Quantum Spin Liquids: Experimental Enigmas and Theoretical Challenges
6-10 October 2025, Budapest

Quantum Phase Diagram of the Bilayer Kitaev-Heisenberg Model

arXiv:2412.17495

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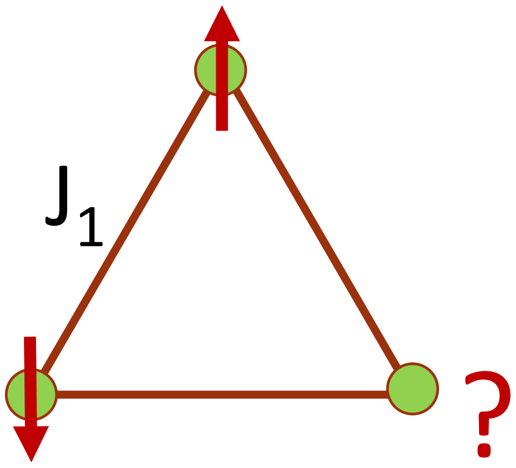
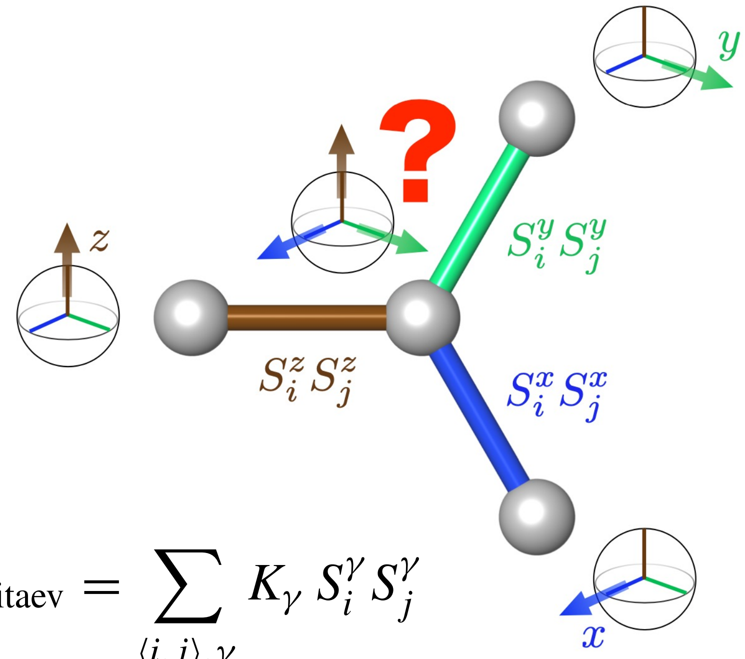
Outline

- Kitaev Quantum Spin Liquids
- Kitaev-Heisenberg Model on the Honeycomb Lattice
- The Bilayer Kitaev-Heisenberg Model
- Tensor Networks for Layered Systems
- Phase Diagram
- Results and Discussion

Frustration, Root to Spin Liquids



$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z$$



$$\mathcal{H}_{\text{Kitaev}} = \sum_{\langle i,j \rangle, \gamma} K_\gamma \, S_i^\gamma S_j^\gamma$$

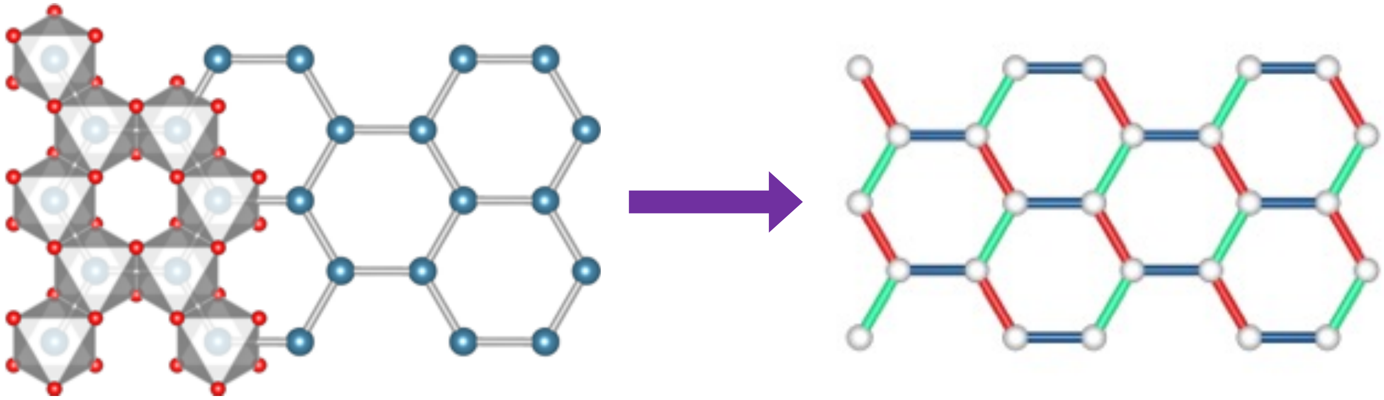
Frustration:

- **Geometric frustration:** Antiferromagnetic Couplings + Odd Loops (Triangular, Kagome lattices)
- **Exchange frustration:** Competition between different exchange paths

- Total energy of the system does not correspond to minimum of each interaction term in the Hamiltonian

Introduction to Frustrated Magnetism: Materials, Experiments, Theory, Editors: F Mila, C Lacroix, P Mendels, Springer, (2011)

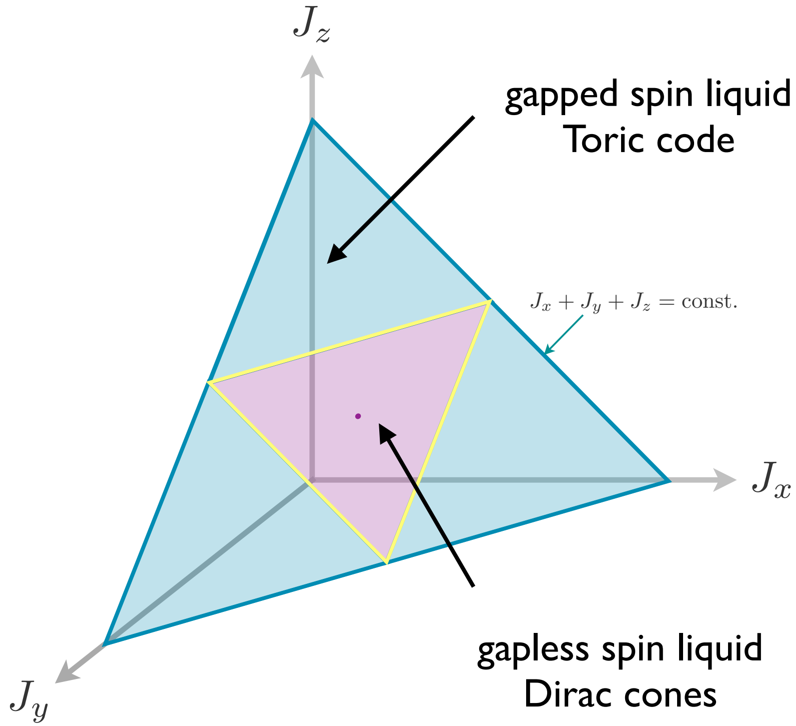
Kitaev Spin Liquid in 2D



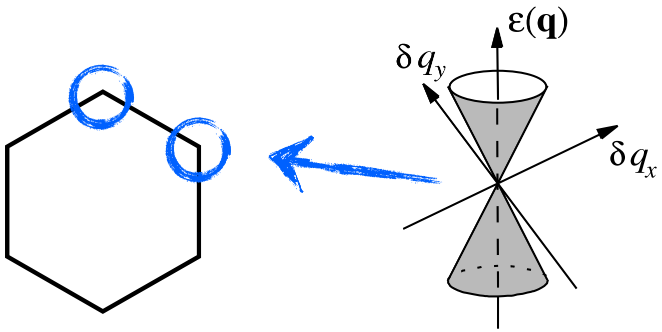
Singh et al., PRL 108, 127203 (2008)

Strong Spin-Orbit Coupling leads to bond-anisotropic exchange interactions

$$H = -\sum_{\gamma-\mathrm{bond}} J_\gamma \sigma_j^\gamma \sigma_k^\gamma$$



Exactly Solvable on all trivalent lattices in 2D, 3D

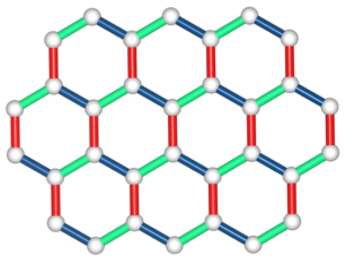


A. Kitaev, Annals of Physics 321, 2 (2006)

Isotropic Kitaev QSL Properties

$$\mathcal{H}_{\mathrm{KIF}} = J \sum_{\substack{\alpha-\text{links} \\ \alpha=x,y,z \\ <i,j>}} S_i^{\alpha} S_j^{\alpha}$$

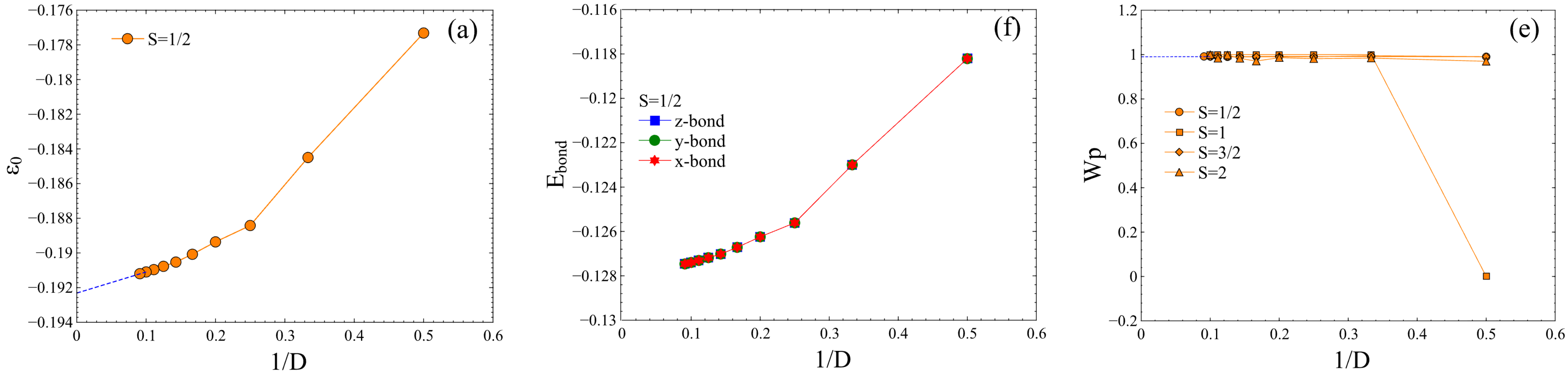
$$W_p = e^{i\pi(S_1^x + S_2^y + S_3^z + S_4^x + S_5^y + S_6^z)}$$



- $[H, W_p] = 0$, → W_p constant of motion → conserved quantum number per plaquette p for general S given by the eigenvalues ±1

A. Kitaev, Annals of Physics 321, 2 (2006)

Tensor Networks (iPEPS) Results



Baskaran, G., Mandal, S. Shankar, R., Phys. Rev. Lett.98, 247201 (2007)

S. S. Jahromi, M. Hörmann, P. Adelhardt, S. Fey, H. Karamnejad, R. Orús, K P. Schmidt, Communications Physics, **7**, 319 (2024)

Kitaev-Heisenberg Model in 2D

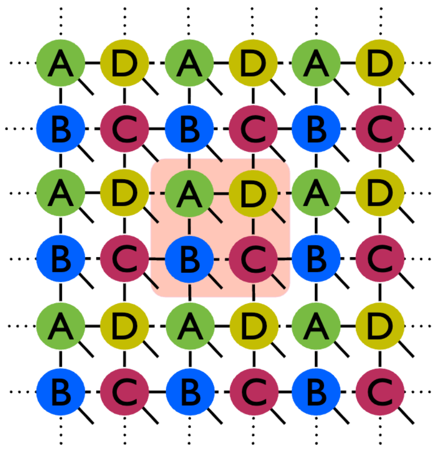
Kitaev-Heisenberg Phase diagram on the Honeycomb lattice:

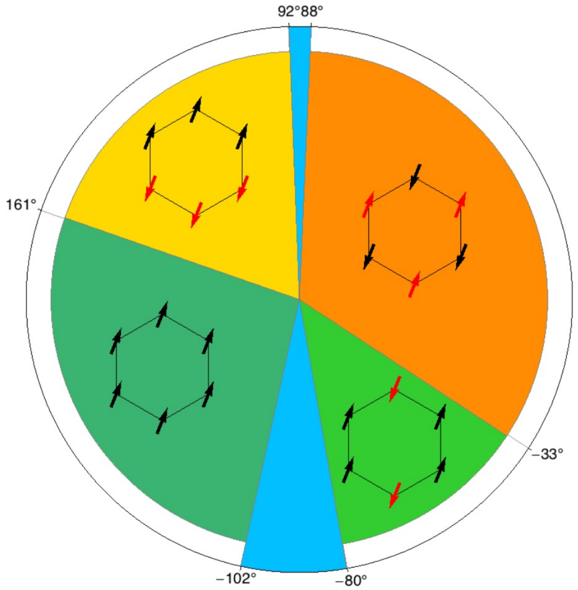
- The interplay of Kitaev and Heisenberg interaction leads to a rich phase diagram

$$\mathcal{H}_{ij}^{(\gamma)} = 2KS_i^\gamma S_j^\gamma + J\boldsymbol{S}_i \cdot \boldsymbol{S}_j.$$

$K = A\sin\varphi$ and $J = A\cos\varphi$

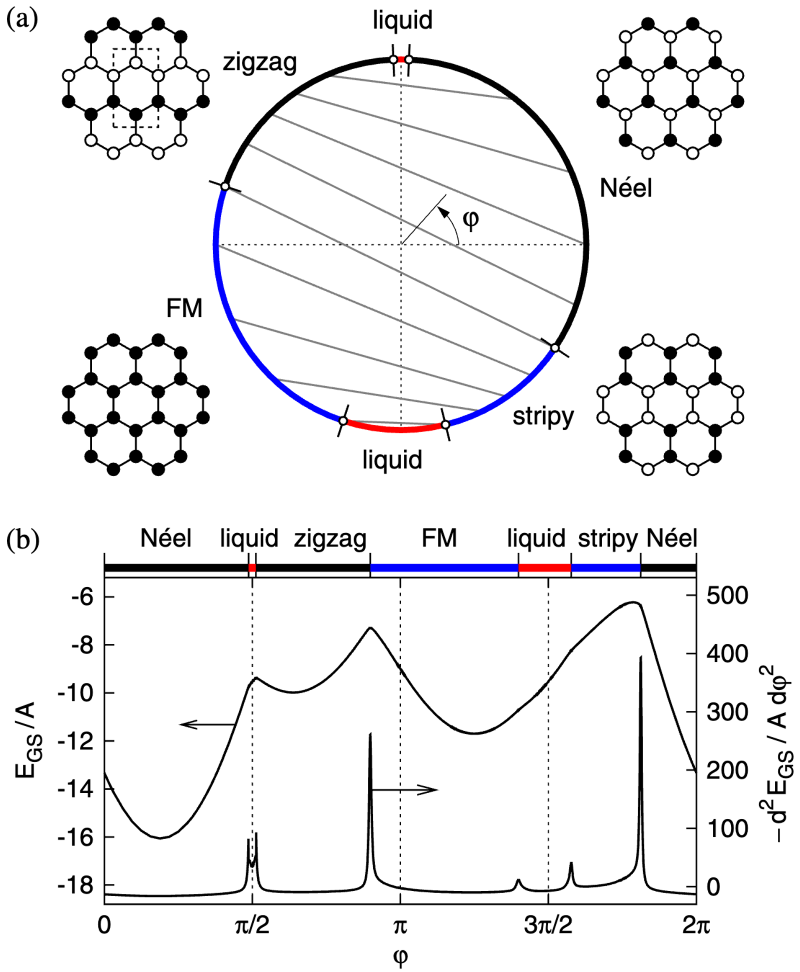
Tensor Networks (iPEPS)





J. Osorio Iregui, P. Corboz, M. Troyer, PRB 90, 195102 (2014)

Exact Diagonalization



J. Chaloupka, G. Jackeli, G. Khaliullin,
PRL 105, 027204 (2010), PRL 110, 097204 (2013)

Beyond 2D: Bilayer Structure

New Physics and Phase Diagram?

- What is the phase diagram of the Kitaev-Heisenberg model on bilayer honeycomb lattice?
- Can we observe any new phase not present in the monolayer?

Geometrical Challenges for Tensor Network Algorithms:

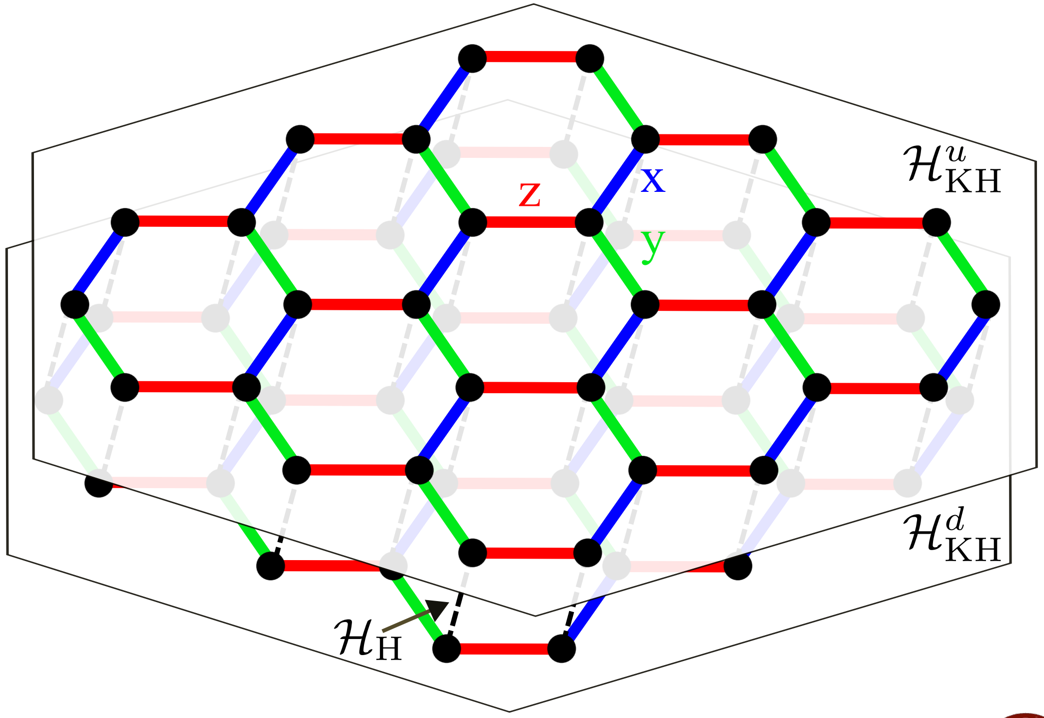
- How to simulate bilayer systems with tensor networks?

Intralayer interactions:

$$\mathcal{H}^{\ell}_{\mathrm{KH}} = K \sum_{\langle ij \rangle_\alpha} S^{\alpha}_{i,\ell} S^{\alpha}_{j,\ell} + J \sum_{\langle ij \rangle} \mathbf{S}_{i,\ell} . \mathbf{S}_{j,\ell},$$

Interlayer interactions:

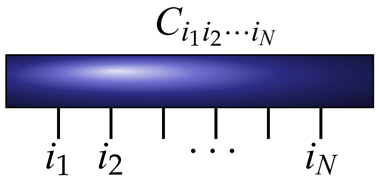
$$\mathcal{H}_{\mathrm{H}} = J_{\perp} \sum_{i} \mathbf{S}_{iu} . \mathbf{S}_{id}$$



Tensor Network Representation of a Wave-Function

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_N}^{p} c_{i_1,i_2,\ldots,i_N} |i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_N\rangle$$

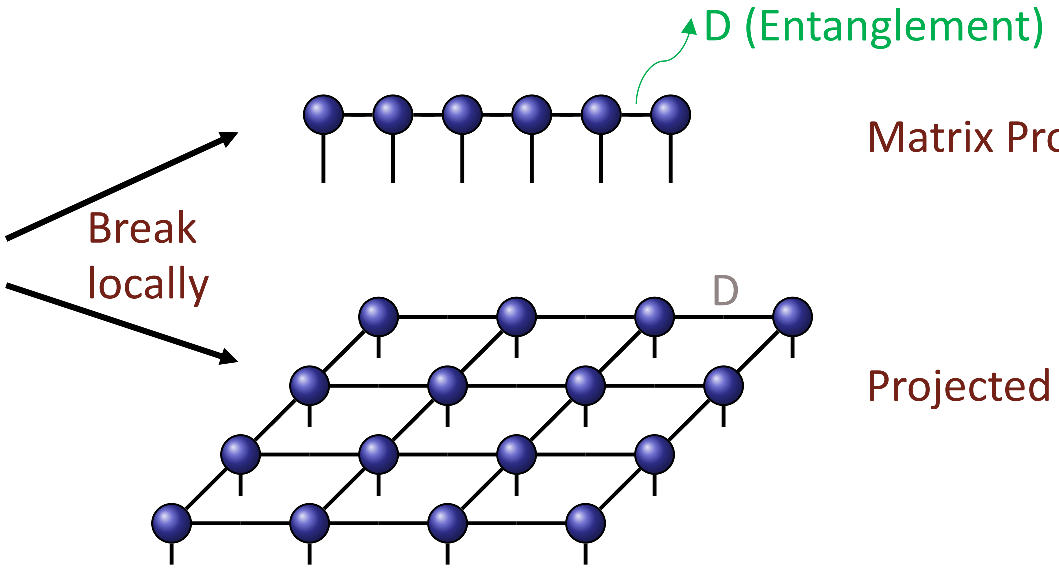
$\mathbb{V}$: local Hilbert space
e.g. $\{|\uparrow\rangle, |\downarrow\rangle\}$



Tensor with N indices

$O(P^N)$

Inefficient



Matrix Product States

Projected Entangled-Pair State (PEPS)

O(poly(P,N,D))

Efficient

Some of the advantages of Tensor Network Methods:

- TNs are build on genuine quantum correlations → Beyond Mean-Field calculations
- No Fermionic sign problem → Beyond QMC calculations
- Simulate systems in the thermodynamic limit → Beyond finite size Exact Diagonalization

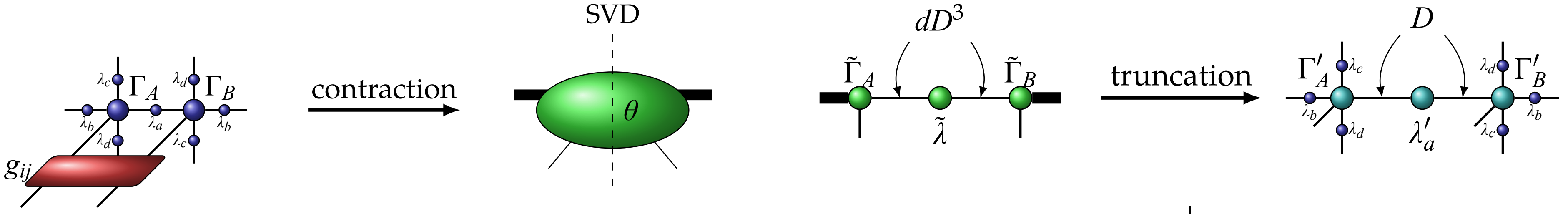
Verstraete et al, PRL, (206), Orus, Ann. Phys. (2014), Orus et al, PRB (2009), Corboz et al, PRB (2010), Corboz et al, PRB (2012)

Infinite Projected Entangled-Pair State

Finding the ground state of Local Hamiltonians? DMRG, TEBD, PEPS

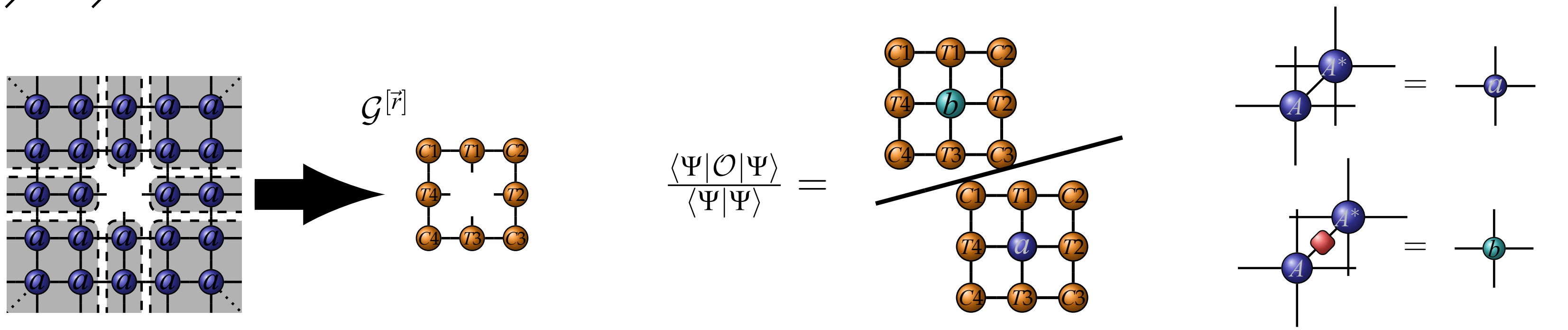
Simple Update:

Jiang et al, PRL, (2008)
Corboz et al, PRB (2010)



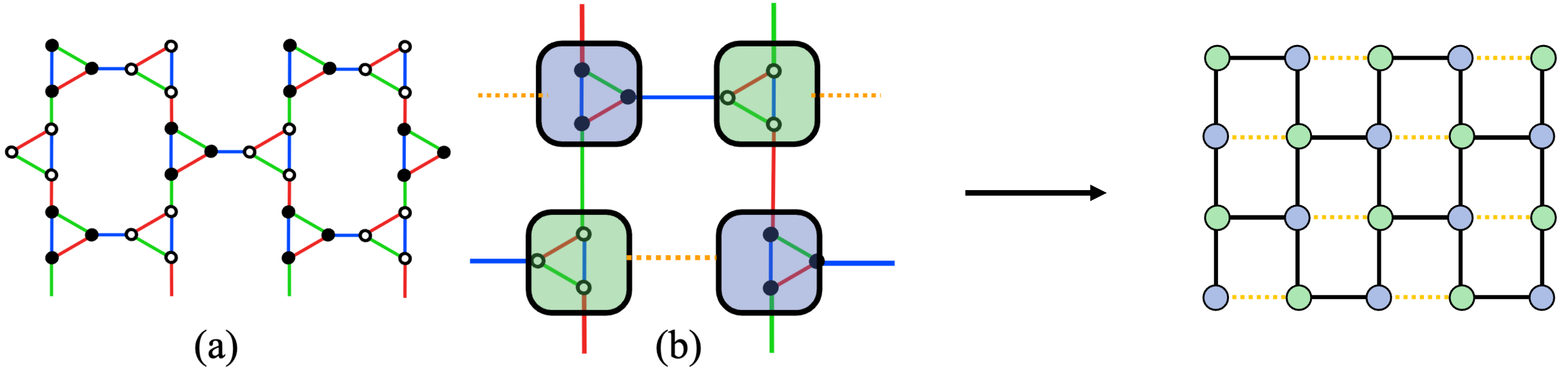
CTMRG:

Nishino et al, JPSJ, (1996)
Orus et al, PRB (2009)
Corboz et al, PRB (2010)
Corboz et al, PRB (2014)



Tensor Network for the Honeycomb-like lattices

iPEPS with coerce-graining three spin-½ into a block site with $d=2^3$ to form a square TN of block-sites

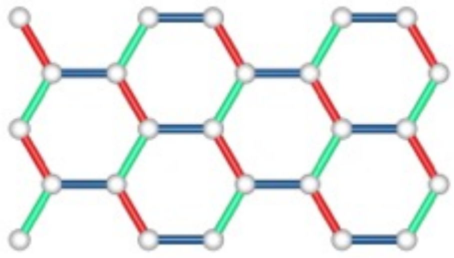


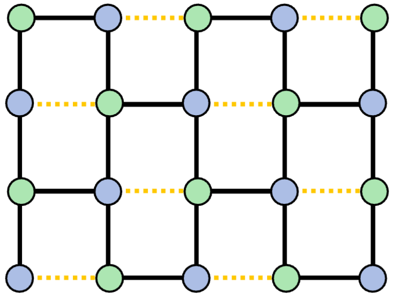
Corboz et al, PRB, (2012)
Corboz et al, PRL (2014)
Jahromi et al, PRB, (2018), (2019)

Tensor Networks for Layered Systems

From Honeycomb to Square Geometry:

- Reshape the Honeycomb lattice to Brick-Wall structure and add dummy link to obtain a Square lattice

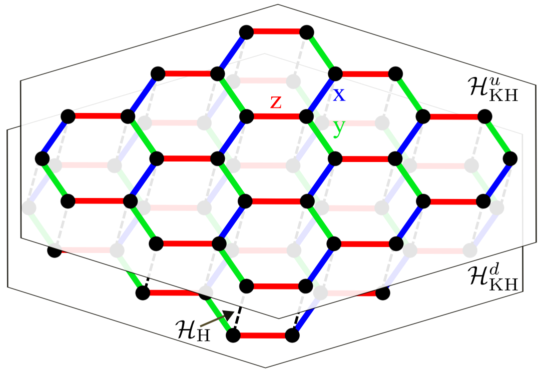


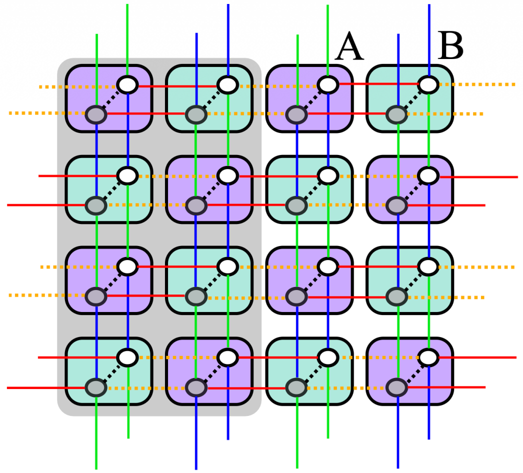


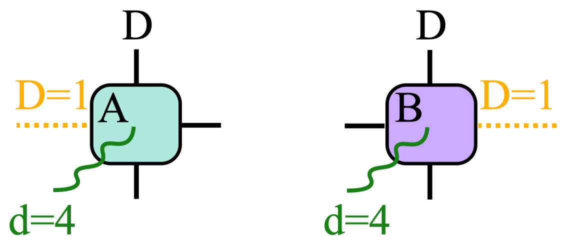
S. S. Jahromi, R. Orus, M. Kargarian, A. Langari, PRB 97, 115161 (2018)

- **From Bilayer to Monolayer:**

- Course-grain the two spins of a rung dimer at each site and replace it with a block-site with local Hilbert space dimension $2^2 = 4$. Then assign a rank-5 iPEPS tensor to each site with one dummy virtual leg



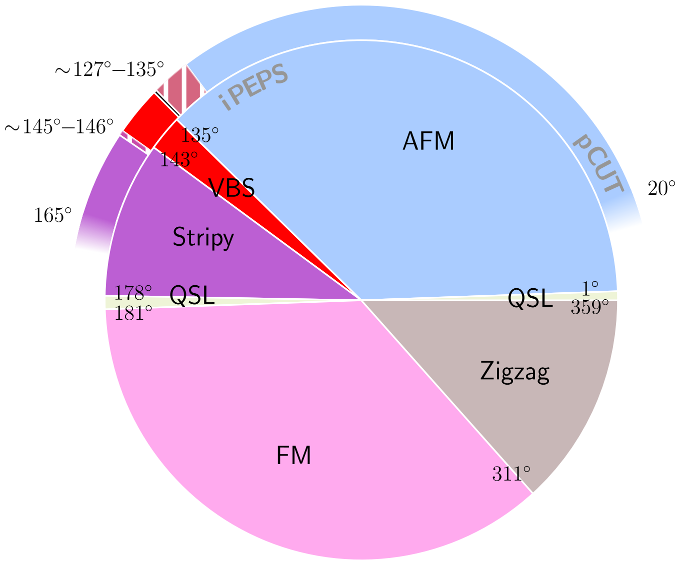




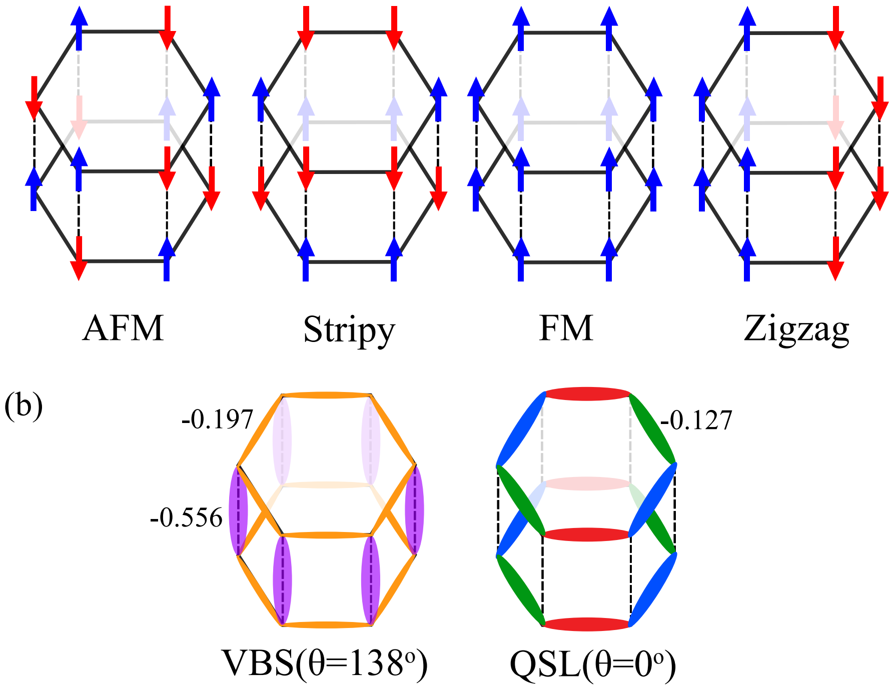
Phase Diagram

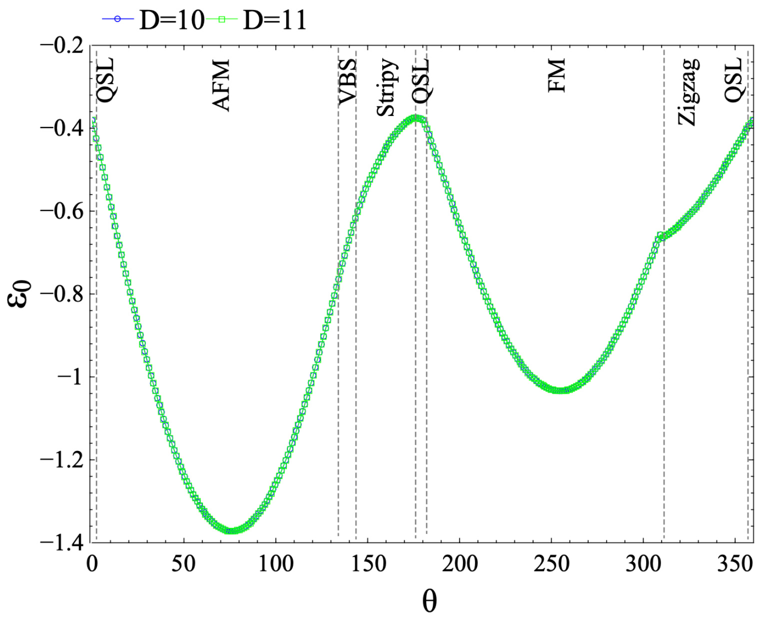
$$\mathcal{H}^{\ell}_{\rm KH} = K \sum_{\langle ij \rangle_\alpha} S^{\alpha}_{i,\ell} S^{\alpha}_{j,\ell} + J \sum_{\langle ij \rangle} \mathbf{S}_{i,\ell}.\mathbf{S}_{j,\ell}, \qquad \mathcal{H}_{\rm H} = J_{\perp} \sum_{i} \mathbf{S}_{iu}.\mathbf{S}_{id}$$

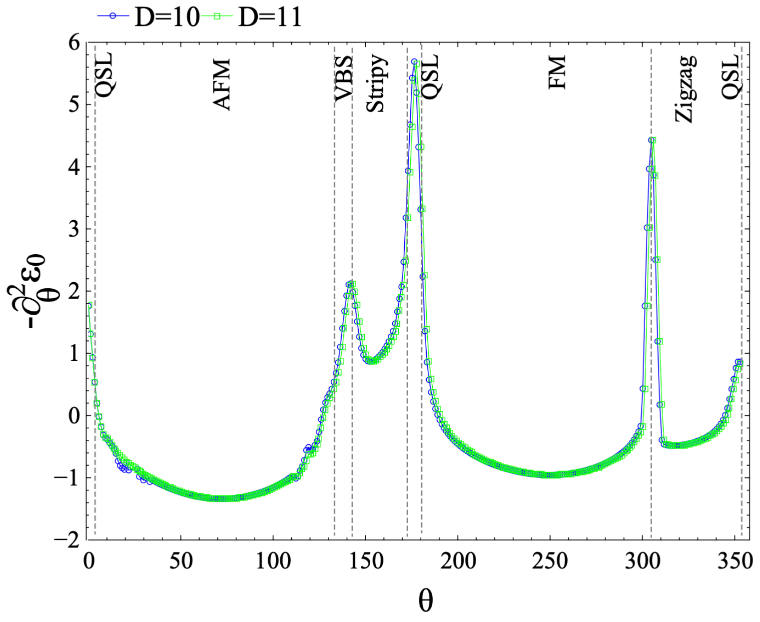
$$\mathcal{H} = \mathcal{H}^{u}_{\rm KH} + \mathcal{H}^{d}_{\rm KH} + \mathcal{H}_{\rm H} \qquad J_{\perp} = J \qquad K = \cos\theta \text{ and } J = \sin\theta$$



(a)



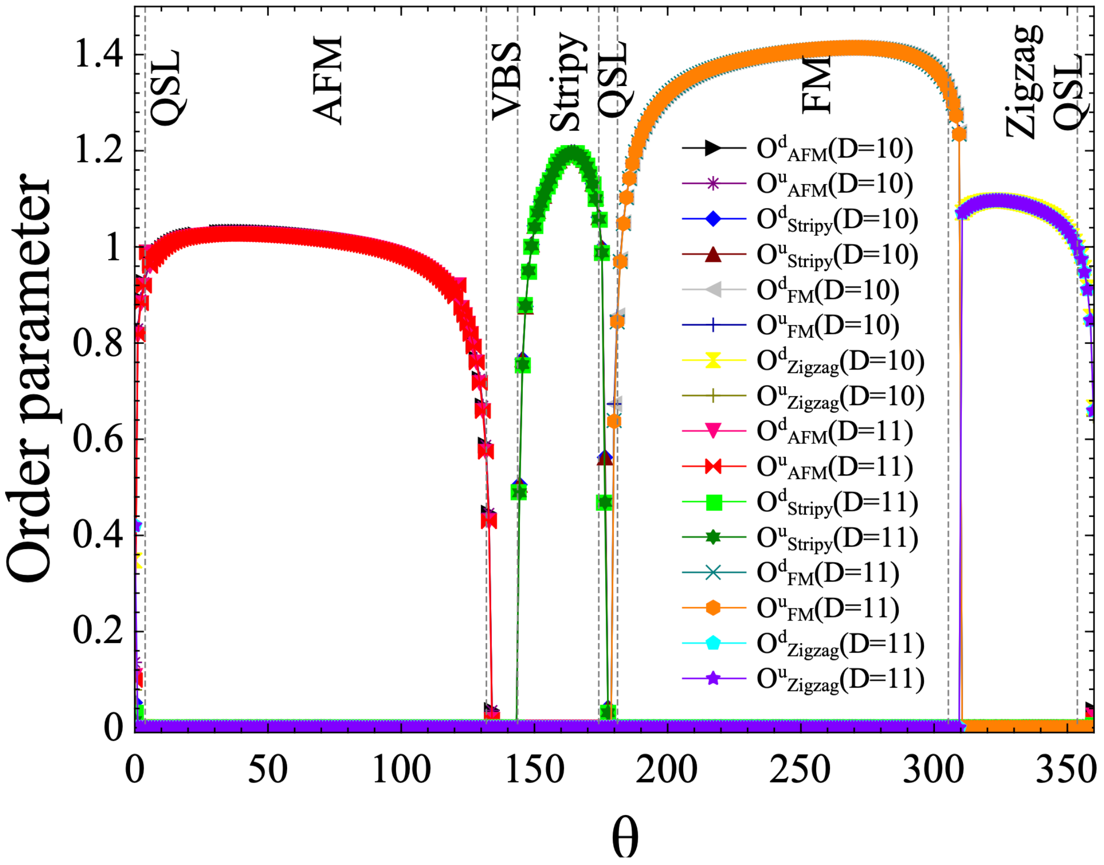


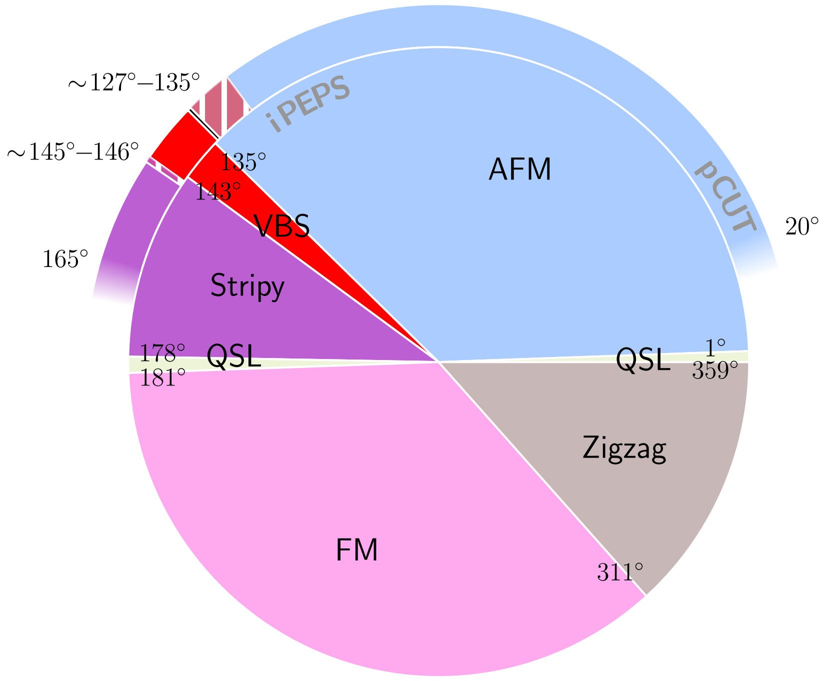


E. Samimi, A. Duft, P. Adelhardt, K. P. Schmidt, S. S Jahromi, arXiv:2412.17495

Phase Diagram

$$\mathcal{H}^{\ell}_{\mathrm{KH}} = K \sum_{\langle ij \rangle_\alpha} S^{\alpha}_{i,\ell} S^{\alpha}_{j,\ell} + J \sum_{\langle ij \rangle} \mathbf{S}_{i,\ell} . \mathbf{S}_{j,\ell}, \qquad \mathcal{H}_{\mathrm{H}} = J_{\perp} \sum_{i} \mathbf{S}_{iu} . \mathbf{S}_{id} \qquad \mathcal{H} = \mathcal{H}^{u}_{\mathrm{KH}} + \mathcal{H}^{d}_{\mathrm{KH}} + \mathcal{H}_{\mathrm{H}}$$





(a)

E. Samimi, A. Duft, P. Adelhardt, K. P. Schmidt, S. S Jahromi, arXiv:2412.17495

Phase Diagram

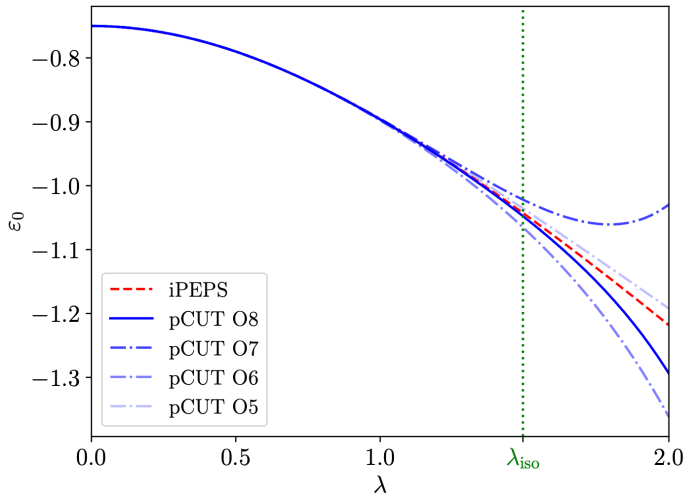
Series Expansion for the VBS Phase

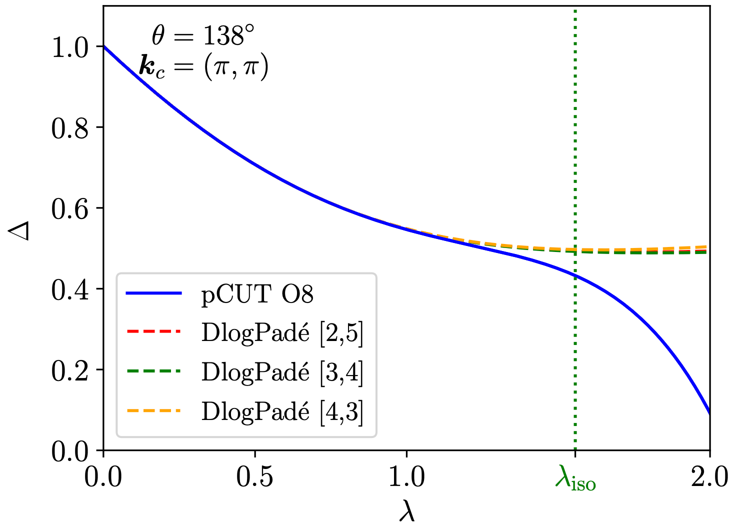
$$\mathcal{H}^{\ell}_{\mathrm{KH}} = K \sum_{\langle ij \rangle_\alpha} S^{\alpha}_{i,\ell} S^{\alpha}_{j,\ell} + J \sum_{\langle ij \rangle} \mathbf{S}_{i,\ell} . \mathbf{S}_{j,\ell}, \qquad \mathcal{H}_{\mathrm{H}} = J_{\perp} \sum_{i} \mathbf{S}_{iu} . \mathbf{S}_{id}$$

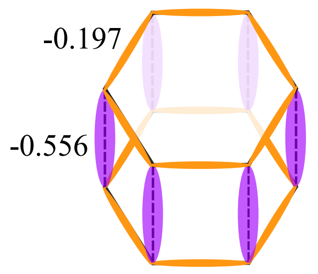
- We performed series expansion around the isolated rung dimers limit.

C. Knetter and G. Uhrig, EPJ B 13, 209 (2000).
C. Knetter et. al., J. Phys. A: Math. Gen. 36, 7889 (2003).

- We rescale the Hamiltonian by $J_{\perp}$ where the ground-state energy is given by and expand in powers of $\lambda_K \equiv K/J_{\perp} = \lambda \cos\theta$ and $\lambda_J \equiv J/J_{\perp} = \lambda \sin\theta.$
- We break the assumption of `isotropic' Heisenberg allowing $J \neq J_{\perp}$ to perform series expansions
- The isotropic Heisenberg interactions is recovered in the end for $\lambda_J = 1$ i.e., $\lambda_{\mathrm{iso}} \equiv 1/\sin\theta$







VBS(θ=138°)

- The triplon gap stays finite at the physically relevant λ_{iso} with no transition → The VBS phase is adiabatically connected to the isolated-dimer limit.

Conclusion

- The ground-state phase diagram of the spin-½ Kitaev-Heisenberg model on the bilayer honeycomb lattice was studied.
- We Combined the iPEPS tensor-network simulations in the thermodynamic limit with high-order series expansions from the isolated-dimer limit to obtain ground-state and excitation properties.
- We Identified **seven** distinct phases—four magnetically ordered, two quantum spin-liquid (QSL) states, and one interlayer valence-bond solid (VBS).
- While the FM, AFM, Zigzag and Stripy phases exist in the monolayer Kitaev-Heisenberg model, the VBS phase uniquely emerges due to the bilayer structure.
- Alternative approaches for TN simulation of layered or 3D systems: gPEPS (graph projected entangled pair state).

S. S. Jahromi, R. Orus, PRB 99, 195105 (2019)
S. S. Jahromi, H. Yarloo, R. Orus, Phys. Rev. Research 3, 033205 (2021)

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Thanks for your attention