Probing the stability of the spin-liquid phases in the Kitaev-Heisenberg model using iPEPS

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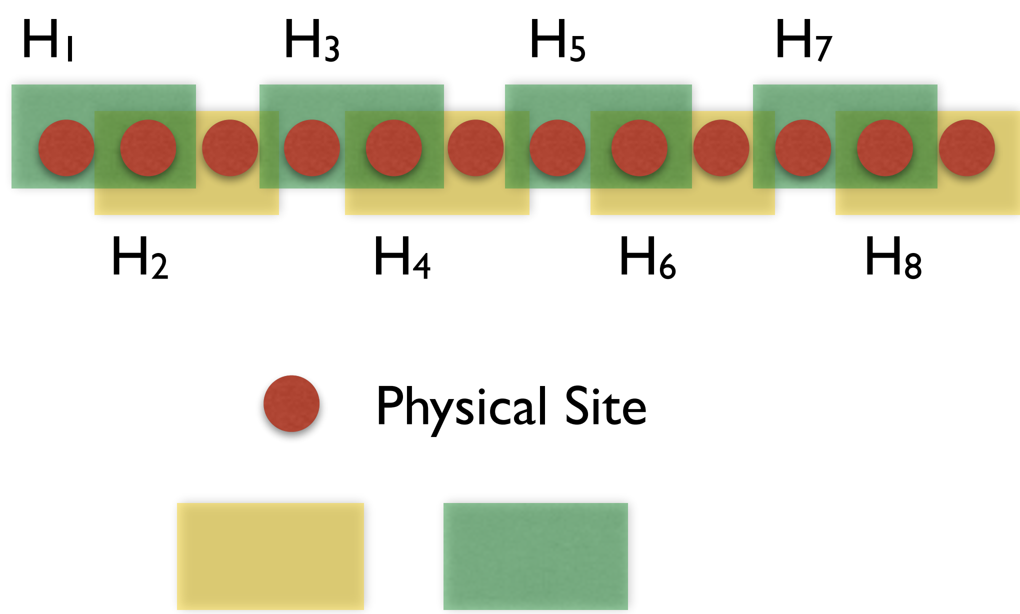
Tensor Networks

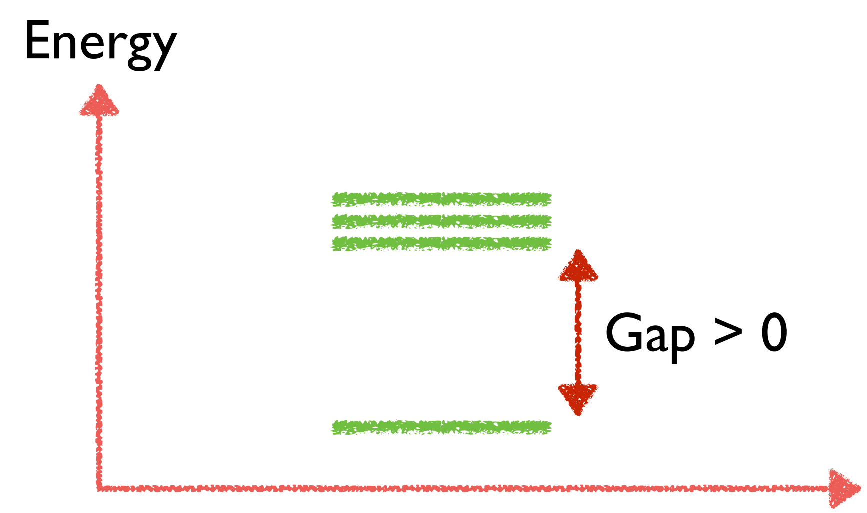
Entanglement-based approach

M. Hastings, arXiv:0705.2024
F. Brandao, M. Horodecki, arXiv: 1206.2947

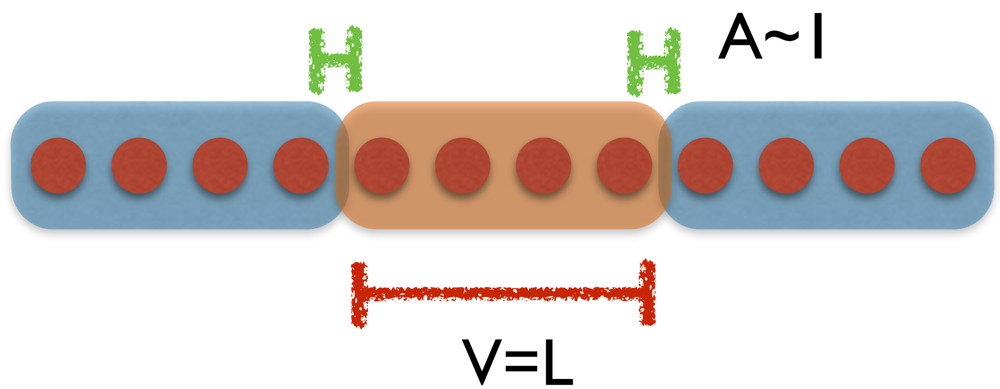


Local H terms

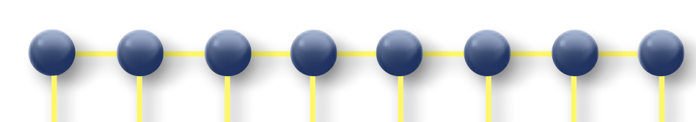
+



Area Law for Entanglement Entropy
S(A) ~ A



Matrix Product State (MPS)
Efficient Representation



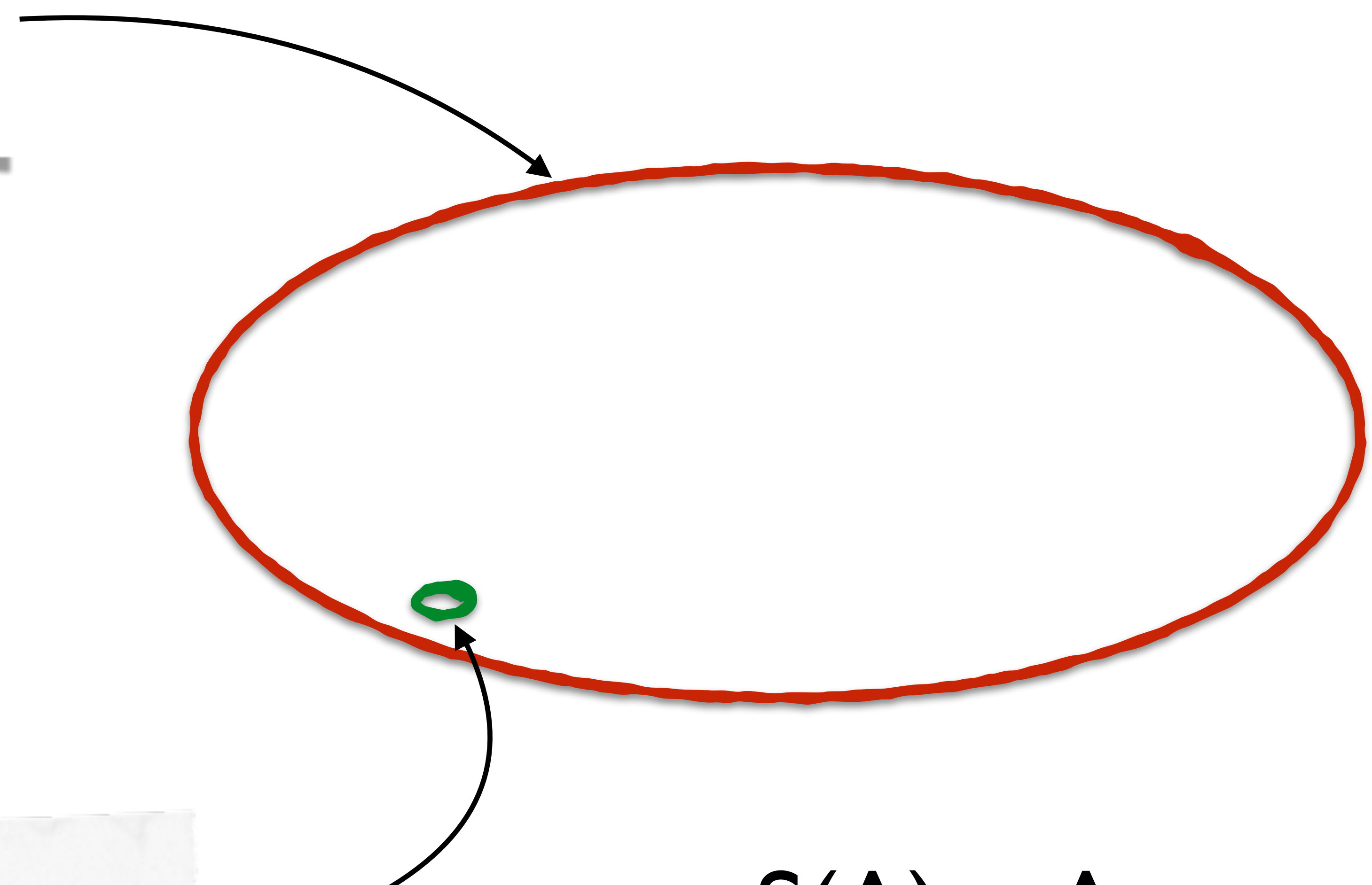
Tensor Networks

Entanglement-based approach

Hilbert Space

$H \sim V^N$

Exponential growth



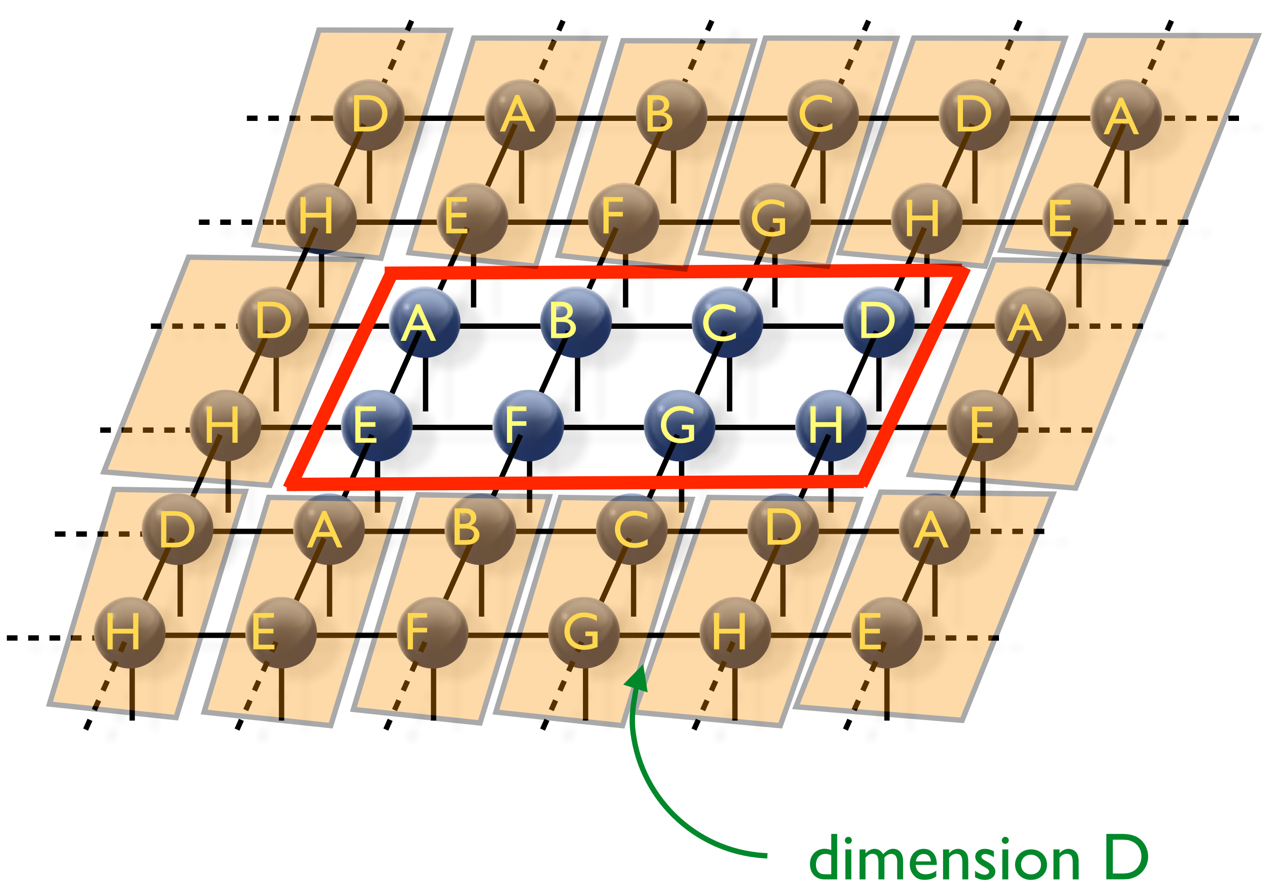
low entanglement corner

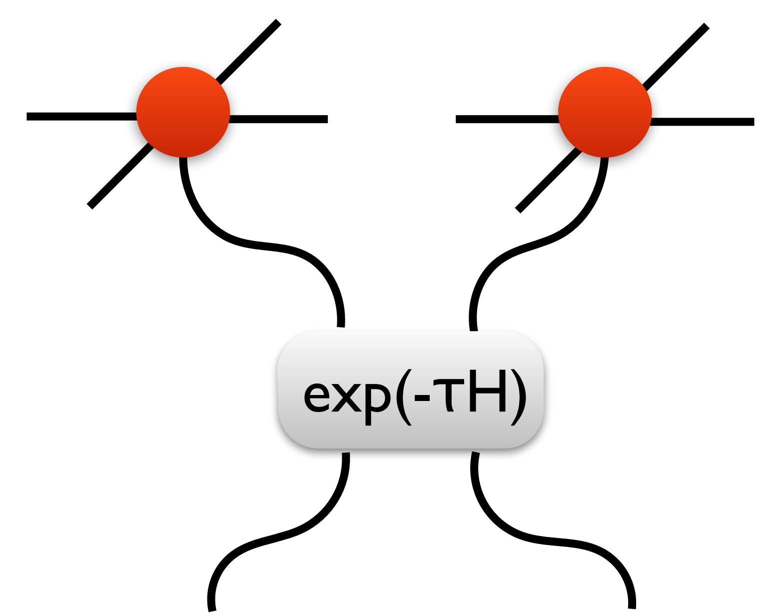
$S(A) \sim A$

Area law growth for entanglement entropy

iPEPS

- infinite Projected Entangled-Pair States
- Define arbitrary structure and size of unit cell.
- Include effect of infinite system via so-called environment tensors.





Typically perform ground state search using imaginary-time evolution.

(Full Update)

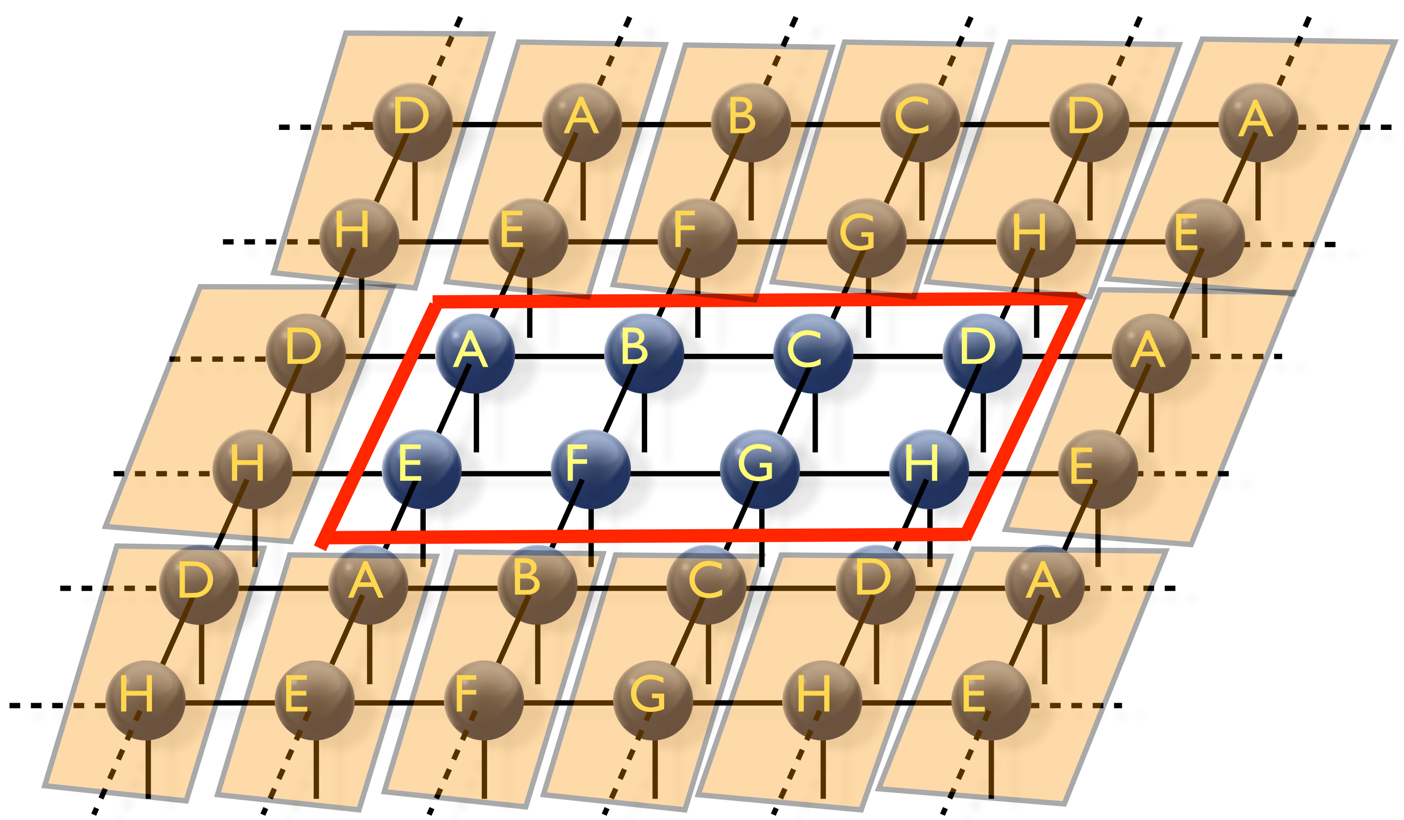
Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

Contracting the network

Corner Transfer Matrix (CTM)

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)

$C(D,\chi) \sim \chi^3 D^4$



PEPS contraction

Cost ~ Exp(N)

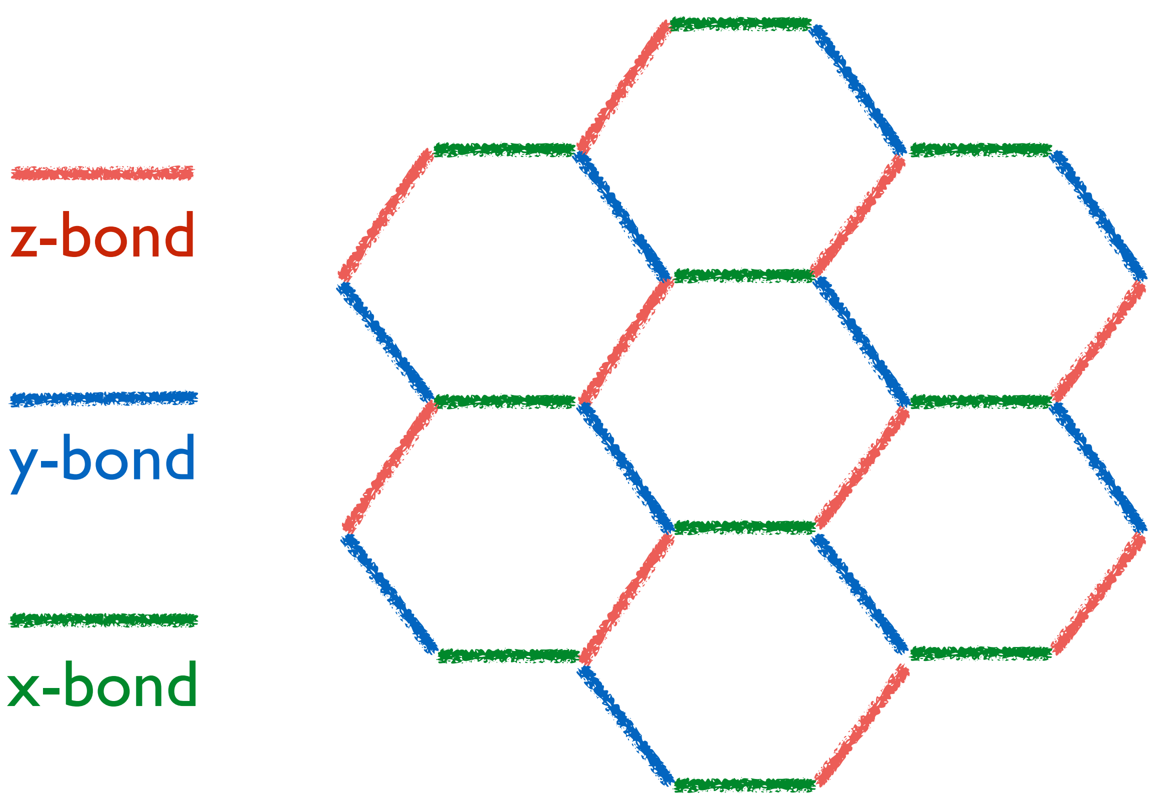
Approximations Required!

Kitaev-Heisenberg model

The Hamiltonian

J. Chaloupka, G. Jackeli, G. Khaliullin, arXiv:1004.2964v2.
J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).

$$H_{i,j}^{(\gamma)} = \cos\varphi\; \vec{S}_i \cdot \vec{S}_j + 2\sin\varphi\; S_i^{(\gamma)} S_j^{(\gamma)}$$



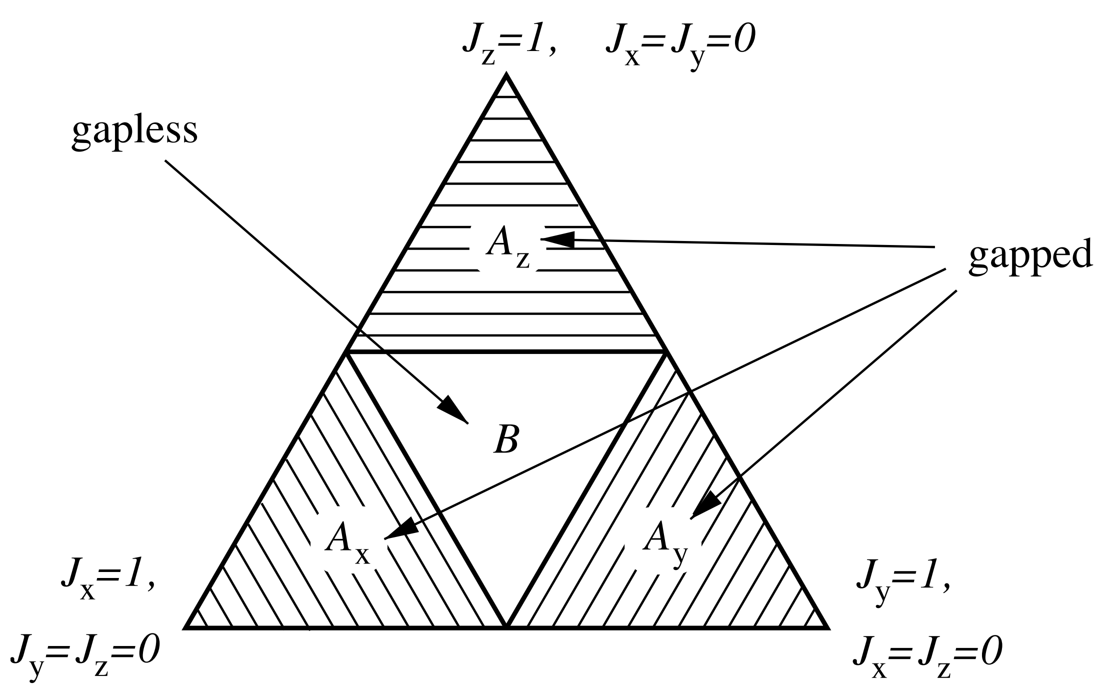
- Proposed by Chaloupka et al. as effective model for (layered) Iridate compounds A_2IrO_3 (A = Li,Na).
- Nearest-neighbor (pseudo-)spin interactions composed of isotropic Heisenberg + anisotropic Kitaev terms.
- Small system studies show that (zigzag) magnetic order found in Iridate compounds is natural ground state of KH model.

Kitaev's Honeycomb model

Hamiltonian/Phase Diagram

A. Kitaev, Annals of Physics 321 (2006).

$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z$$



Gapped (A) phase can be mapped to the toric code.

Gapless (B) phase hosts non-abelian anyonic excitations.

Gapless region defined by:

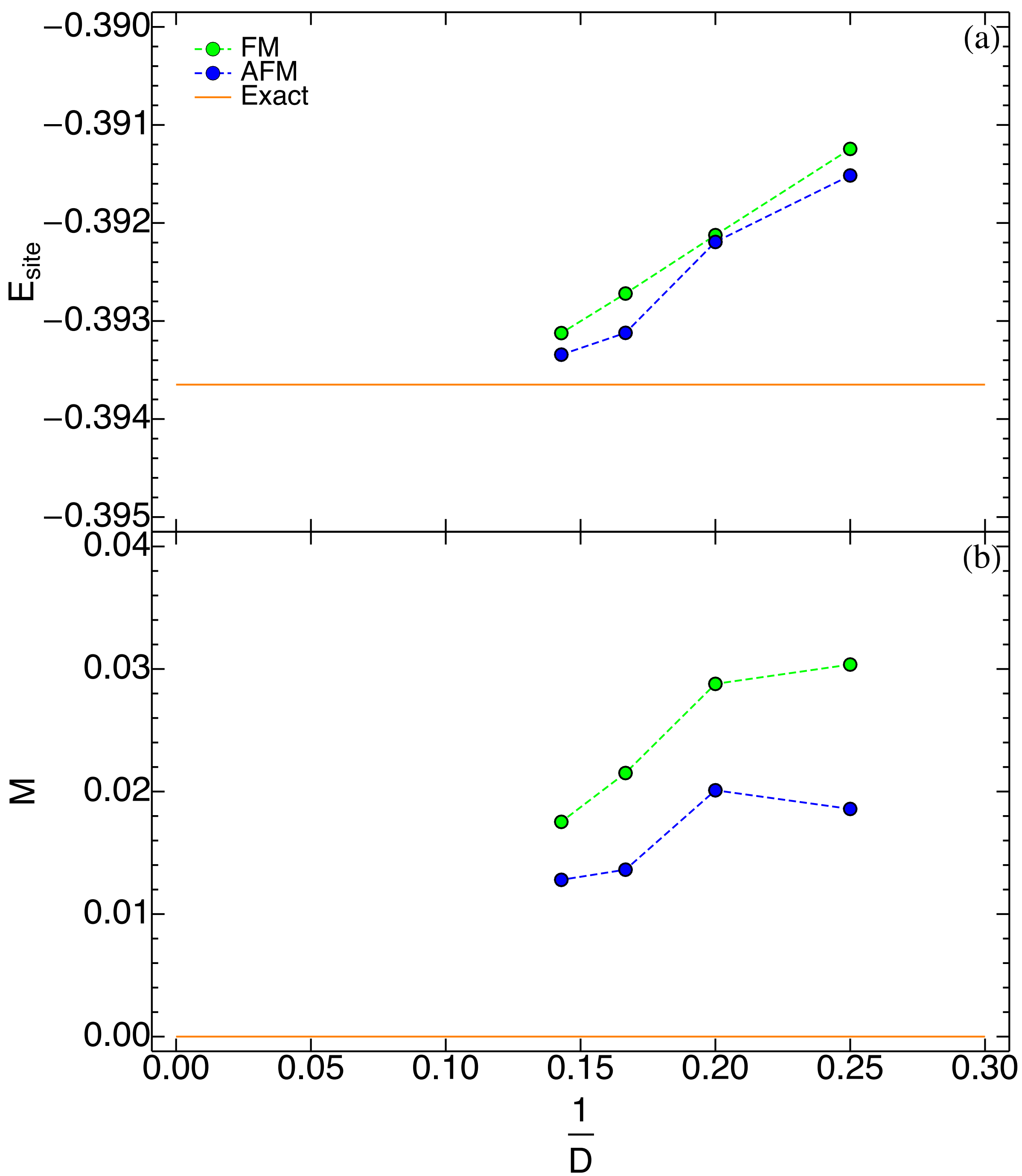
$$|J_x| \leqslant |J_y| + |J_z|$$
$$|J_y| \leqslant |J_x| + |J_z|$$
$$|J_z| \leqslant |J_x| + |J_y|$$

We expect iPEPS to perform well inside gapped (A phase) region. What about the gapless region?

Perfect benchmark.

Kitaev's Honeycomb model

Energy/Magnetization



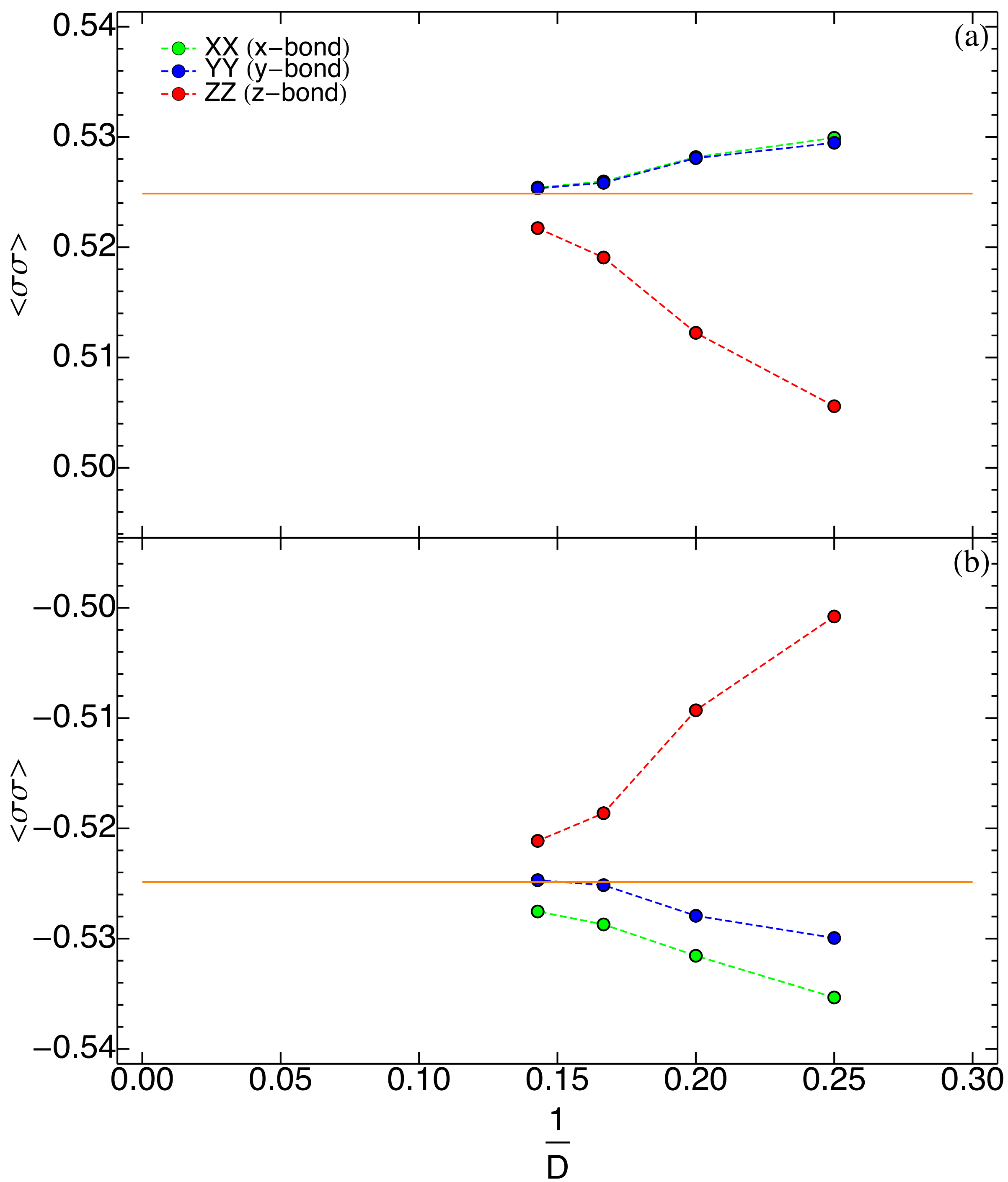
- Isotropic $J_x=J_y=J_z$ point (B-phase).
- Exact energy per site: -0.3936.
- iPEPS energy:
  - D=7 (AFM): -0.3933
  - D=7 (FM): -0.3931
- Monotonic decrease with D.

- Spin liquid ground state > Zero magnetization expected.
- iPEPS results:
  - D=7 (AFM): 0.01
  - D=7 (FM): 0.02
- Monotonic decrease with D.
- Infinite D extrapolation yields vanishing magnetization.

A. Kitaev, Annals of Physics 321 (2006).
G.Baskaran, S.Mandal, R. Shankar, PRL 98 (2007).
JOI, P. Corboz, M.Troyer, arXiv:1408.4020.

Kitaev's Honeycomb model

Spin-Spin Correlations



- Results from Baskaran et al. show that only NN correlations of corresponding bond type are non-vanishing, eg.

$$\gamma(i,j) = x \rightarrow \langle \sigma_i^x \sigma_j^x \rangle = 0.525$$
$$\langle \sigma_i^y \sigma_j^y \rangle = 0$$
$$\langle \sigma_i^z \sigma_j^z \rangle = 0$$

- Data not shown < 10^{-3}.
- Systematic improvement upon increasing bond dimension.

G.Baskaran, S.Mandal, R. Shankar, PRL 98 (2007).
JOI, P. Corboz, M.Troyer, arXiv:1408.4020.

Kitaev-Heisenberg model

Previous Results

- Type of transition observed in 4th quadrant differed for small systems vs SP Mean-Field study.
- Survival of QSL phases in TD limit remained under debate.
- Type of phase transitions from AQSL to symmetry broken not certain.

$$H_{i,j}^{(\gamma)} = \cos\varphi \; \vec{S}_i \cdot \vec{S}_j + 2\sin\varphi \; S_i^{(\gamma)} S_j^{(\gamma)}$$

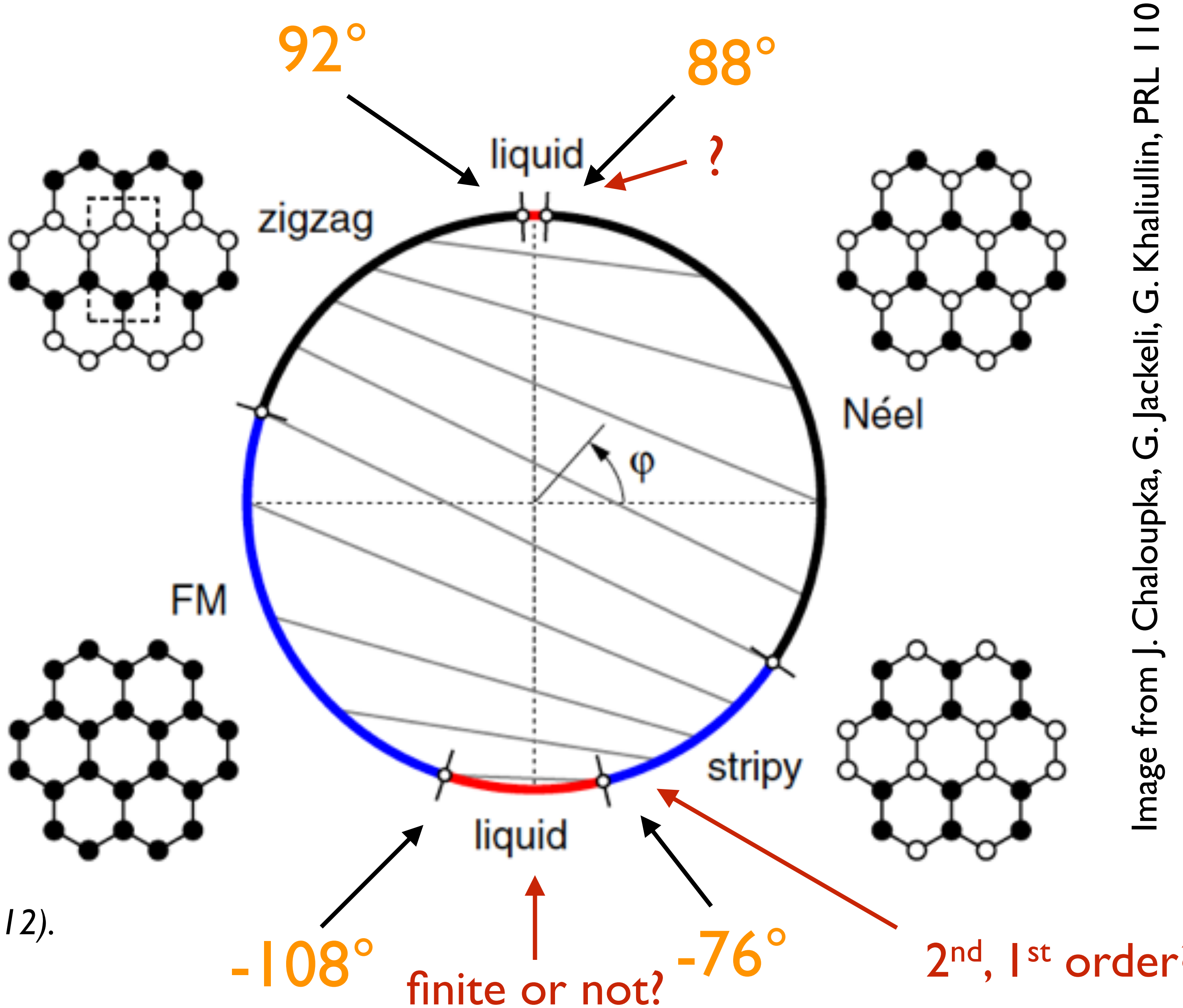


Image from J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).

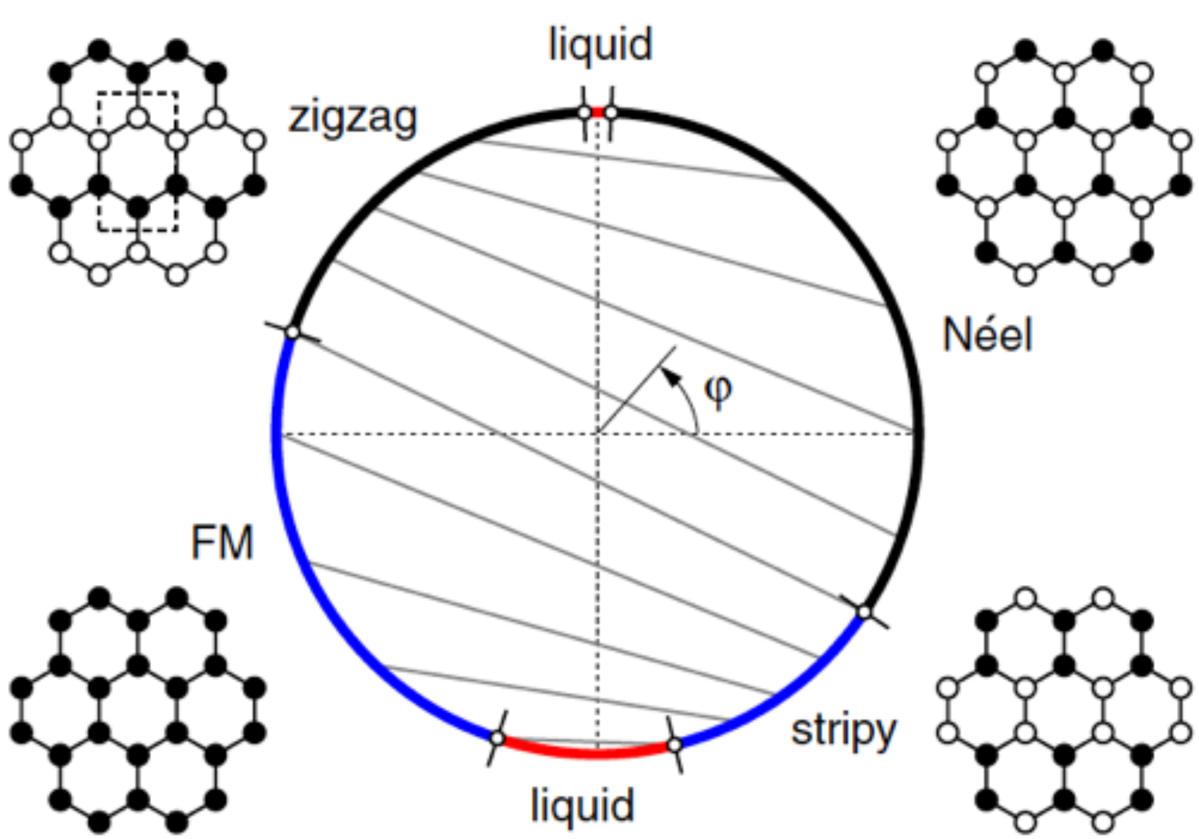
J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).
J. Chaloupka, G. Jackeli, G. Khaliullin, arXiv:1004.2964v2.
R. Schaer, S. Bhattacharjee, and Y. B. Kim, Phys. Rev. B 86, 224417 (2012).
Jiang et al., arXiv:1101.1145v1.
Z. Wang, C. Li, Y. Han, and G. Guo, arXiv:1303.2431 (2013)

Kitaev-Heisenberg model

iPEPS Approach

Energy crossing + OP analysis

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.



- Perform initial runs mapping out phases arising in phase diagram.
- Find representative states deep inside each phase.
- Compare energies + OP of different phases in the vicinity of phase transitions.
- "Hysteretic" behavior will hint towards 1st order type transitions.

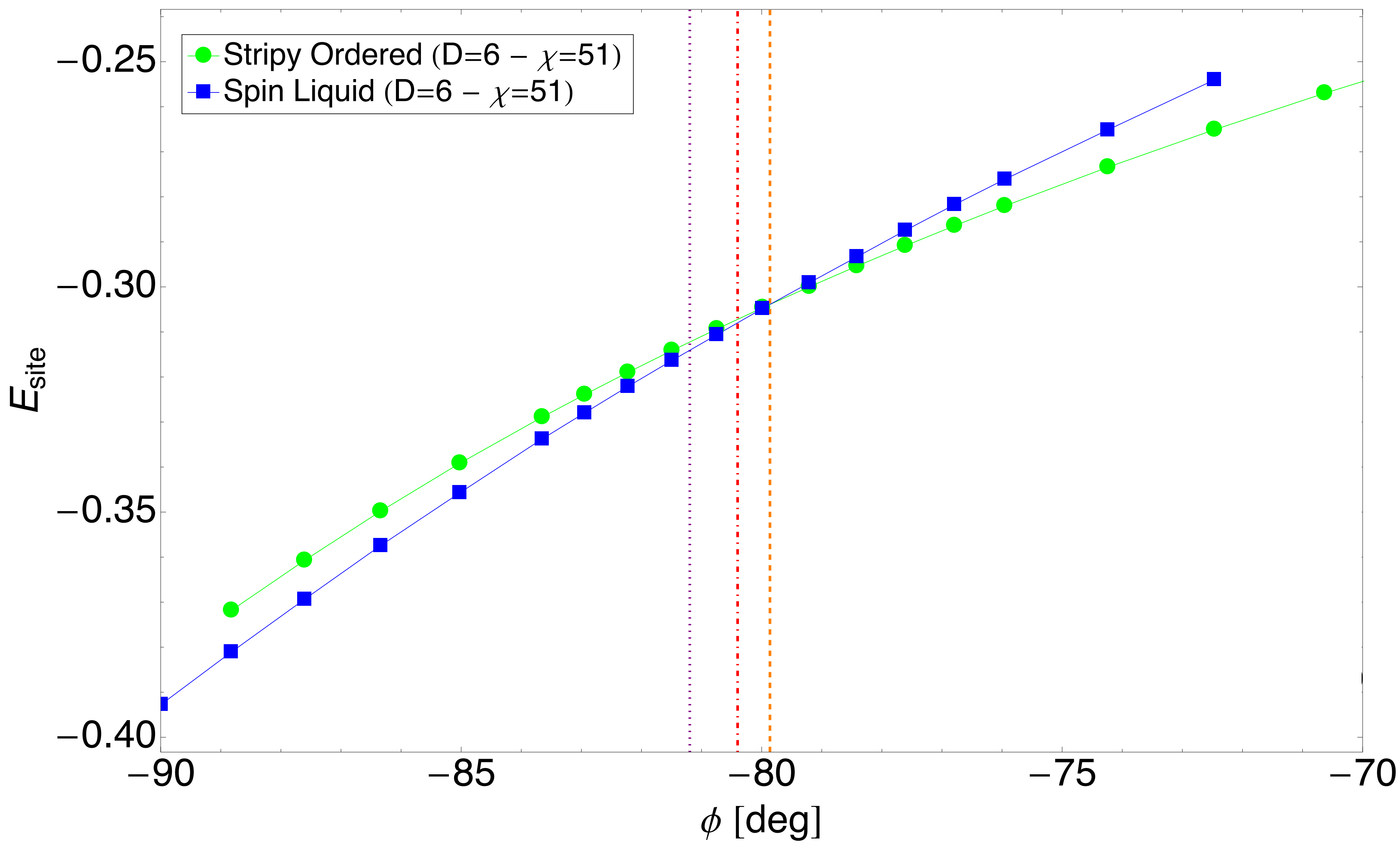
Image from J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).

Kitaev-Heisenberg model

Spin Liquid to Stripy Transition

Energy Crossings

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.



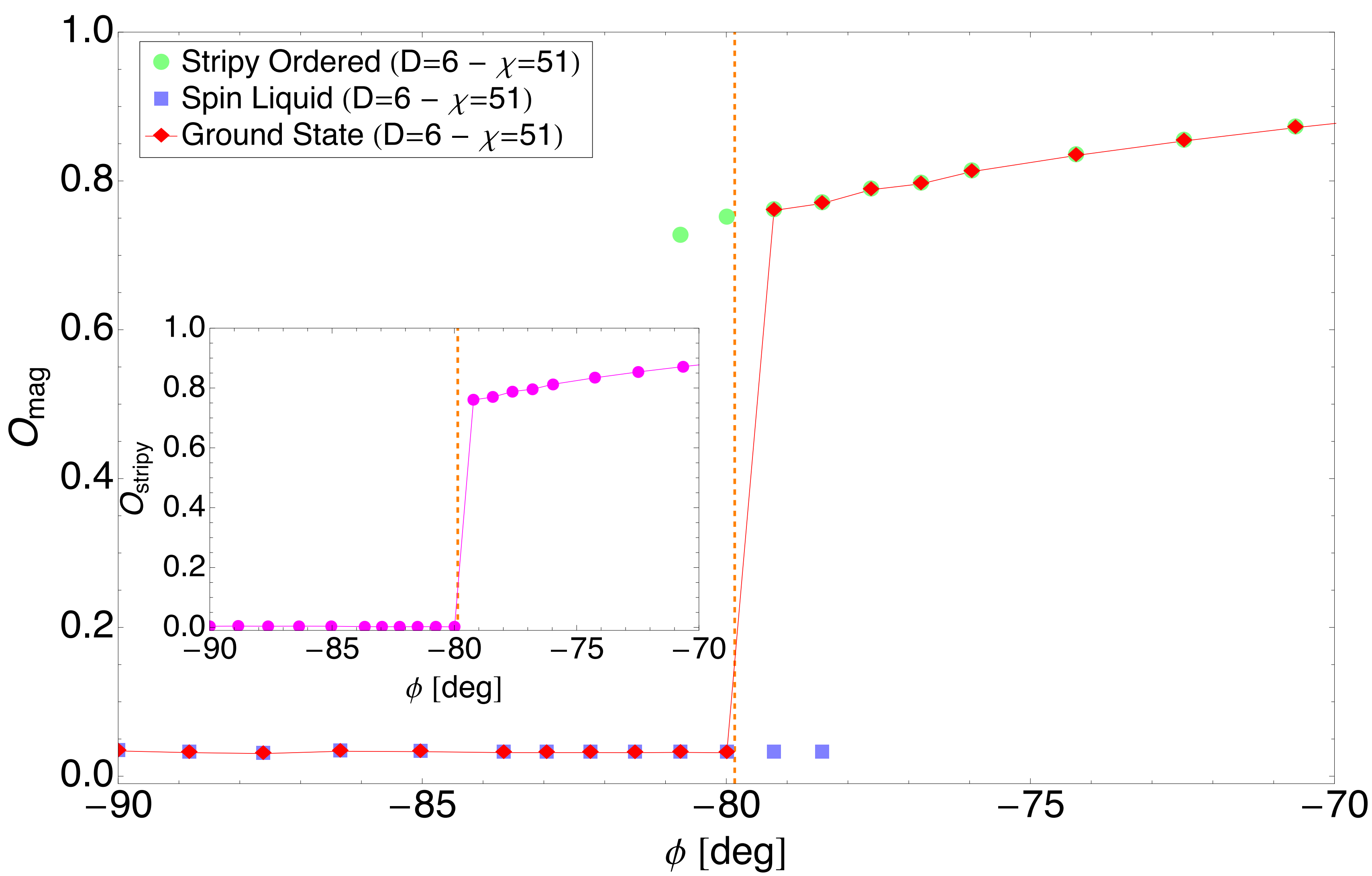
- Weak energy crossing at φ ~ -80° (D=6) suggests 1st order phase transition.
- Transition point shifts towards lower φ with increasing D.

Kitaev-Heisenberg model

Spin Liquid to Stripy Transition

Magnetic Order Parameters

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.



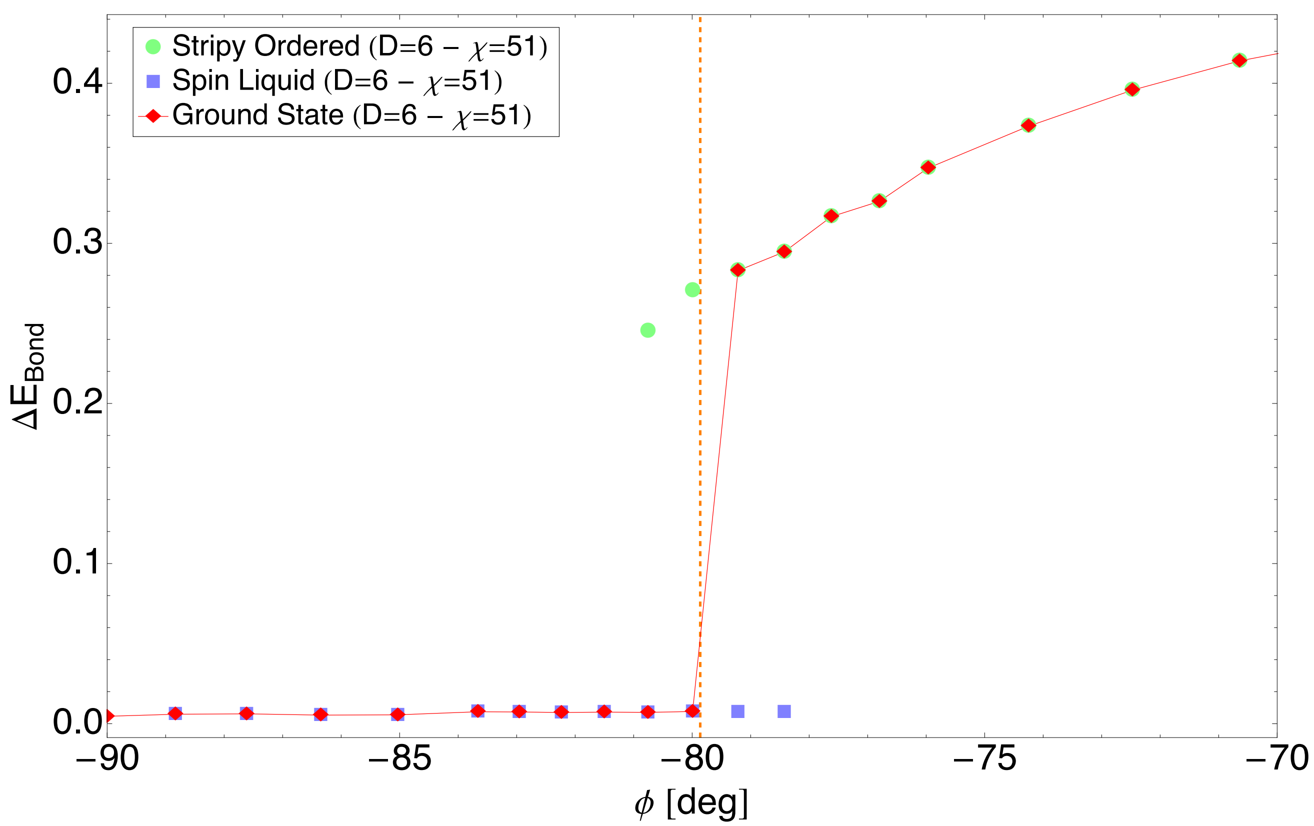
- Discontinuous behavior for Magnetization/Stripy order parameters in GS (red diamonds/cyan circles).
- Green/blue data show OP values for each of the phases.
- Discontinuity expected to remain finite in infinite D limit.

Kitaev-Heisenberg model

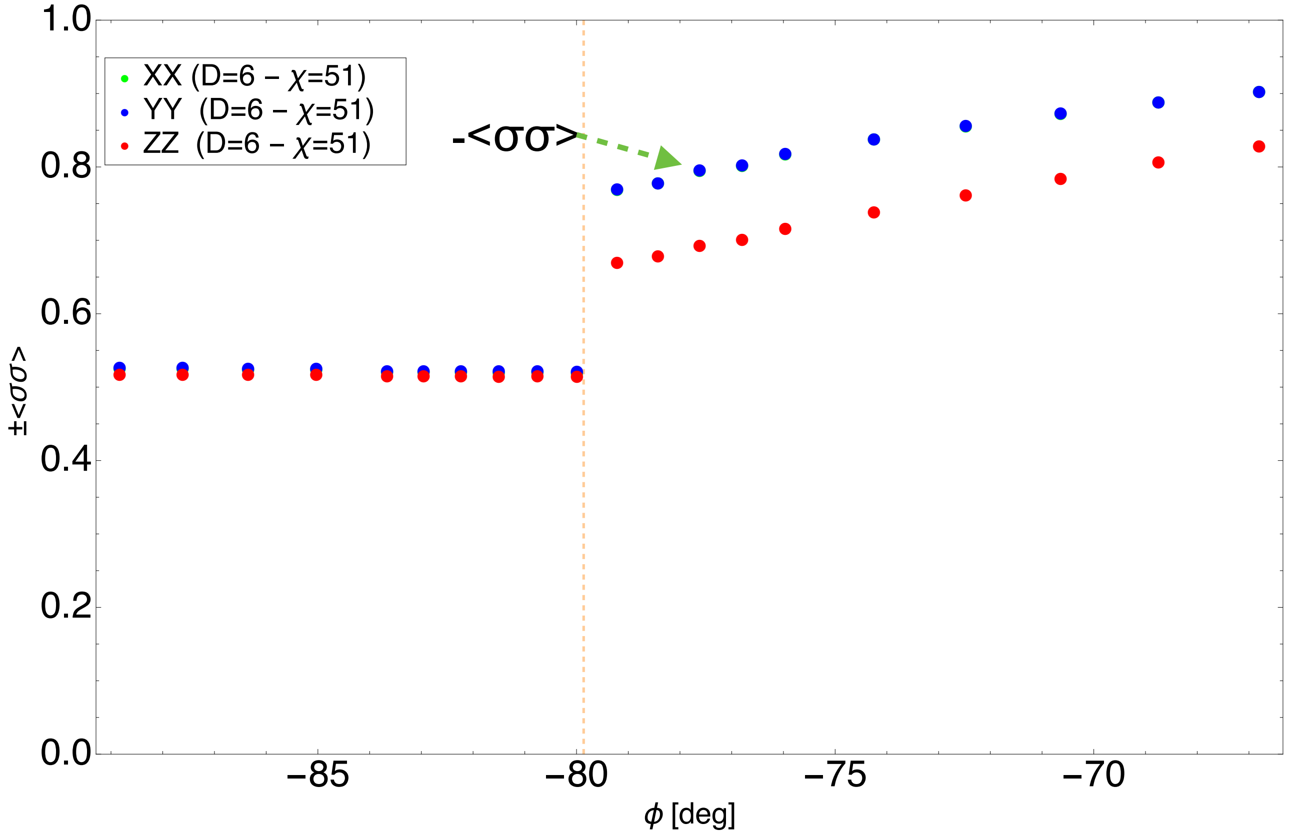
Spin Liquid to Stripy Transition

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.

Bond Order Parameter



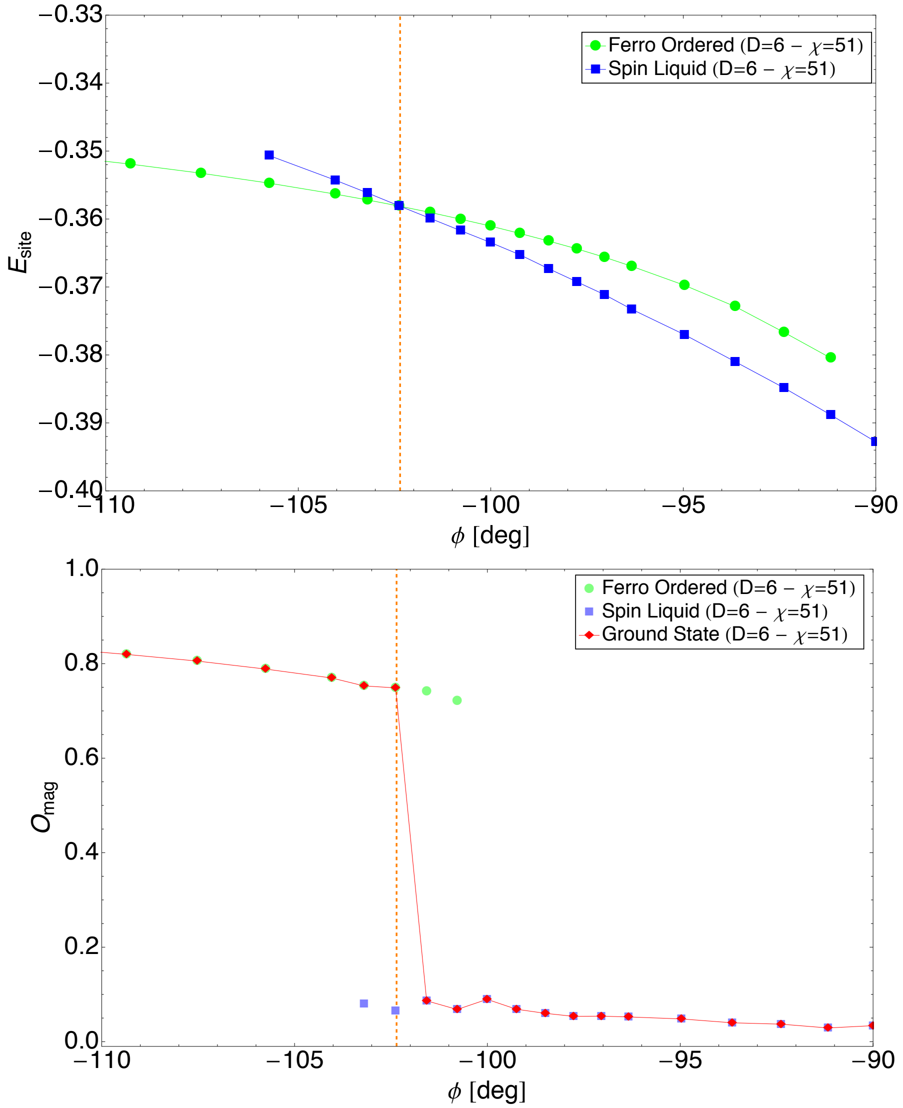
Dominant NN Correlations



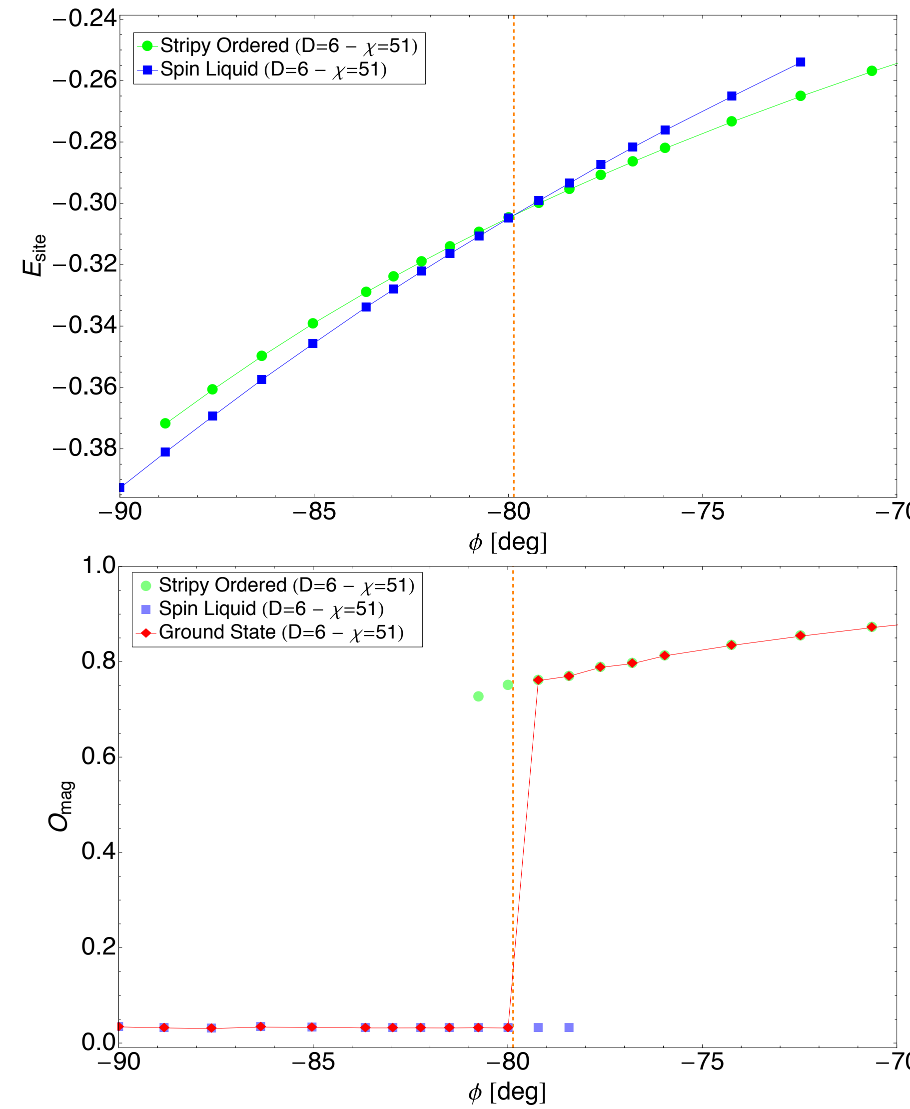
Kitaev-Heisenberg model

FM Spin Liquid to Symmetry-broken

FSL - Ferro



FSL - Stripy

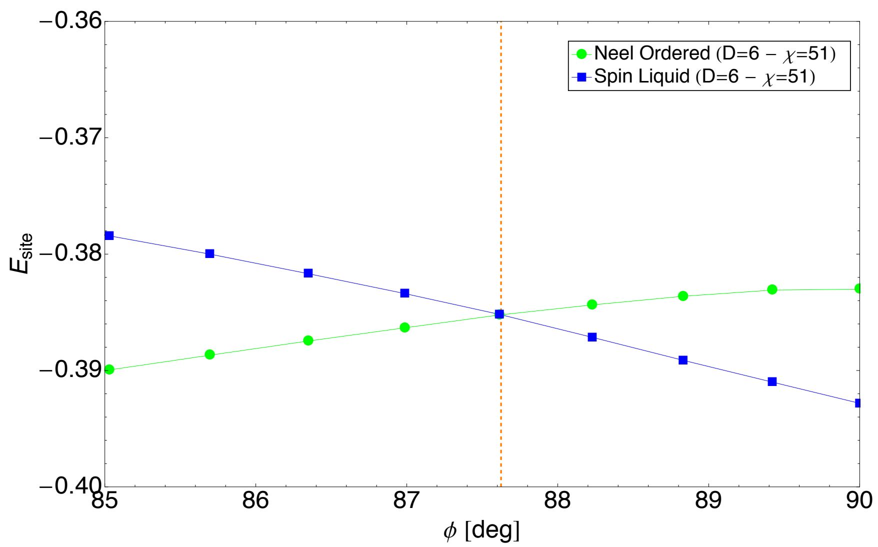


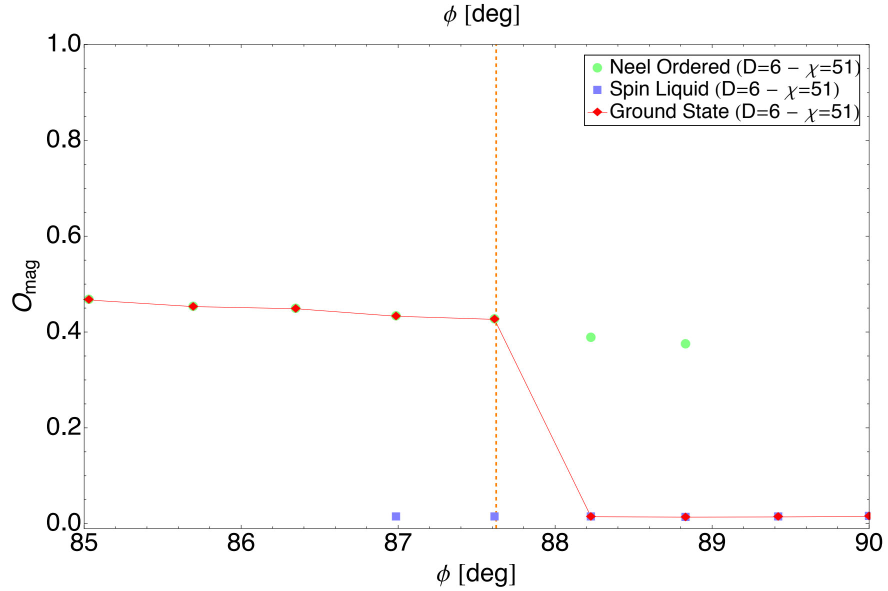
JOI, P. Corboz, M. Troyer, arXiv:1408.4020.

Kitaev-Heisenberg model

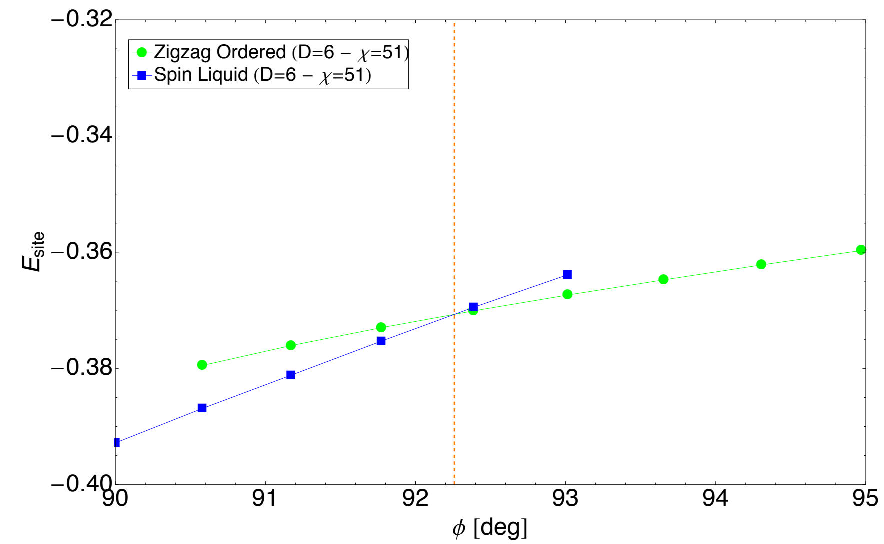
AFM Spin liquid to symmetry broken

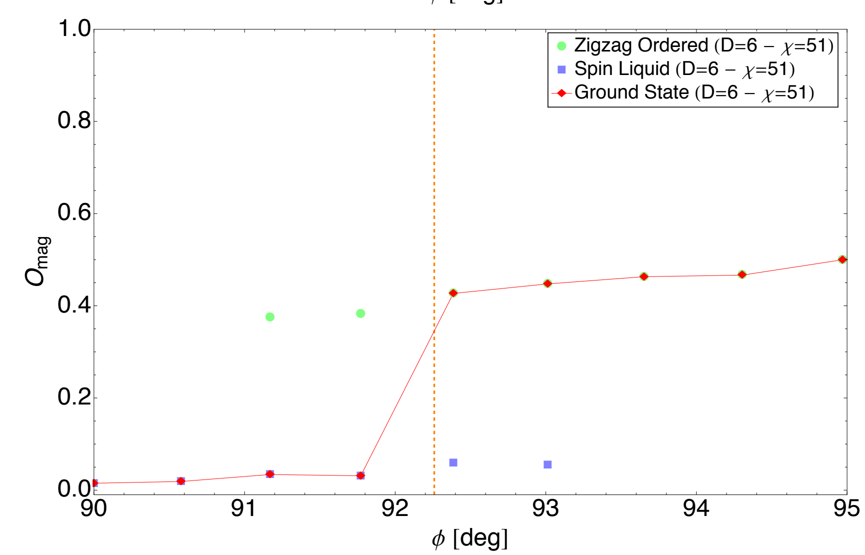
ASL - Néel





ASL - Zigzag

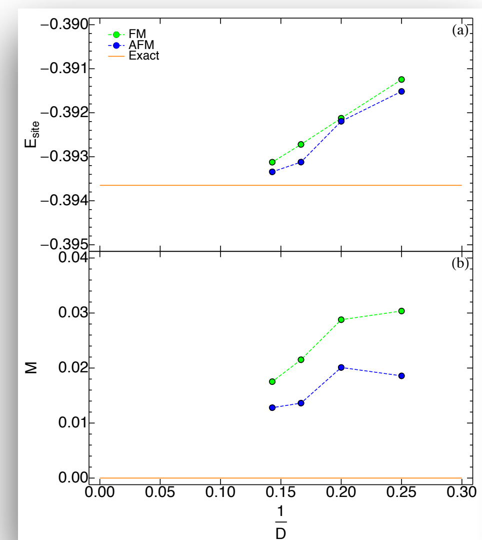


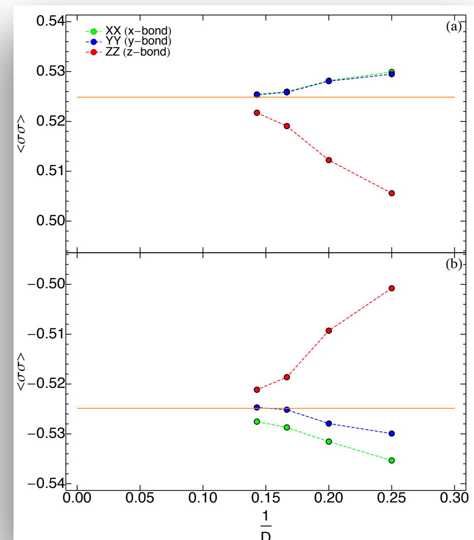


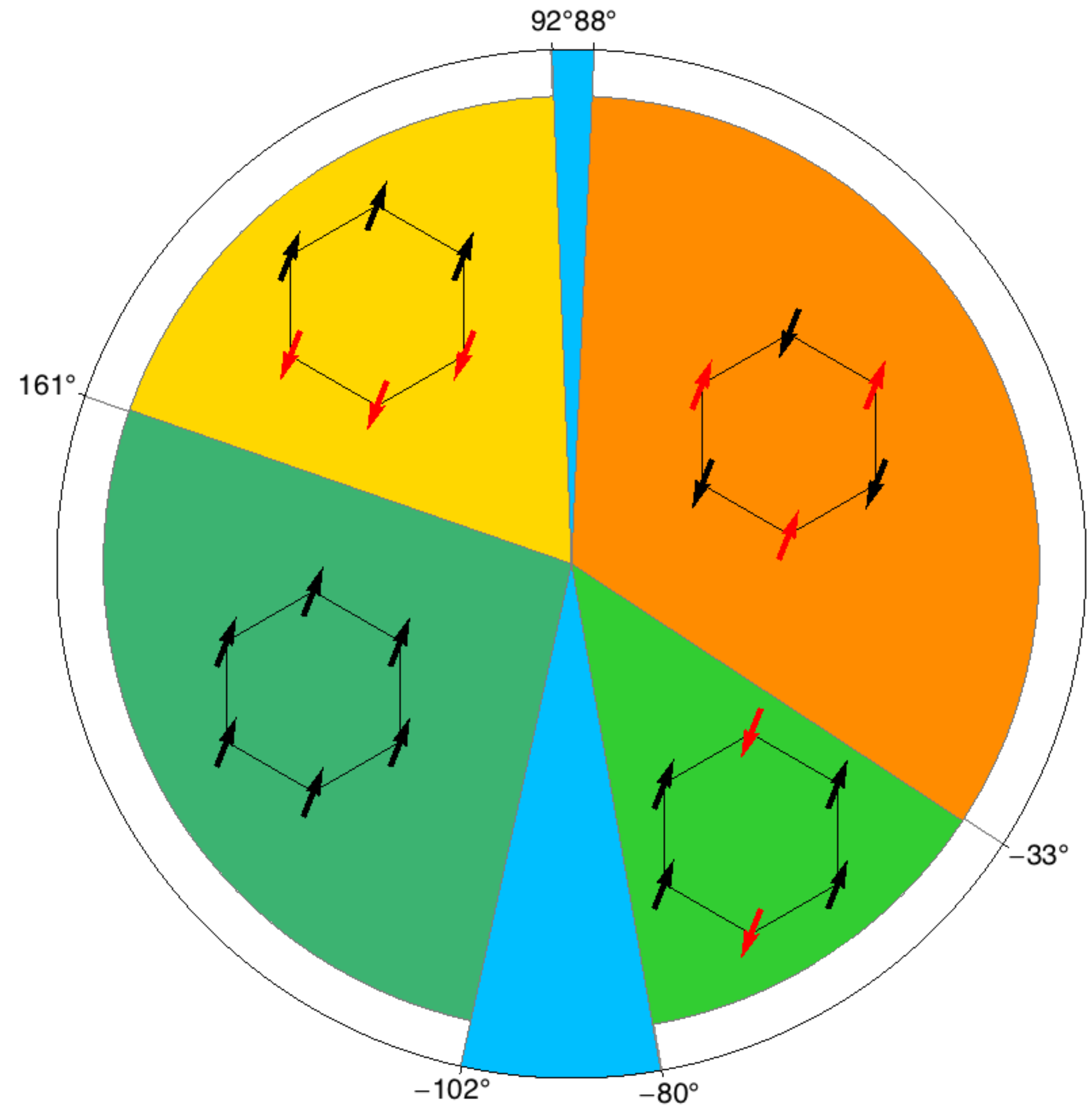
JOI, P. Corboz, M. Troyer, arXiv:1408.4020.

Kitaev-Heisenberg model

Summary







	iPEPS	Lanczos
ASL - Néel	88°	88°
ASL - Zigzag	92°	92°
FSL - Stripy	-80°	-76°
FSL - Ferro	-102°	-108°
Ferro - Zigzag	161°	162°
Stripy - Néel	-33°	-34°