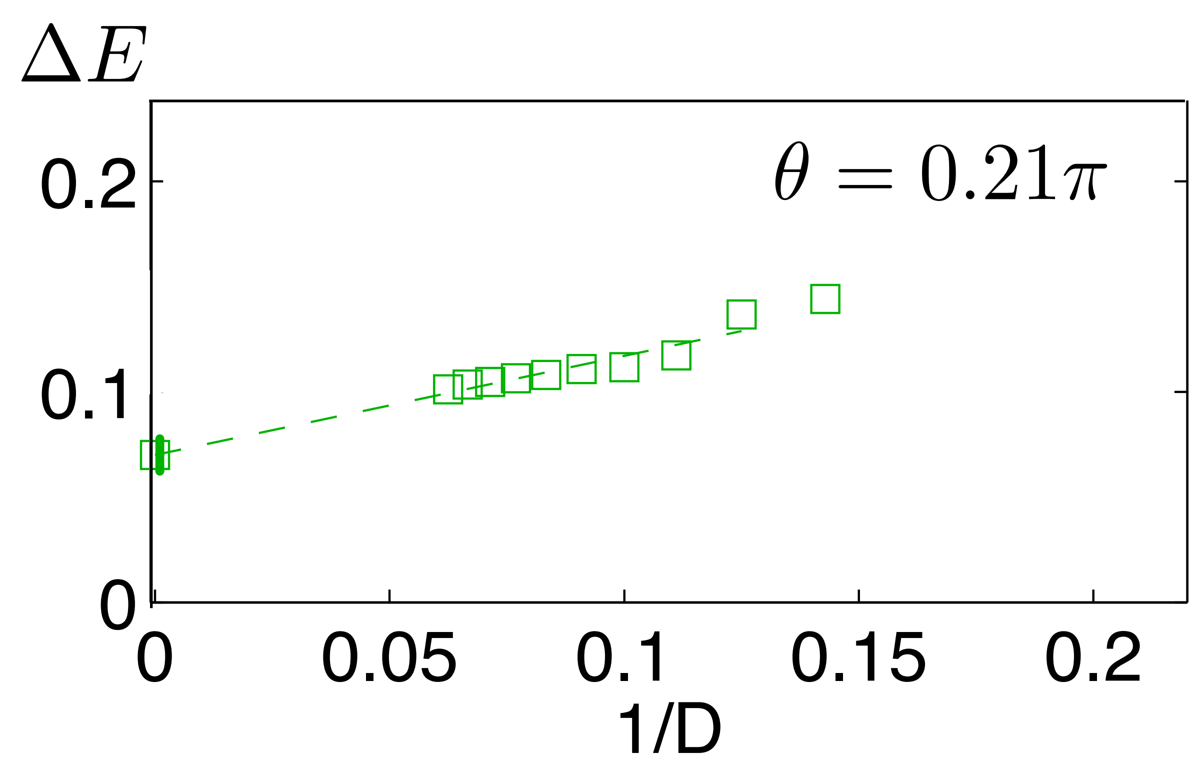
Magnetization **vanishes** beyond $\theta/\pi = 0.189(2)$ **!!**

i.e. BEFORE entering the 3-sublattice phase

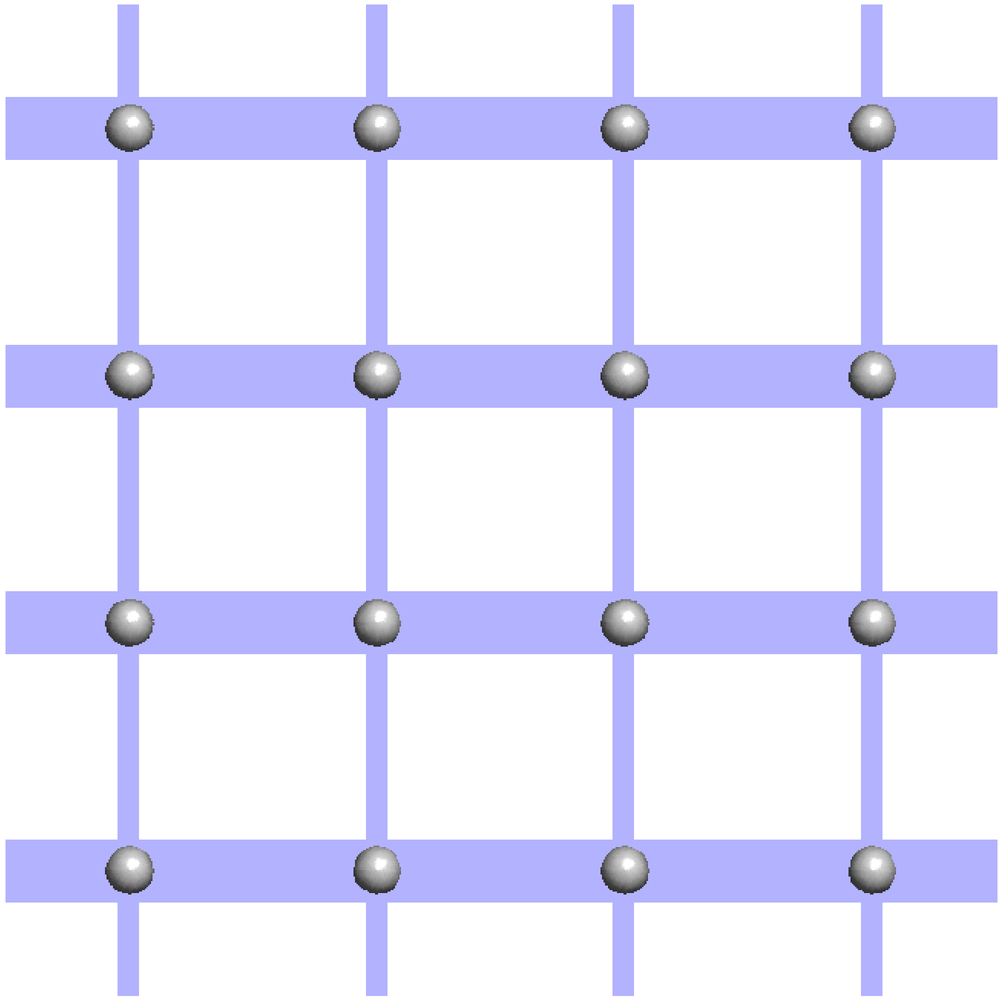
Intermediate phase?



- Vanishing magnetic moment (and vanishing quadrupolar order)
  No SU(2) symmetry breaking
- Same state can also be obtained using a 1x1 unit cell ansatz
  No translational symmetry breaking
- Energies different in x- / y- direction
  Rotational symmetry breaking



Intermediate phase?



- **No SU(2) & translational symmetry breaking**
- **BUT rotational symmetry breaking**

?

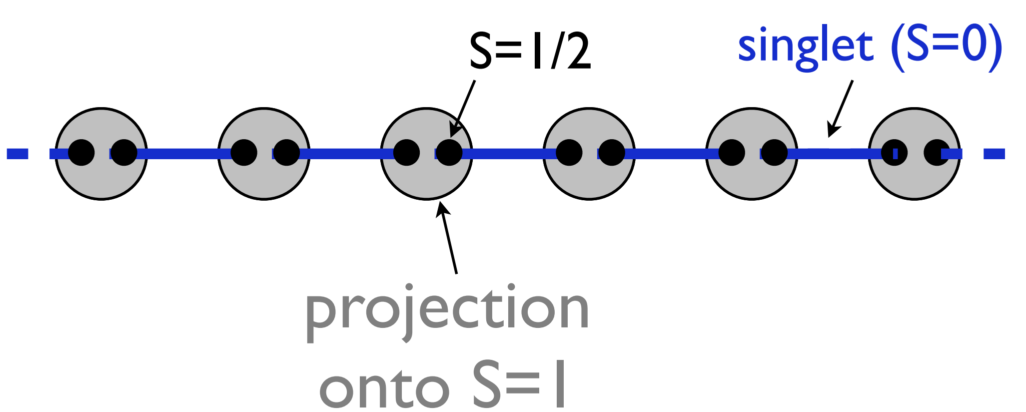
- **Reminiscent of coupled 1D chains!**
- **Is it linked to 1D physics?**

Reminder: S=1 chains in 1D

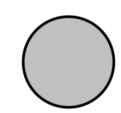
- Bilinear-biquadratic S=1 chain:

  Haldane phase for $-1/4 < \theta/\pi < 1/4$

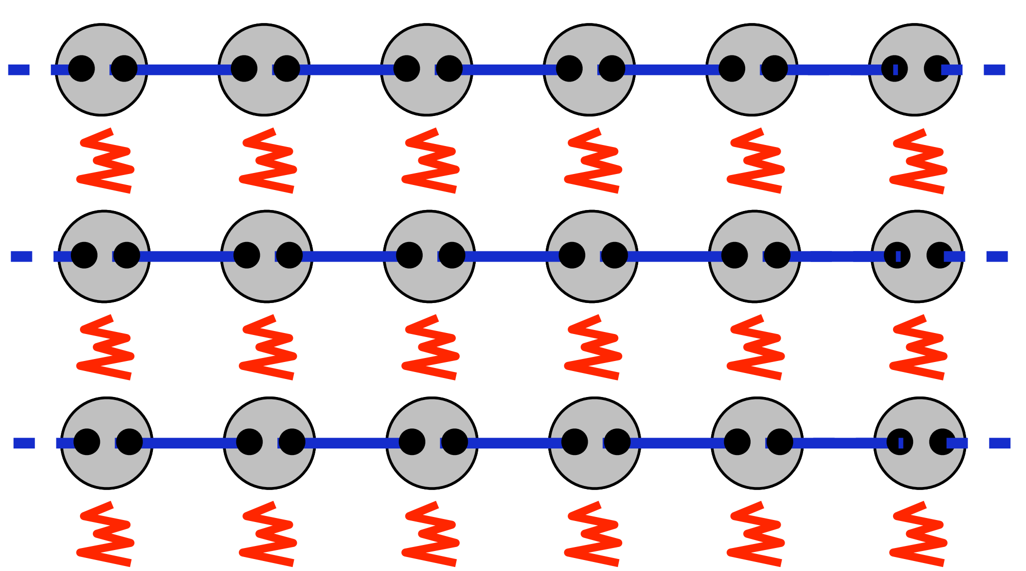
  with exact AKLT ground state for $\theta/\pi = 0.1024$



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

 $= |+\rangle\langle\uparrow\uparrow| + |0\rangle \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$

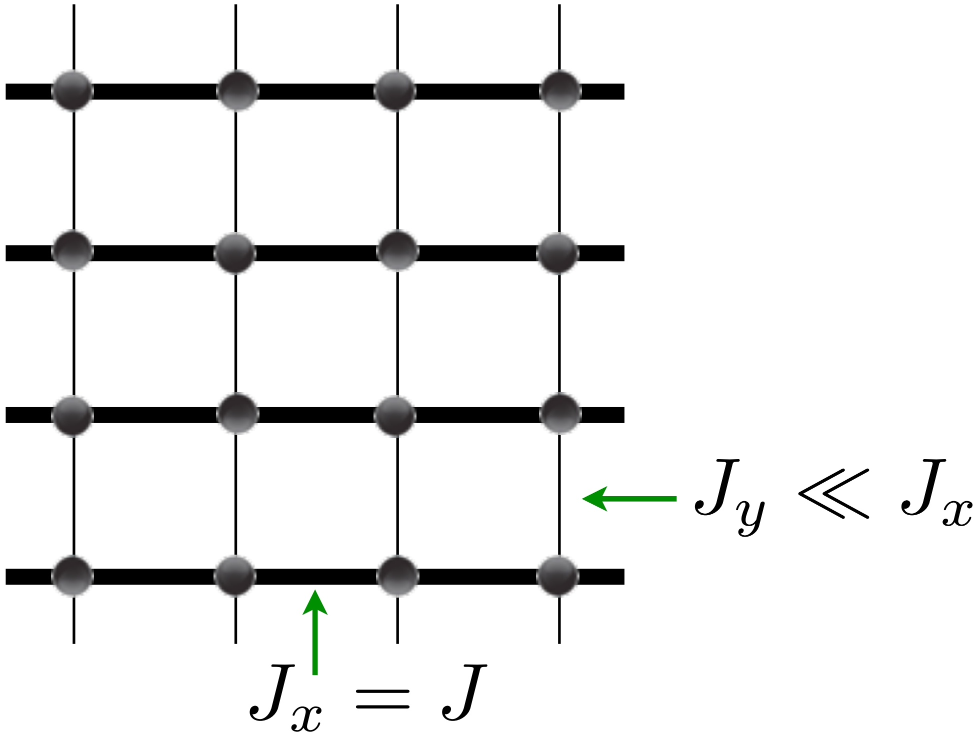
- What happens upon coupling many 1D Haldane chains?



?

Coupled S=1 Heisenberg chains

- Heisenberg case ($\theta = 0$): accessible by QMC simulations



Sakai & Takahashi, J. Phys. Soc. Jpn. 58 (1989)
Koga & Kawakami, PRB 61 (2000)
Kim & Birgeneau, PRB 62 (2000)
Matsumoto, Yasuda, Todo & Takayama, PRB 65 (2001)
Wierschem & Sengupta, PRL 112 (2014)

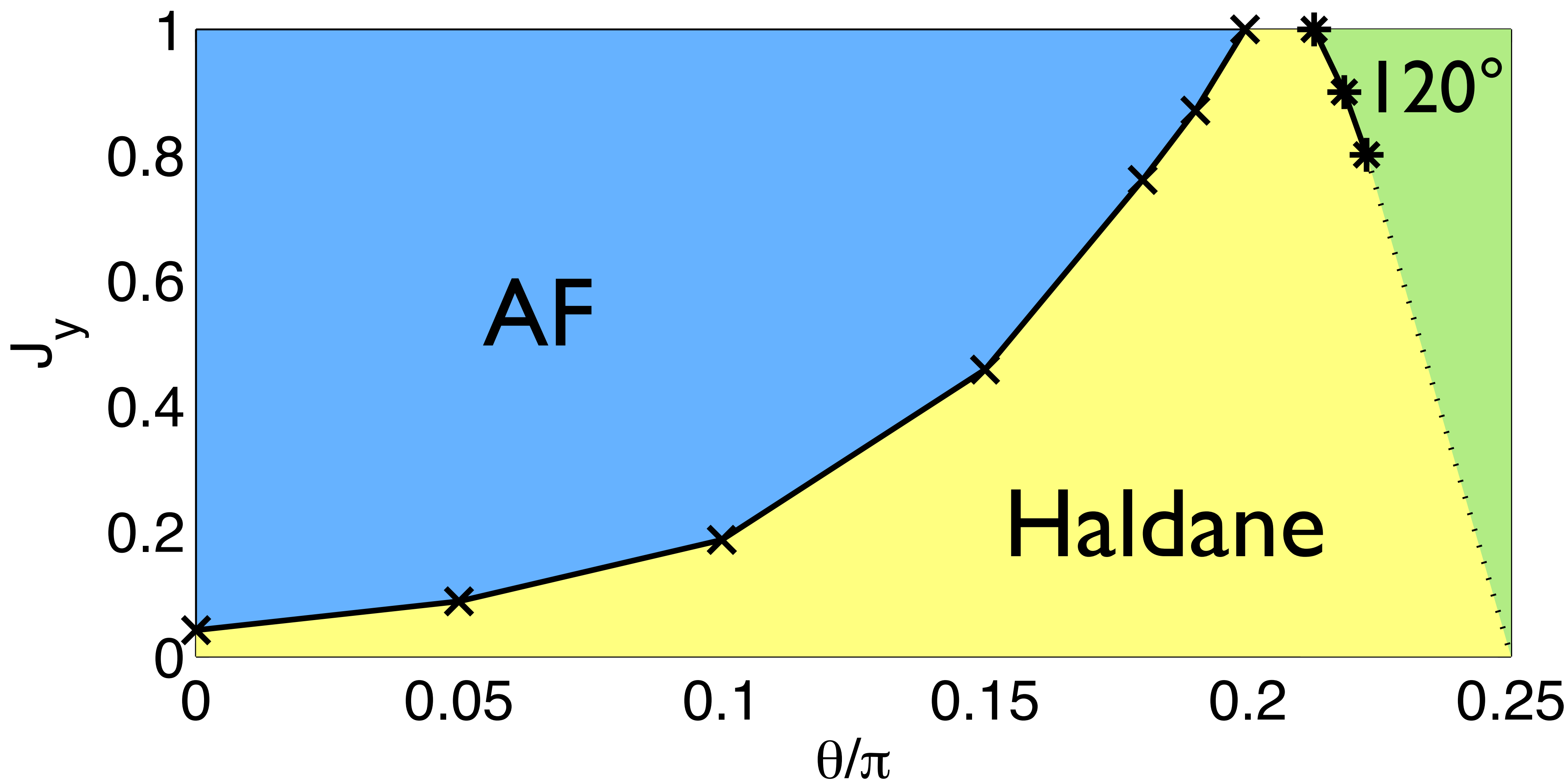
- Haldane phase stable only up to $J_y/J \approx 0.0436$

  before entering AF phase, i.e far away from the isotropic limit!

- **But for $\theta > 0$?**

Anisotropic S=1 bilinear-biquadratic model

- iPEPS phase diagram (simple update D=10)



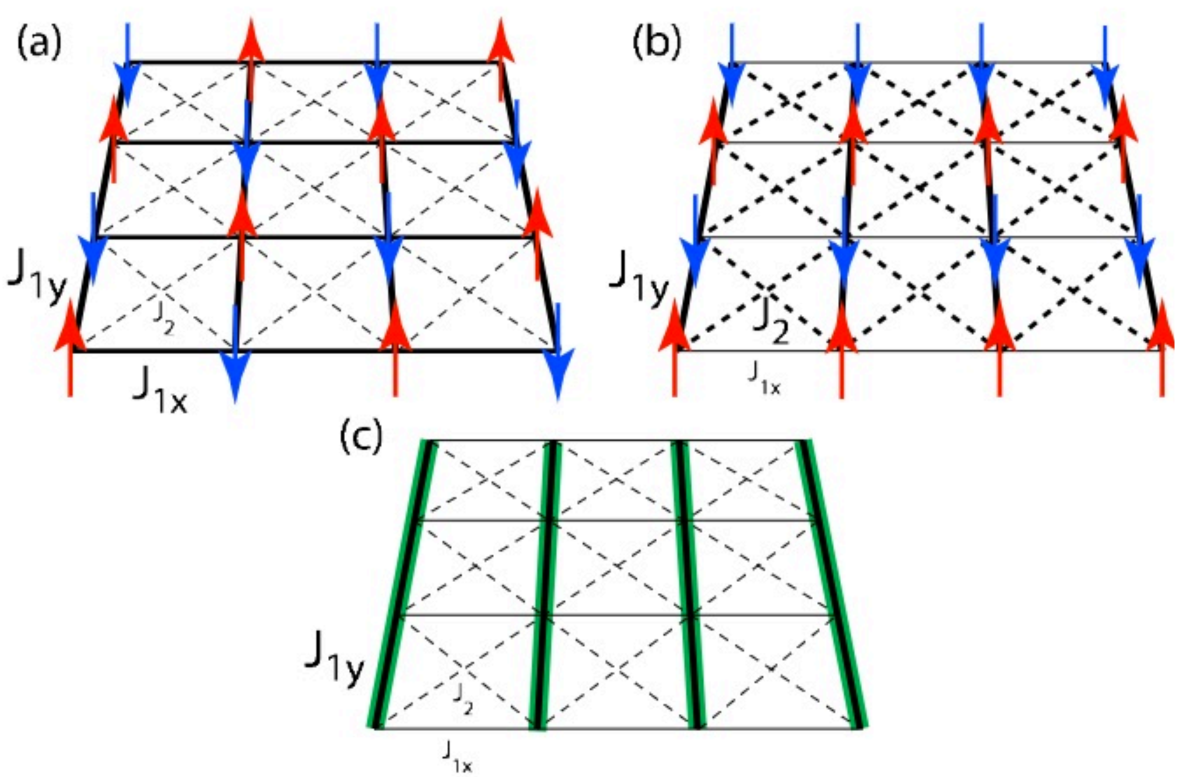
- $\theta = 0$ case: consistent with QMC $(J_y^c \approx 0.042)$
- J_y^c increases with θ

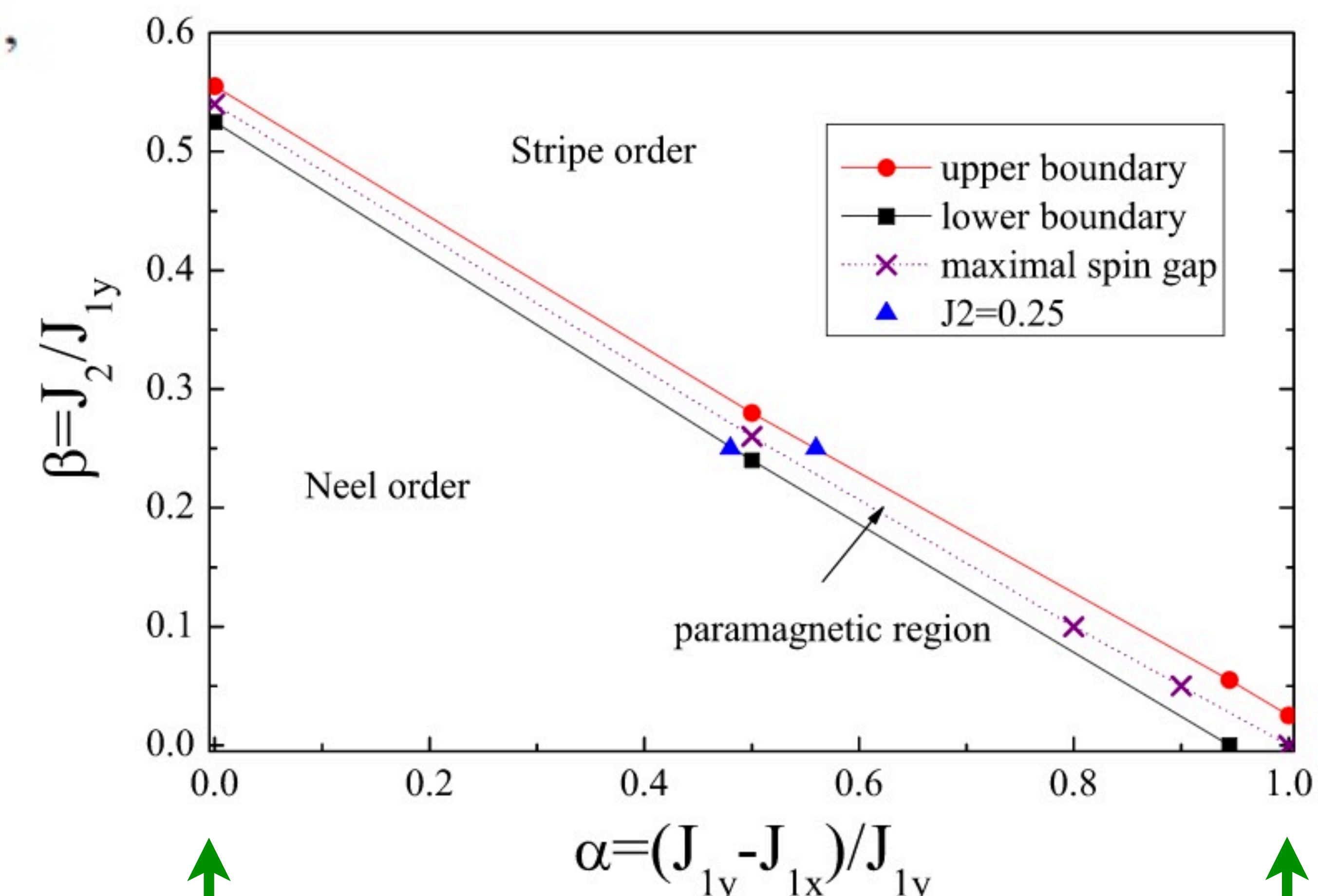
- **Haldane phase persists up to the isotropic 2D limit!**

Similar situation: frustrated S=1 anisotropic Heisenberg model

DMRG + SBMFT study: Jiang, Krüger, Moore, Sheng, Yaanen, and Weng, PRB 79 (2009)

$$H = J_{1x}\sum_{\langle i,j\rangle_x} \mathbf{S}_i\mathbf{S}_j + J_{1y}\sum_{\langle i,j\rangle_y} \mathbf{S}_i\mathbf{S}_j + J_2\sum_{\langle\langle i,j\rangle\rangle} \mathbf{S}_i\mathbf{S}_j,$$





isotropic limit

decoupled chains

- Also in this case: Haldane phase persists up to the isotropic 2D limit!

Transition between Haldane - 3 sublattice 120° phase

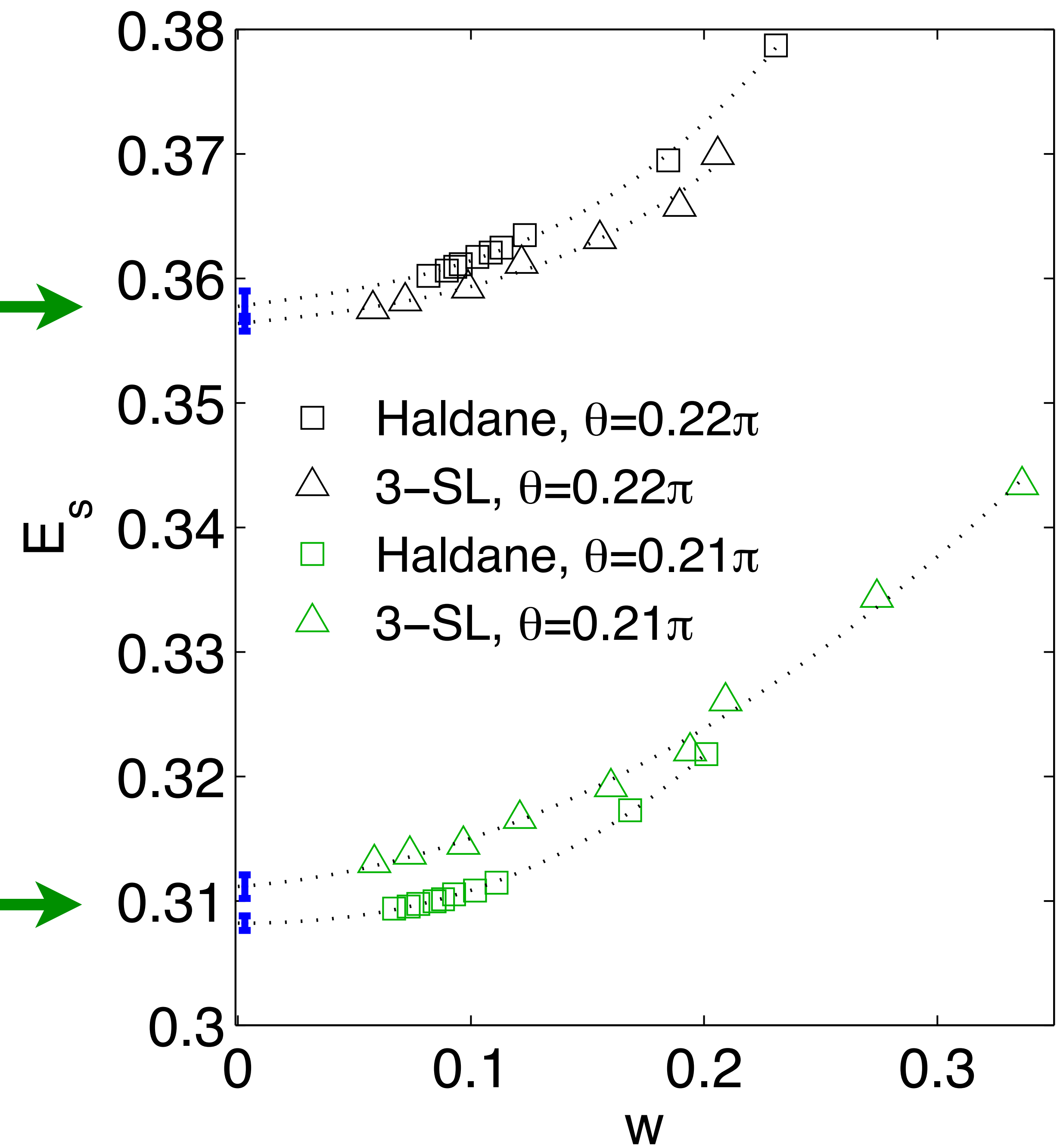
- Push full update simulations up to D=16 (D=10)

$\theta/\pi = 0.22$

3-sublat. phase lower

$\theta/\pi = 0.21$

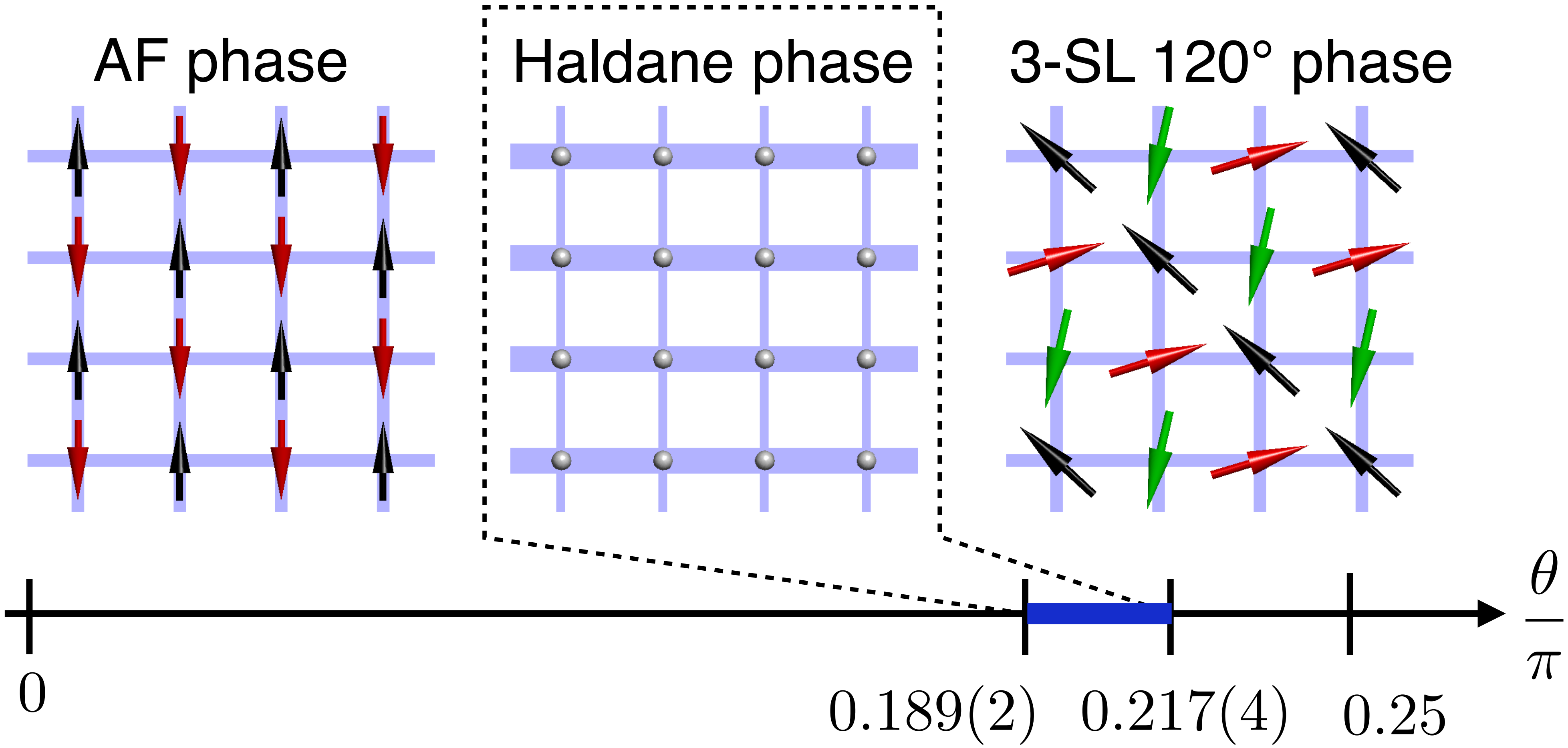
Haldane phase lower



- Energies intersect at $\theta/\pi = 0.217(4)$

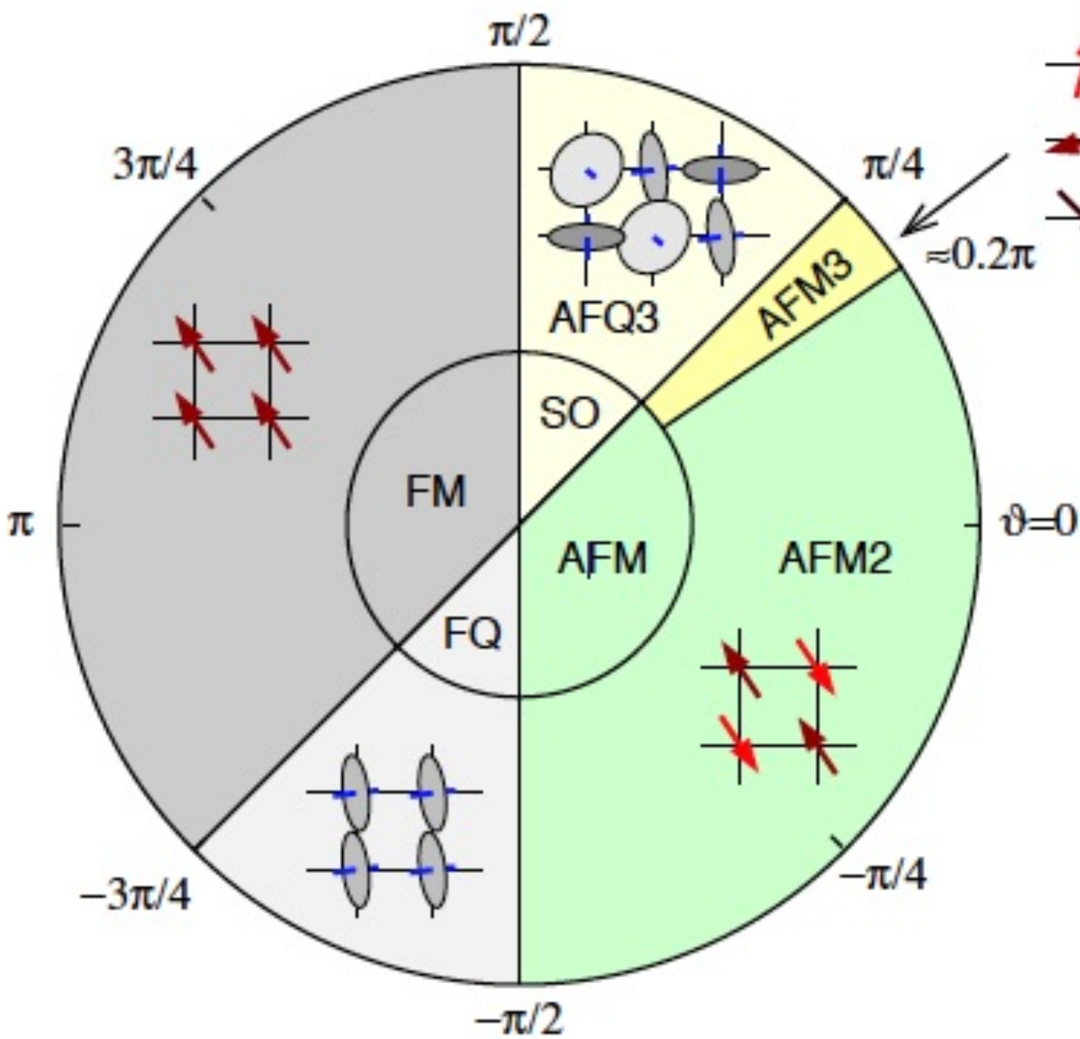
iPEPS (full update) phase diagram $(0 \leq \theta/\pi \leq 1/4)$

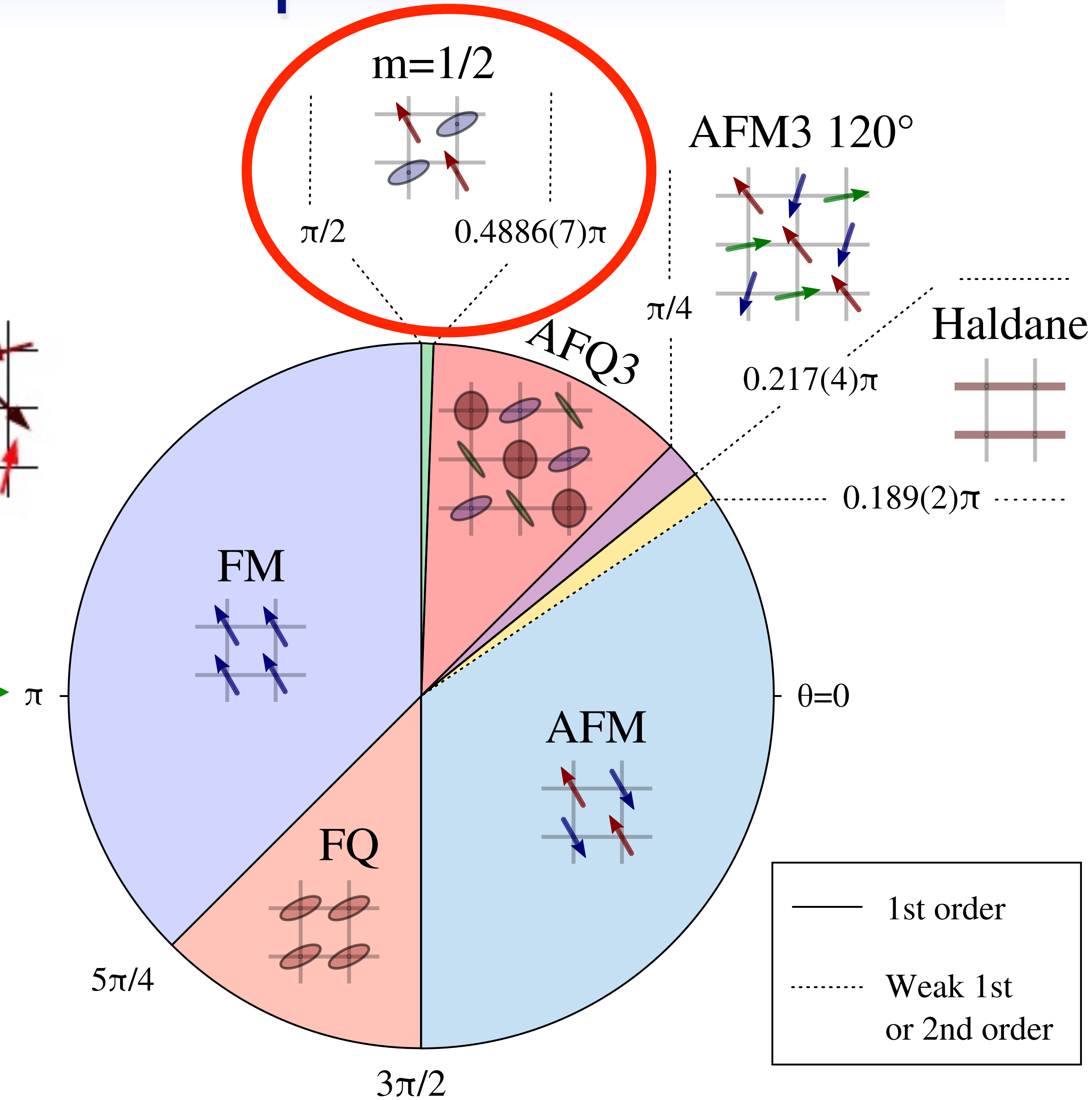
I. Niesen & PC, PRB 95 (2017)



- in contrast to previous predictions of a direct transition between AF and 3-SL phase

Full phase diagram: another surprise





ED / LFWT

Tóth, et al, PRB 85 (2012)

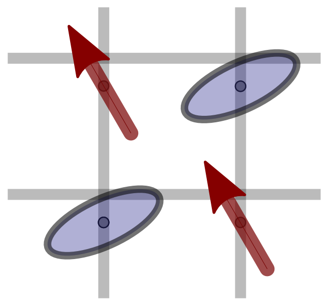
iPEPS

Niesen & PC, SciPost Phys. 3 (2017)

m=1/2 half magnetized half nematic phase

- Spontaneous m=1/2 for

$$0.4886(7) < \theta/\pi < 0.5$$

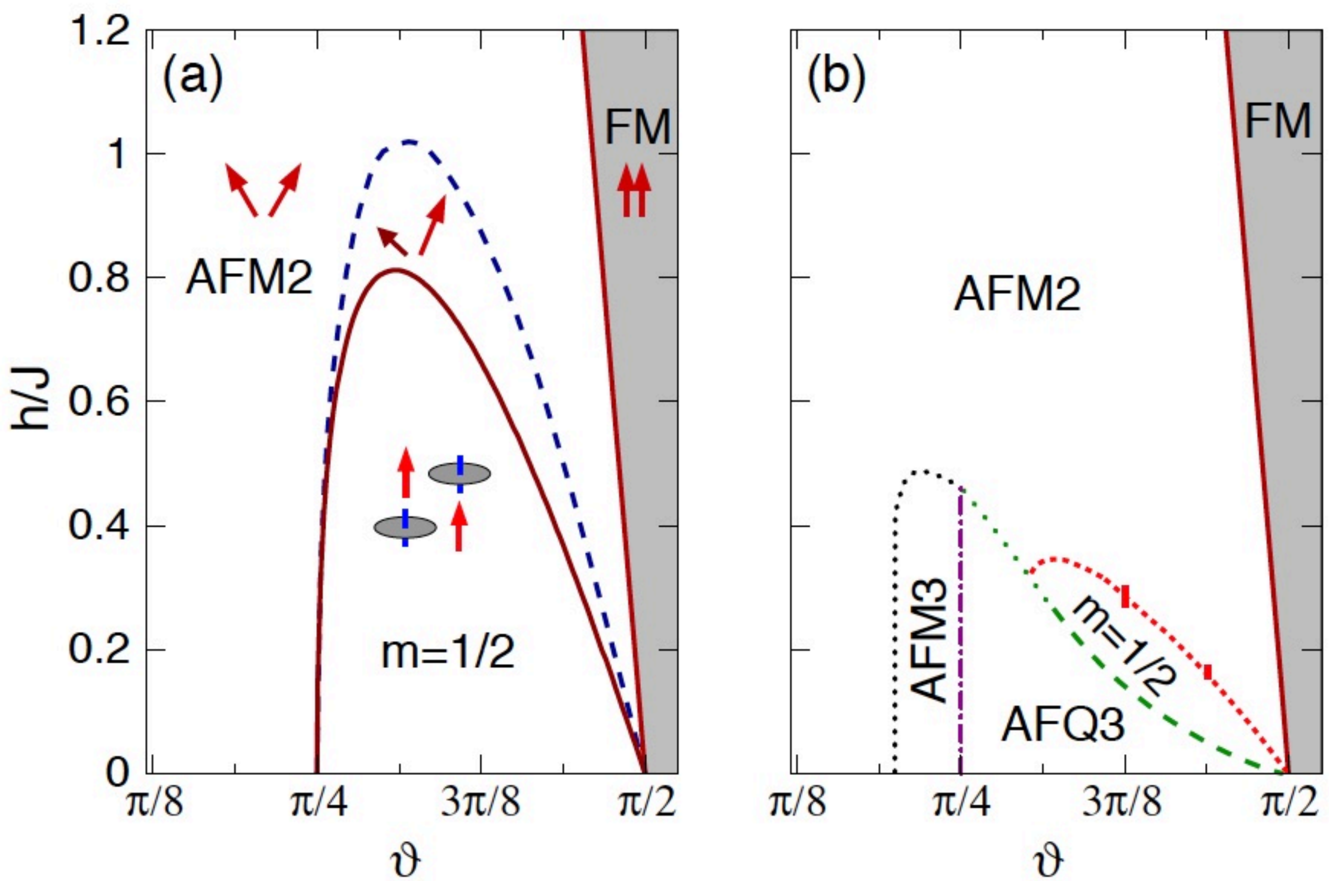


$$|\uparrow\rangle \quad |0\rangle$$

$$|0\rangle \quad |\uparrow\rangle$$

- Previously predicted to occur only when applying an external magnetic field

product state: **ED:**

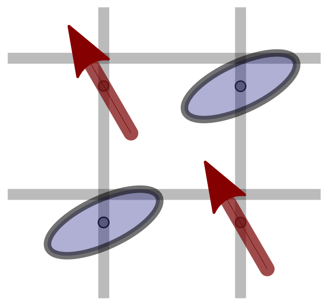


Tóth, Läuchli, Mila & Penc, PRB 85 (2012)

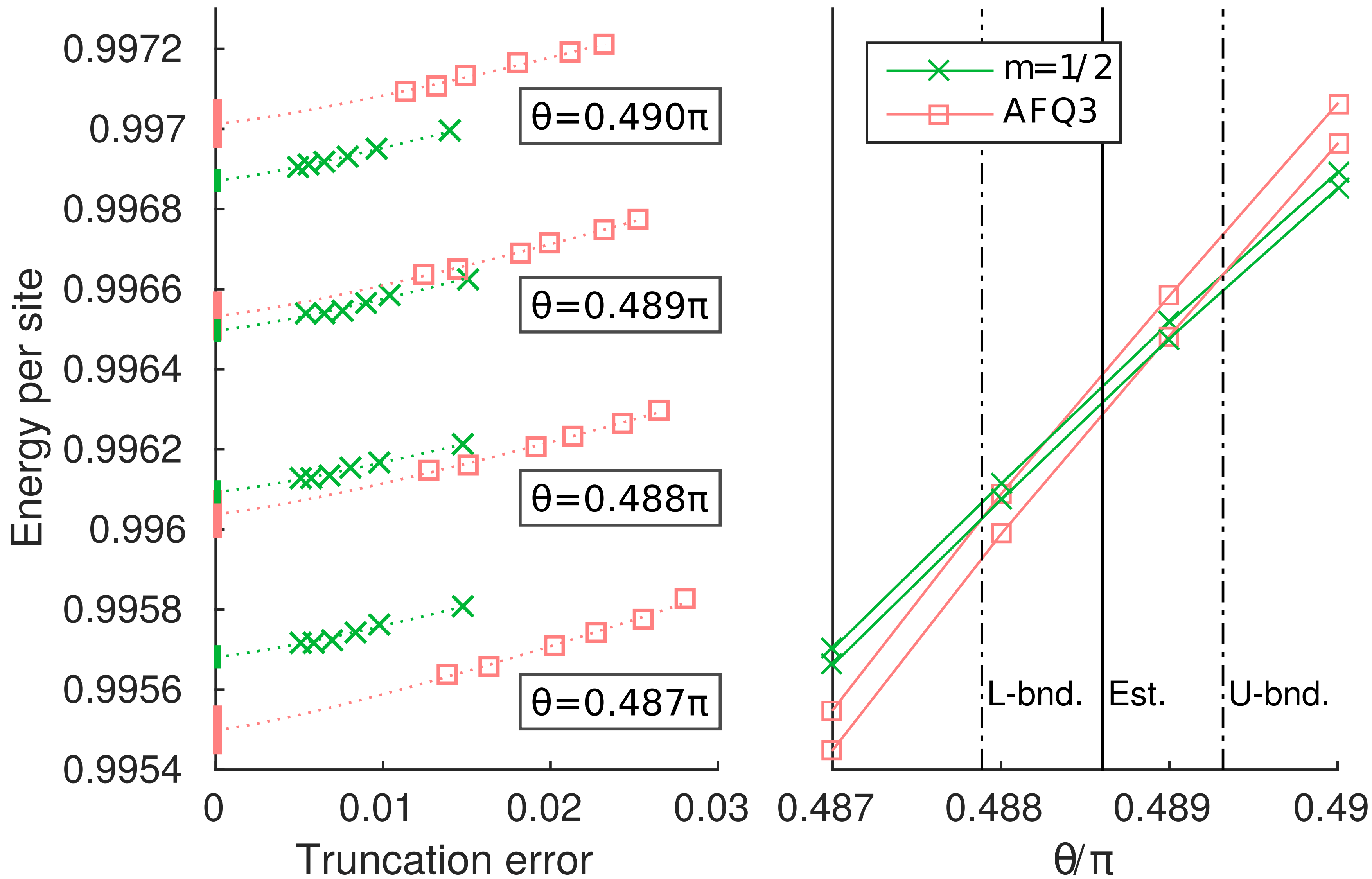
m=1/2 half magnetized half nematic phase

- Spontaneous m=1/2 for

$$0.4886(7) < \theta/\pi < 0.5$$



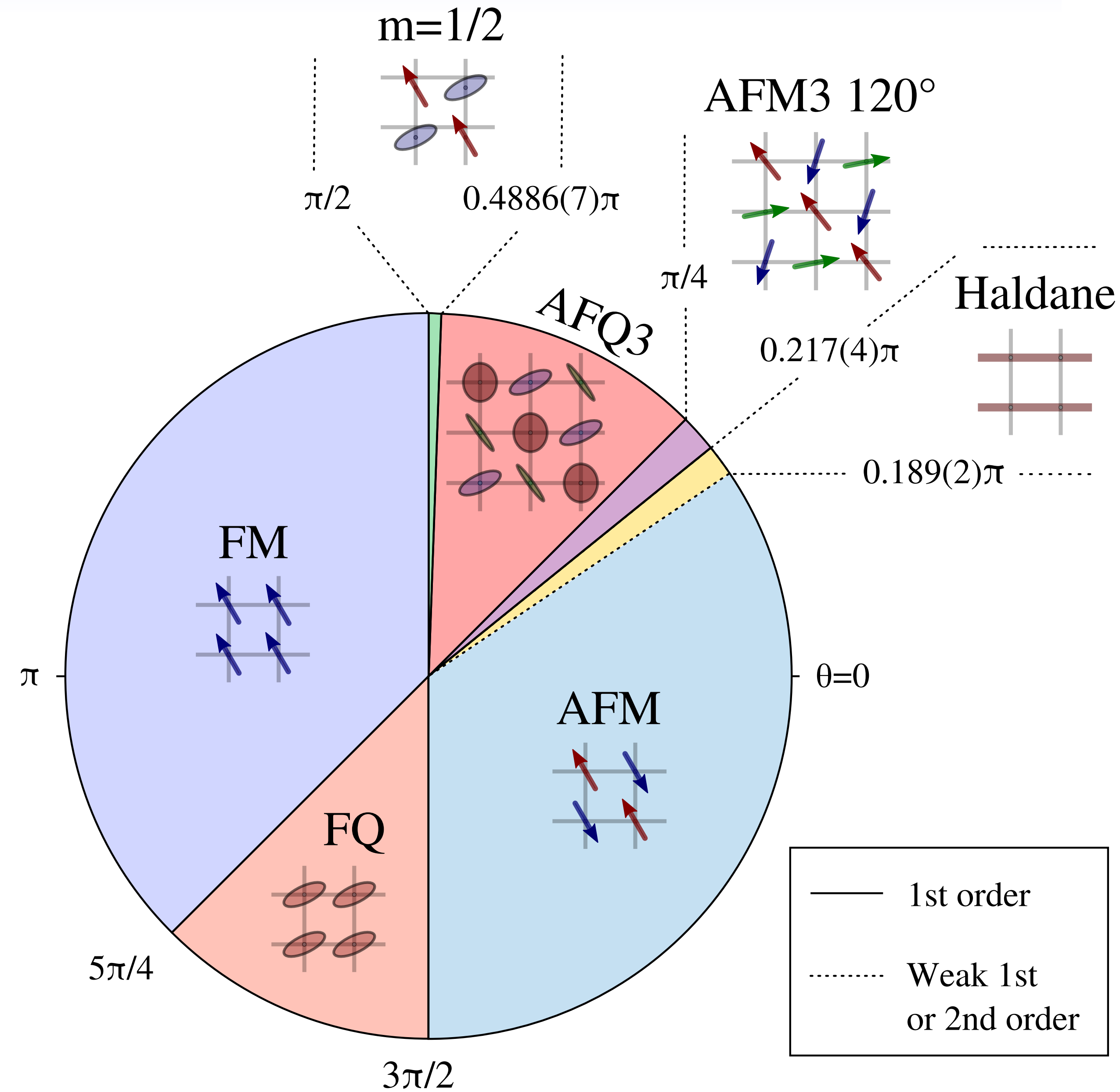
iPEPS (full update):



Summary: S=1 bilinear-biquadratic Heisenberg model

- Using accurate iPEPS simulations we found a rich phase diagram with 2 new phases:
  - Haldane phase in between 2-sublattice and 3-sublattice antiferromagnetic phases
  - m=1/2 phase in between anti-ferroquadrupolar and ferromagnetic phase

- Haldane phase appears also in the S=1 J_1-J_2 Heisenberg model
- Probably appears also in other systems with competing S=1 magnetic orders



Comparison: iMPS vs iPEPS on infinite cylinders

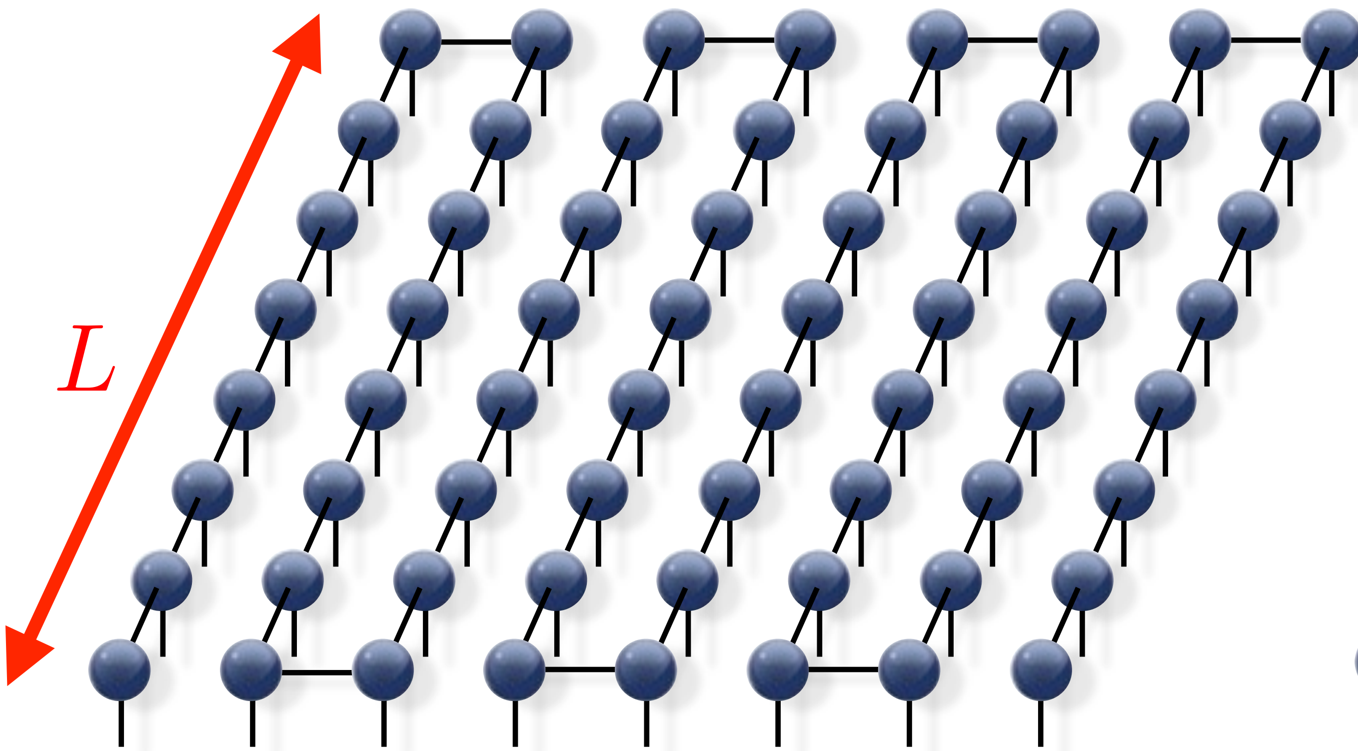
J. Osorio Iregui, M. Troyer & PC, PRB 96 (2017)

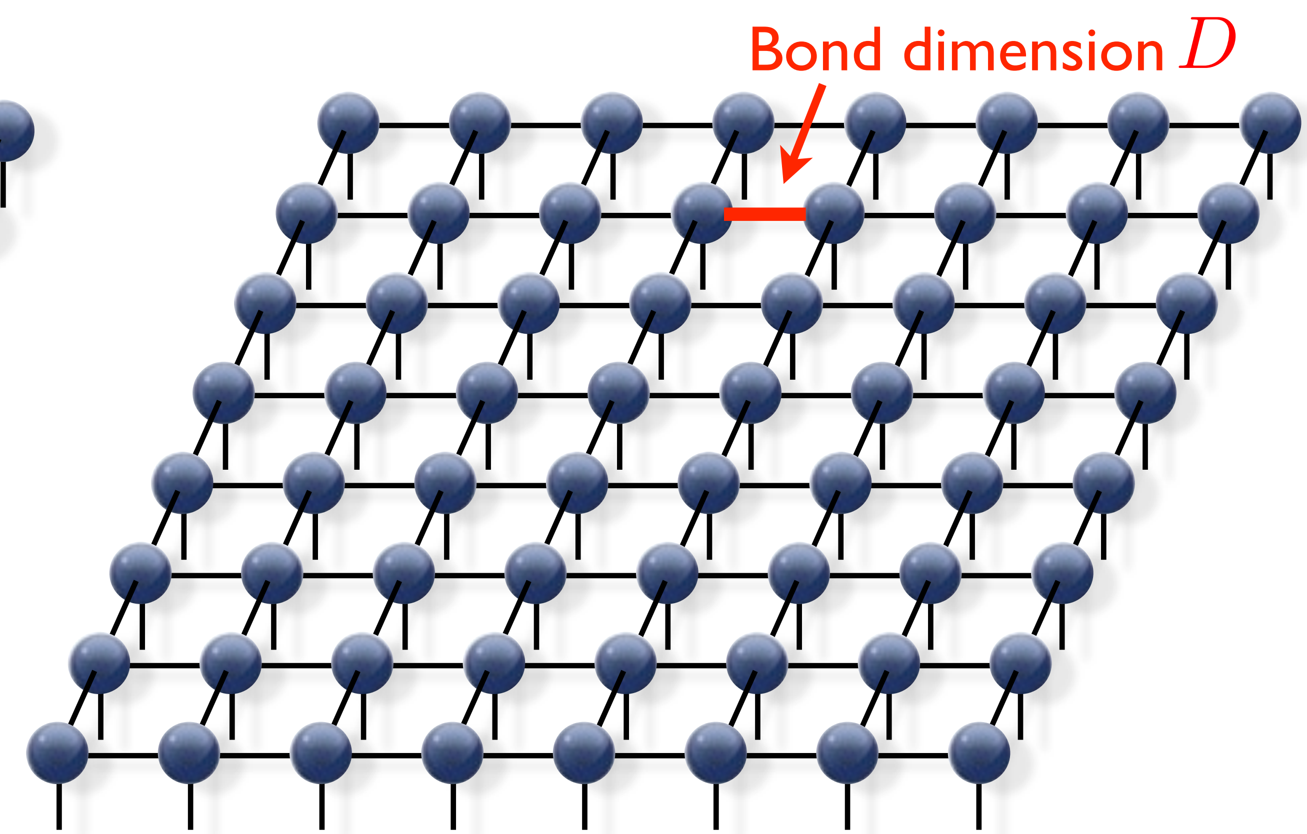
Juan Osorio Iregui

Comparison: iMPS vs iPEPS on infinite cylinders

J. Osorio Iregui, M. Troyer & PC, PRB 96 (2017)

Snake MPS **vs** **(i)PEPS**





★ Scaling of algorithm: D^3

★ Simpler algorithms & implementation

★ Very accurate results for "small" L

\- inaccurate beyond certain L because *D~exp(L)*

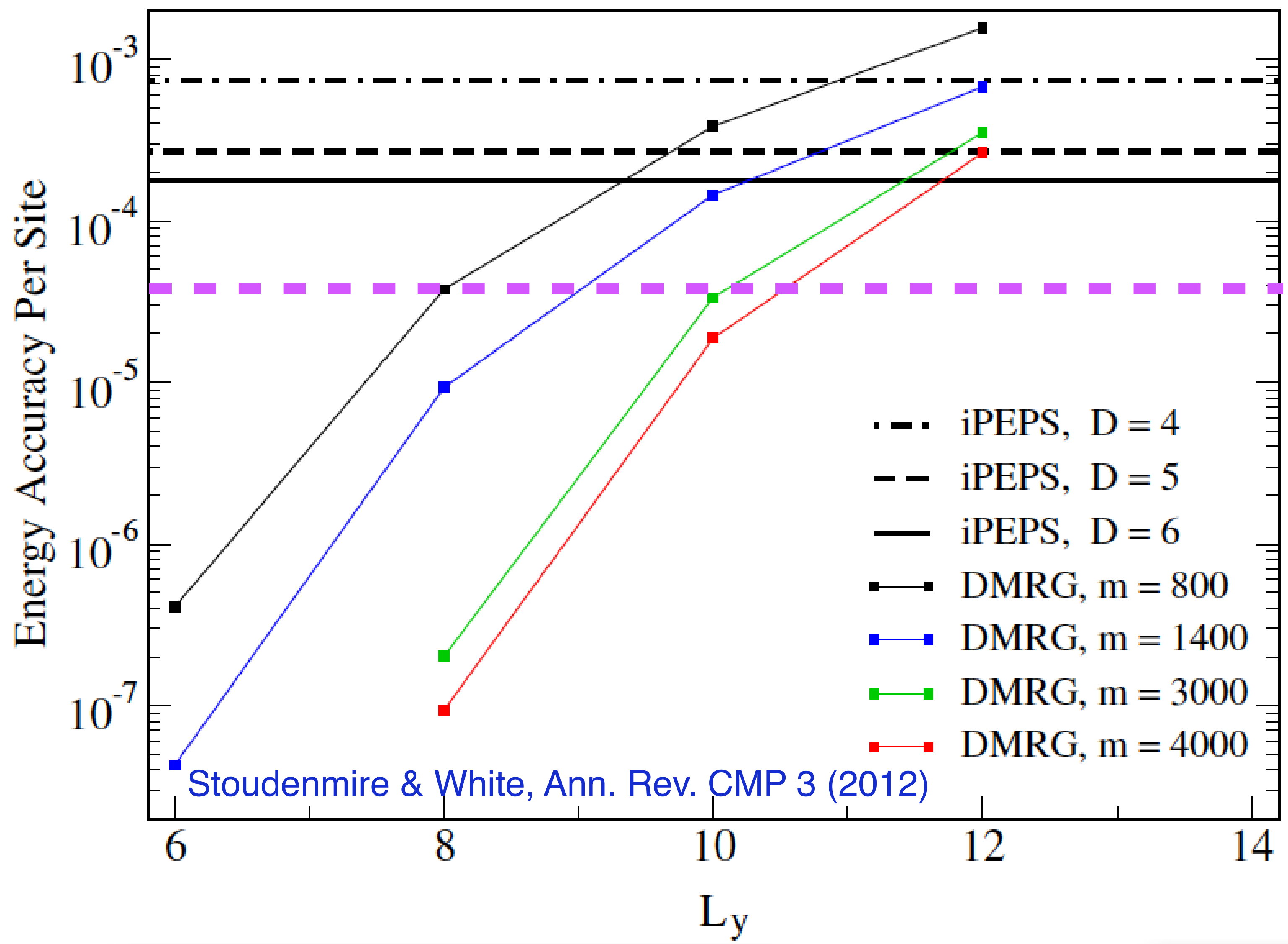
★ Large / infinite systems (scalable)!

★ Much fewer variational parameters because much more natural 2D ansatz

\- Algorithms more complicated

\- Large cost of roughly D^{10}

Comparison 2D DMRG & iPEPS: 2D Heisenberg model



← iPEPS D=6
(variational optimization)

iPEPS D=6 in the thermodynamic limit

~ 2'600 variational pars.

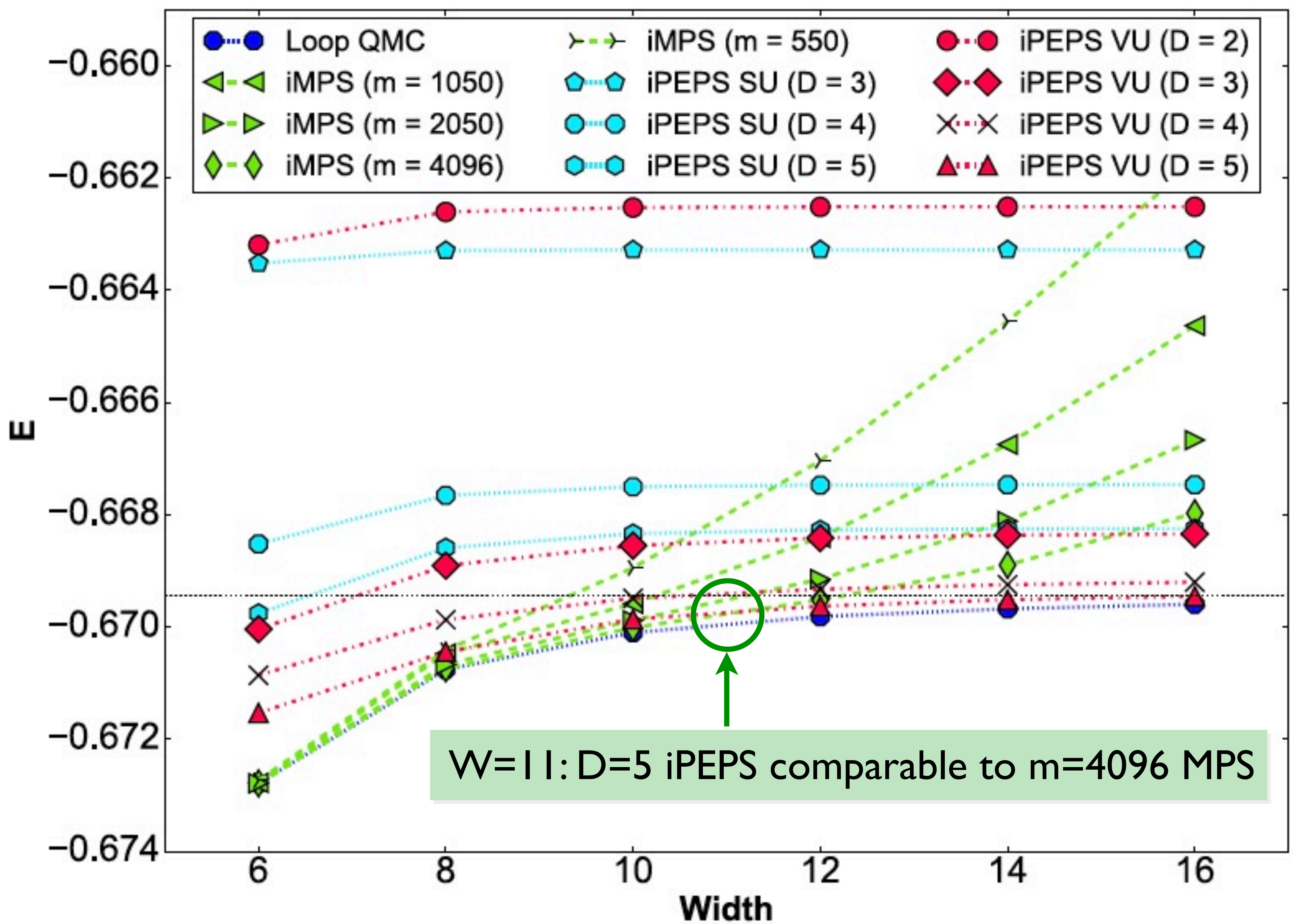
similar accuracy ~

MPS D=3000 on finite Ly=10 cylinder

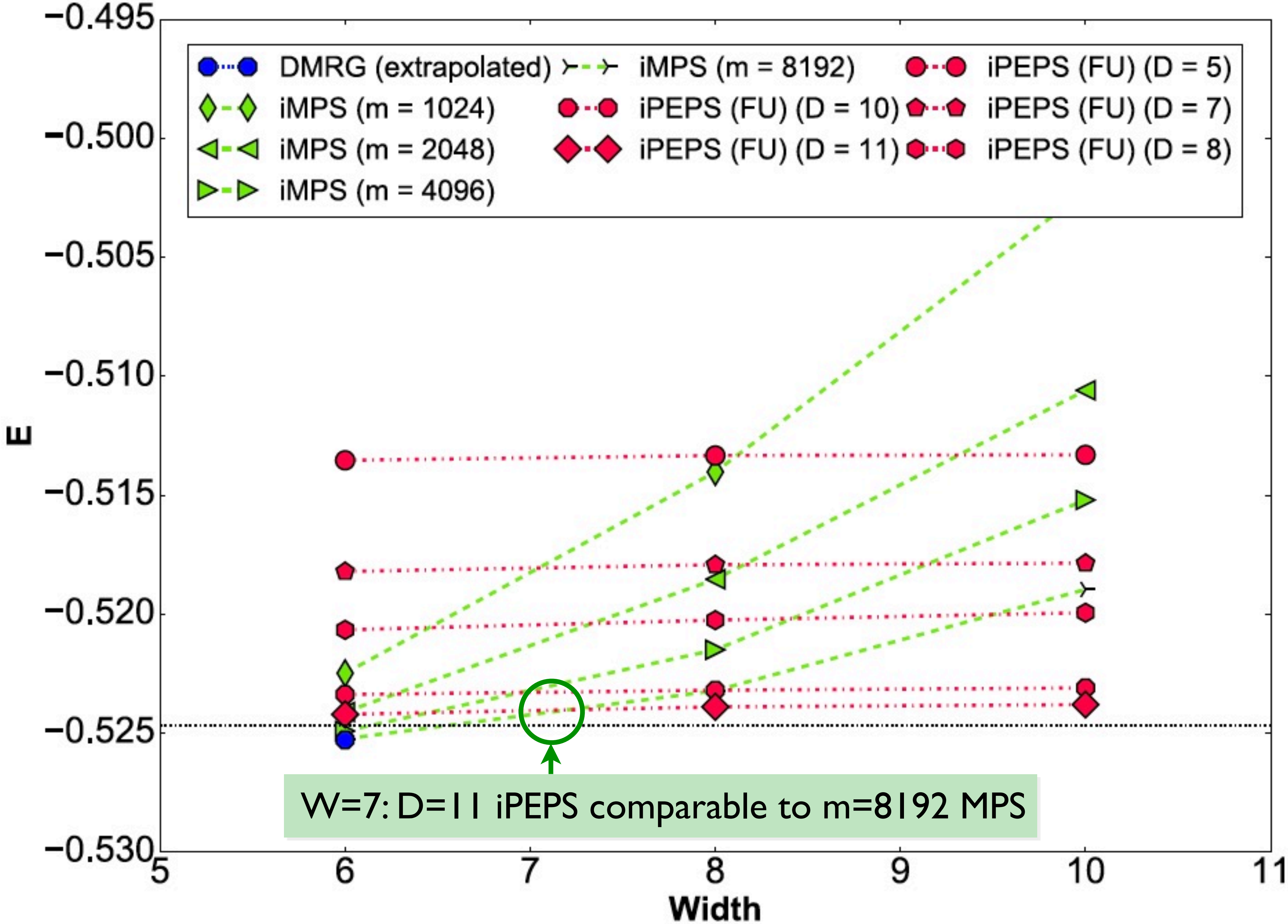
~ 18'000'000

4 orders of magnitude fewer parameters (per tensor)

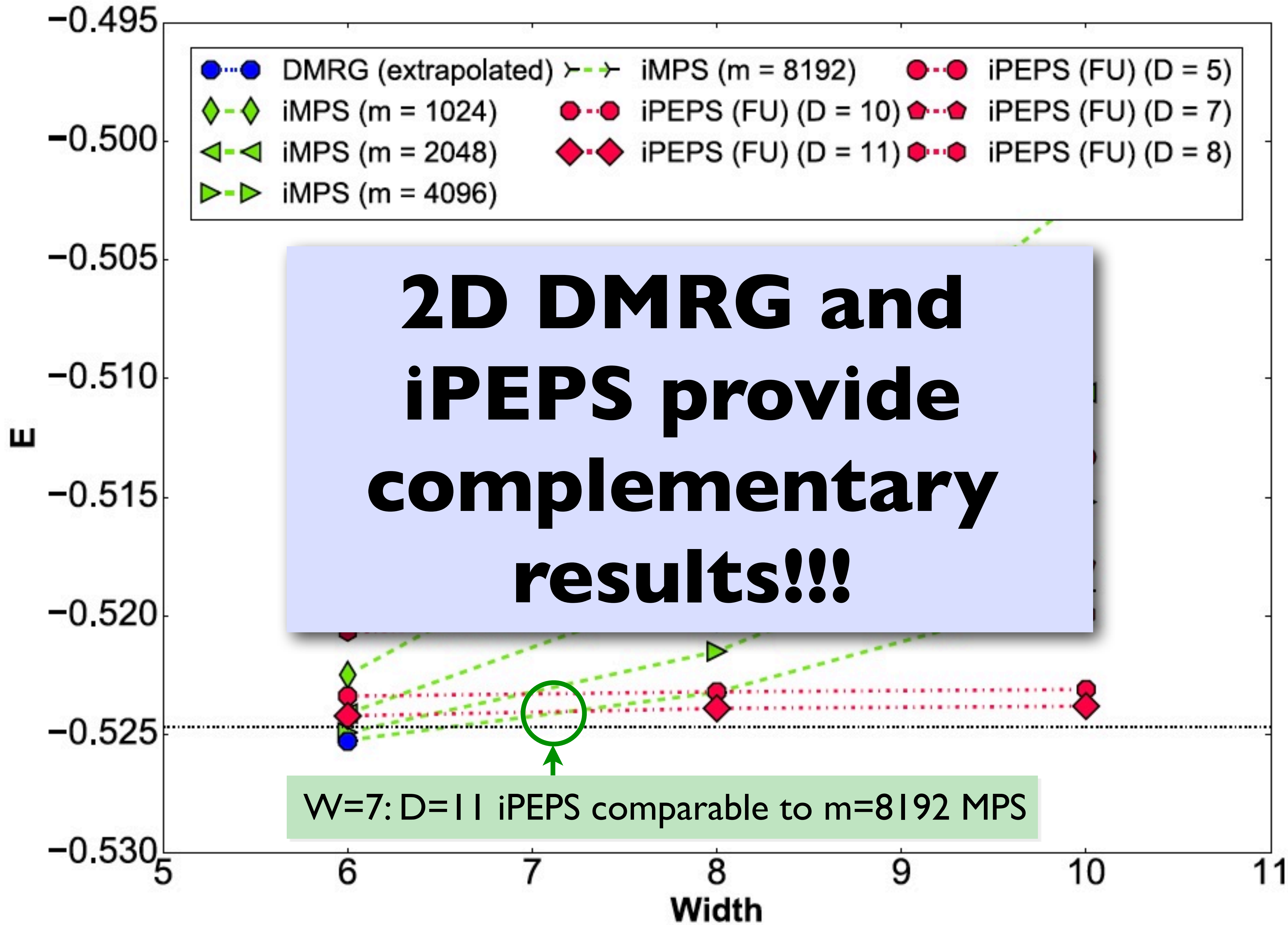
iMPS vs iPEPS on infinite cylinders: Heisenberg model



iMPS vs iPEPS on infinite cylinders: Hubbard model (n=1)



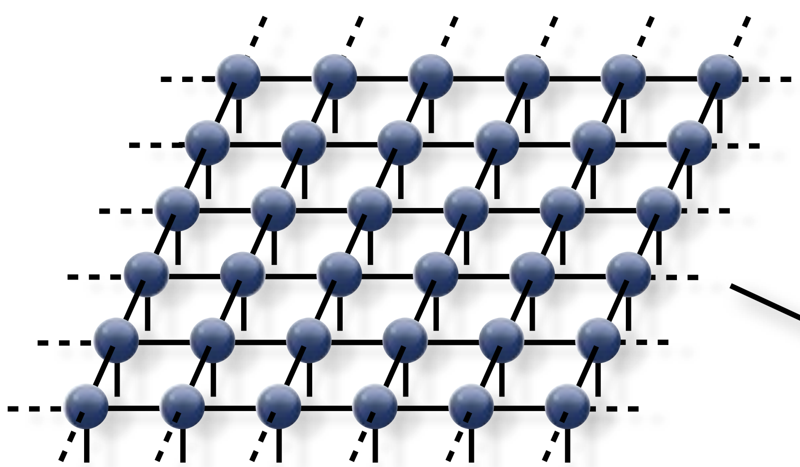
iMPS vs iPEPS on infinite cylinders: Hubbard model (n=1)



2D DMRG and iPEPS provide complementary results!!!

Stripe order in the 2D Hubbard model

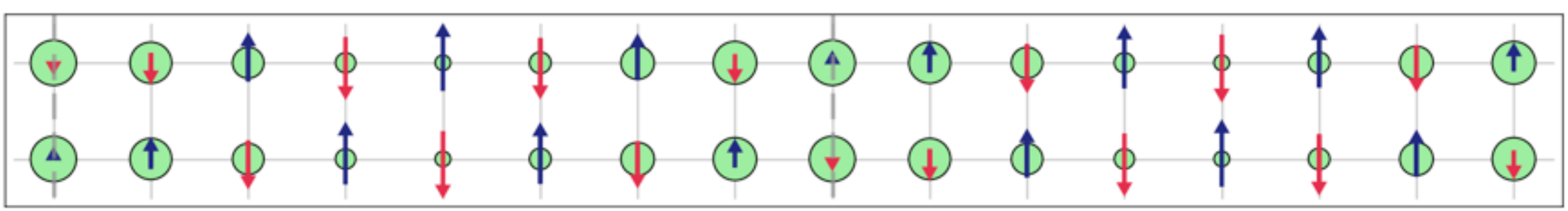
Boxiao Zheng, Chia-Min Chung, PC, Georg Ehlers, Ming-Pu Qin, Reinhard Noack,
Hao Shi, Steven White, Shiwei Zhang, Garnet Chan, arXiv:1701.00054



iPEPS + **DMRG** + **AFQMC** + **DMET**

$$U/t = 8$$
$$\delta = 1/8$$

→ Ground state: **Stripe state**



Conclusion: iMPS

✓ **1D** tensor networks: State-of-the-art for quasi 1D systems

✓ **2D** tensor networks: A lot of progress in recent years!

★ iPEPS has become a powerful & competitive tool

★ Much room for improvement & many extensions

✓ 2D tensor networks and 2D DMRG provide *complementary* results!

✓ Combined studies: promising route to solve challenging problems

Thank you for your attention!

Thank you