Entanglement in Strongly Correlated Systems
09-22 February 2020, Benasque, Spain

Spin-½ Kagome Heisenberg Antiferromagnet with Strong Breathing Anisotropy

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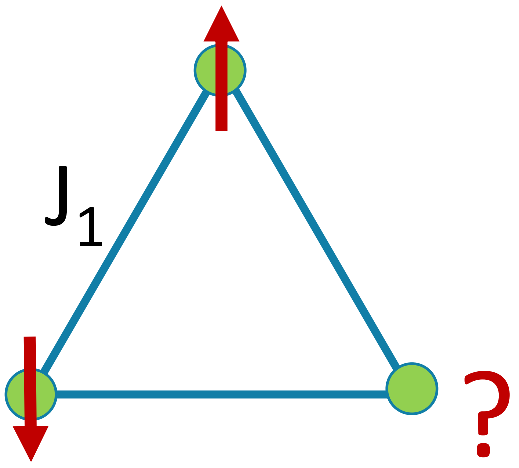
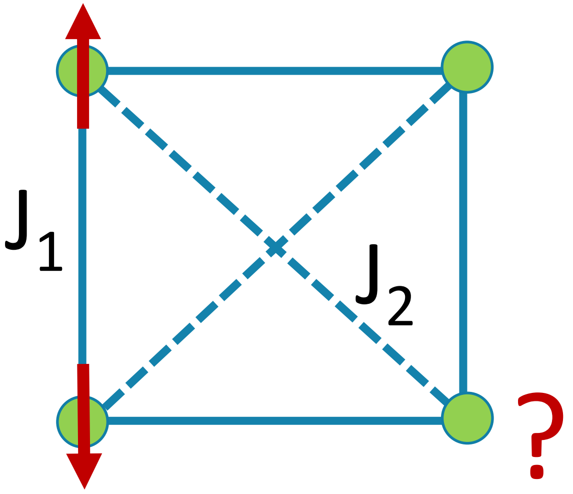
Outline

- Frustrated Spin Systems
- Breathing Kagome Heisenberg Antiferromagnets
- Infinite Projected Entangled Pair (Simplex) States
- Small Breathing Anisotropy Limit
- Large Breathing Anisotropy Limit
- Quantum Phase Transition
- Conclusion and Outlook

Frustrated Spin Systems





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

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z$$

Frustration: Antiferromagnetic Couplings + Odd Loops

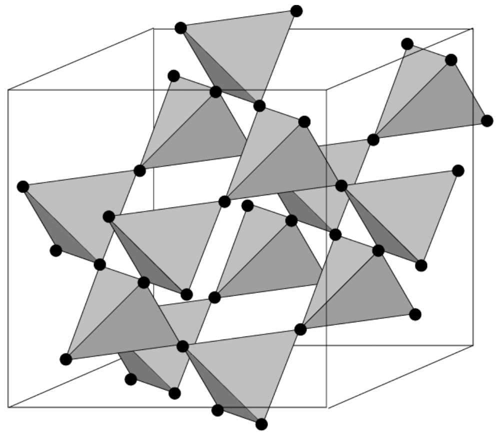
- Geometric: 2D lattice of corner-sharing triangles (Triangular, Kagome)
- Competition between different exchange paths: J_1-J_2 Mode
- Total energy of the system does not correspond to minimum of each interaction term in the Hamiltonian

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

Frustrated Spin Systems

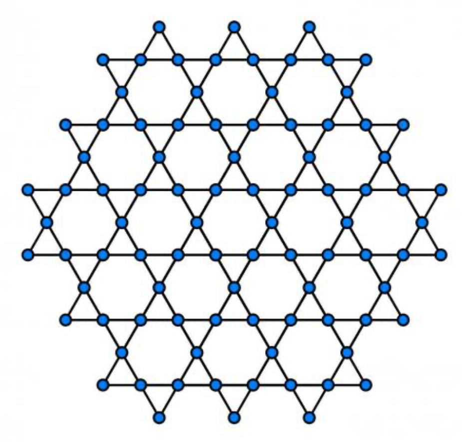
Why study frustrated systems?

- Frustration is typically present in real material in nature
- Exciting and challenging playground for both theorists and experimentalists
- Host exotic phases of matter such as: Spin Liquids, RVB, VBC, Plaquette States



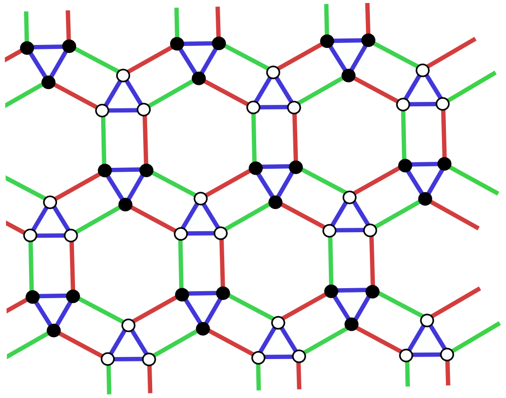
Pyrochlore Lattice

Y. Iqbal et al, PRX (2019)
Bergman et al, PRB, (2006)
Harris et al, Mod. Phys. Lett. B (1996)



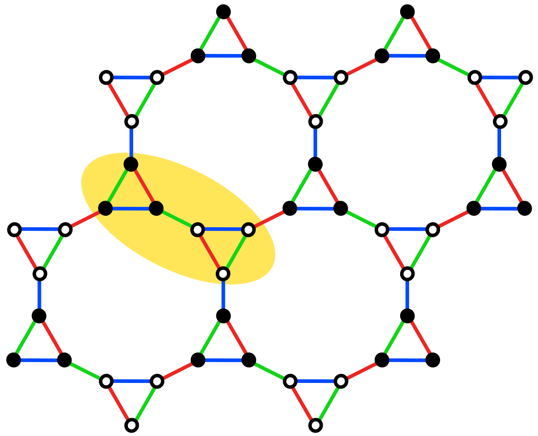
Kagome Lattice

Ran et al, PRL, (2007)
Y. Iqbal et al, PRB (2013)
Liao et al, PRL, (2017)



Ruby Lattice

Kargarian et al, NJP, (2010)
Farnell et al, PRB, (2014)
Jahromi et al, PRB (2018)



Star Lattice

Yao et al, PRL, (2007)
Dusuel et al, PRB, (2008)
Jahromi et al, PRB (2018)

Frustrated Spin Systems

Spin-½ Kagome Heisenberg Antiferromagnet

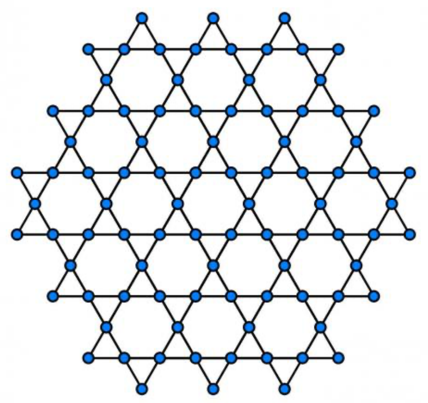
- Presence of corner sharing triangles induce high quantum fluctuation
- Ground-state of the Kagome Heisenberg antiferromagnets has been one of the most hotly debated topics in condensed matter physics
- The ground state is believed to be a Quantum Spin Liquid (QSL)
- The gapped or gapless nature is under debate

Y.C.He et al, PRX (2017)
Picot et al, PRb (2016)
Liao et al, PRL (2017)

Ran et al, PRL (2007)
Y. Iqbal et al, PRB (2014)
Y. Iqbal et al, PRB (2015)

Poilblanc et al, PRB (2012)
Schuch et al, PRB (2012)
Poilblanc et al, PRB (2013)

Jiang et al, Science (2008)
Yan et al, Science (2011)
Depenbrock et al, PRL (2012)



Kagome Lattice

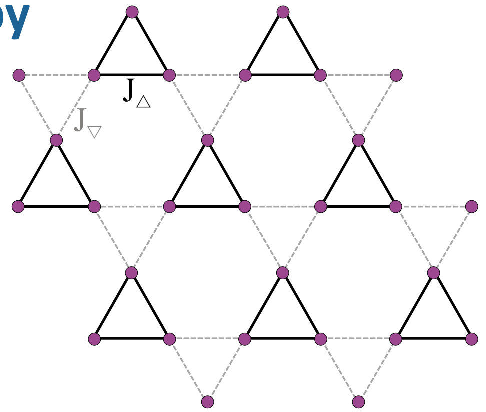
Candidate Materials:

- Volborthite $Cu_3V_2O_7(OH)_2{\cdot}2H_2O$ Yoshida et al, JPSJ, (2001), (2009)
- Vesignieite $BaCu_3V_2O_8(OH)_2$ Okomato et al, JPSJ, (2009)
- Herbertsmithite $ZnCu3(OH)_6Cl_2$ Helton et al, PRL, (2007)

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Breathing Kagome Heisenberg Antiferromagnets

Spin-½ Kagome Heisenberg Antiferromagnetic model with Breathing Anisotropy



$$H = J_\triangle \sum_{\langle ij \rangle \in \triangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_\triangledown \sum_{\langle ij \rangle \in \triangledown} \mathbf{S}_i \cdot \mathbf{S}_j$$

- Naturally, Kagome compound tend to be anisotropic in nature due to impurities or effective perturbations which influence the strength of coupling on different Kagome triangles to Be different
- Can Heisenberg antiferromagnets with Breathing anisotropy host QSL?
- Candidate Material: Vanadium Oxyfluoride compound $[NH_4]_2[C7H_{14}N][V_7O_6F_{18}]$
- Experimental Signatures of a QSL at $J_\triangledown / J_\triangle \approx 0.55$ Orian et al, PRL, (2017)

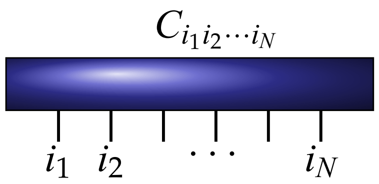
Clark et al, PRL, (2013)
Aidoudi et al, Nat. Chem. (2011)
Orian et al, PRL, (2017)

Phase Diagram?

$J_\triangledown / J_\triangle \ll 1$ QPT? $J_\triangledown / J_\triangle = 1$

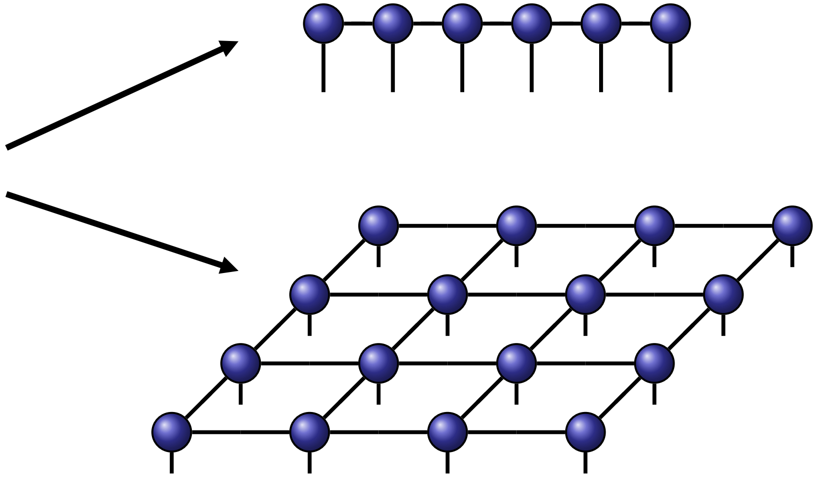
Infinite Projected Entangled-Pair State

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



Tensor with N indices

$O(P^N)$



Matrix Product States

Projected Entangled-Pair State (PEPS)

O(poly(P,N,D))

Some of the advantages of Tensor Network Methods:

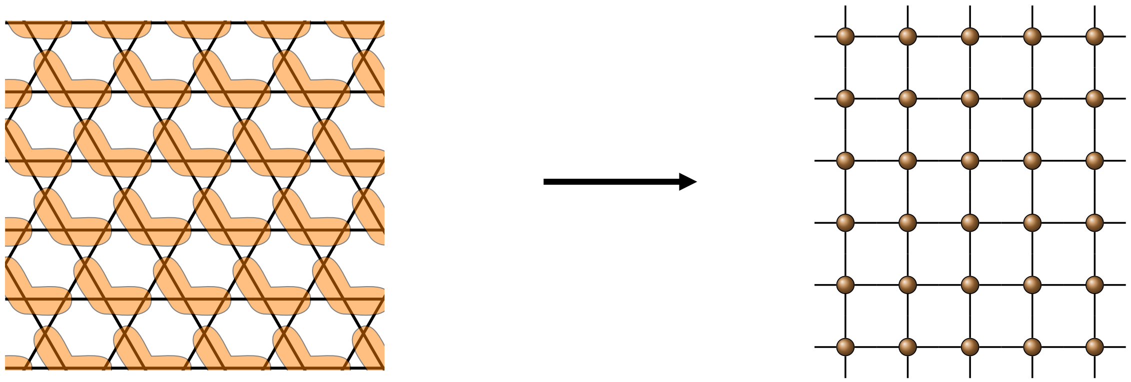
- ❖ TNs are build on genuine quantum correlations → Beyond Mean-Field calculations
- ❖ No Fermionic sign problem → Beyond QMC calculations
- ❖ Simulate systems in the thermodynamic limit → Beyond finite size Exact Diagonalization

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

Tensor Network for the Kagome lattice

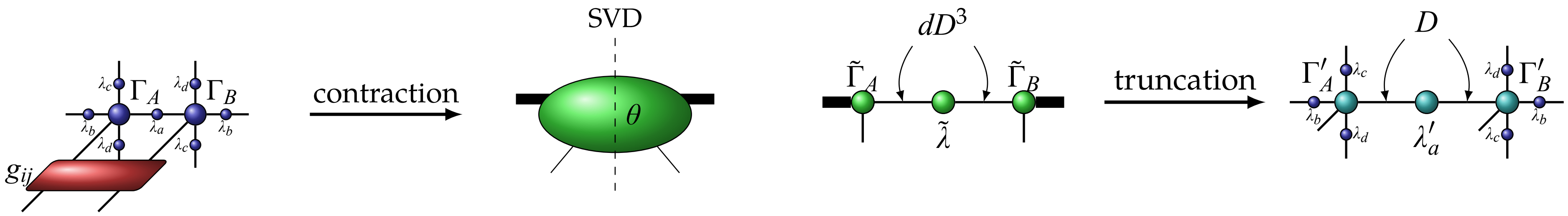
iPEPS with coerce-graining three spin-½ into a block site with d=2³ to form a square TN of block-sites



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

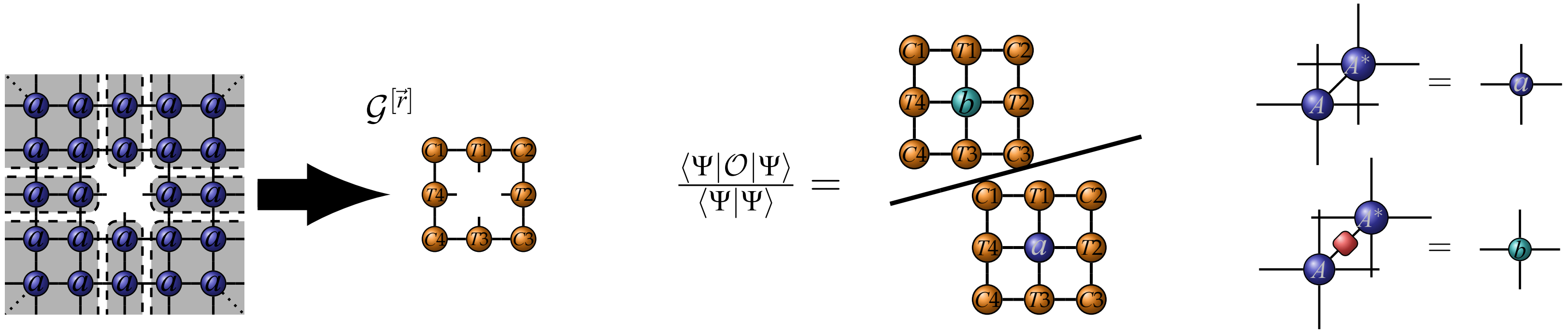
Simple Update:

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



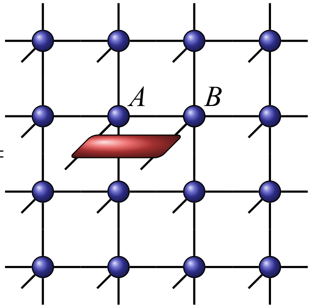
CTMRG:

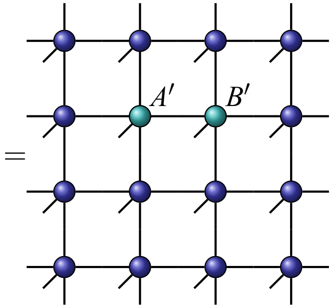
Nishino et al, JPSJ, (1996)
Orus et al, PRB (2009)
Corboz et al, PRB (2010)
Corboz et al, PRB (2014)



Infinite Projected Entangled-Pair State

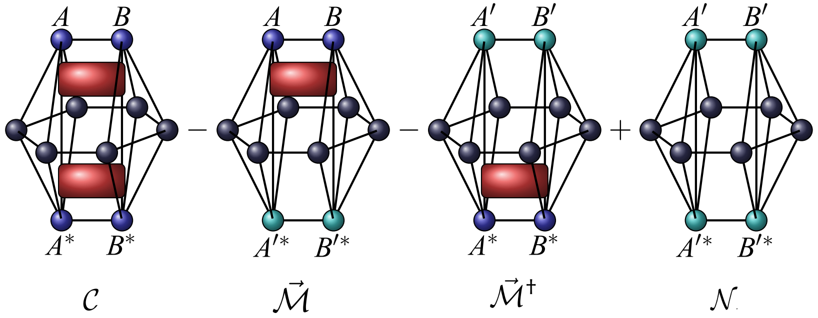
Full Update:

$|\Psi\rangle =$ 

$|\widetilde{\Psi}\rangle =$ 

Corboz, Mila, PRL (2014)
Phien et al, PRB, (2015)
Corboz, Rice et al, PRL (2014)

$$\delta = \left|\left||\Psi\rangle - |\widetilde{\Psi}\rangle\right|\right|^2 = \langle\Psi|\Psi\rangle - \langle\Psi|\widetilde{\Psi}\rangle - \langle\widetilde{\Psi}|\Psi\rangle + \langle\widetilde{\Psi}|\widetilde{\Psi}\rangle$$

$\delta =$ 

$$\min_{A'} \left|\left||\Psi\rangle - |\widetilde{\Psi}\rangle\right|\right|^2 = \min_{A'} \left(\vec{A'}^\dagger \mathcal{N} \vec{A'} - \vec{A'}^\dagger \vec{\mathcal{M}} - \vec{\mathcal{M}}^\dagger \vec{A'} + \mathcal{C}\right) \longrightarrow \frac{\partial}{\partial \vec{A'}^\dagger}\left(\vec{A'}^\dagger \mathcal{N} \vec{A'} - \vec{A'}^\dagger \vec{\mathcal{M}} - \vec{\mathcal{M}}^\dagger \vec{A'} + \mathcal{C}\right) = 0 \longrightarrow \mathcal{N}\vec{A'} = \vec{\mathcal{M}}$$

Projected Entangled-Simplex State

Tensor Network for the Kagome lattice

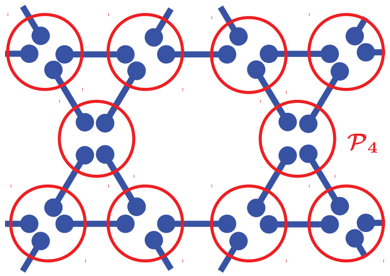


Figure taken from Schuch et al PRB (2012)

Entangled-Pairs (two-partite entangled states) on the bonds

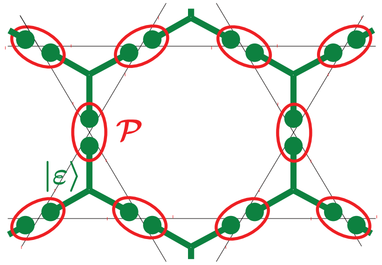
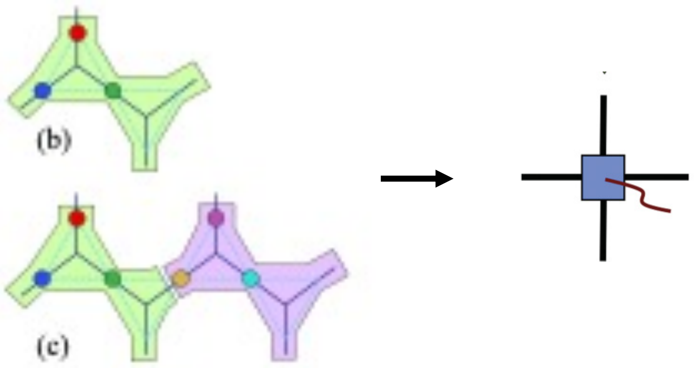
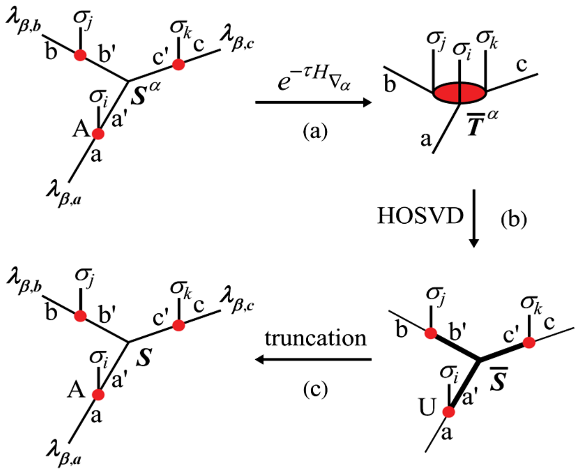


Figure taken from Schuch et al PRB (2012)

Simplex states (three-partite entangled states) on triangles



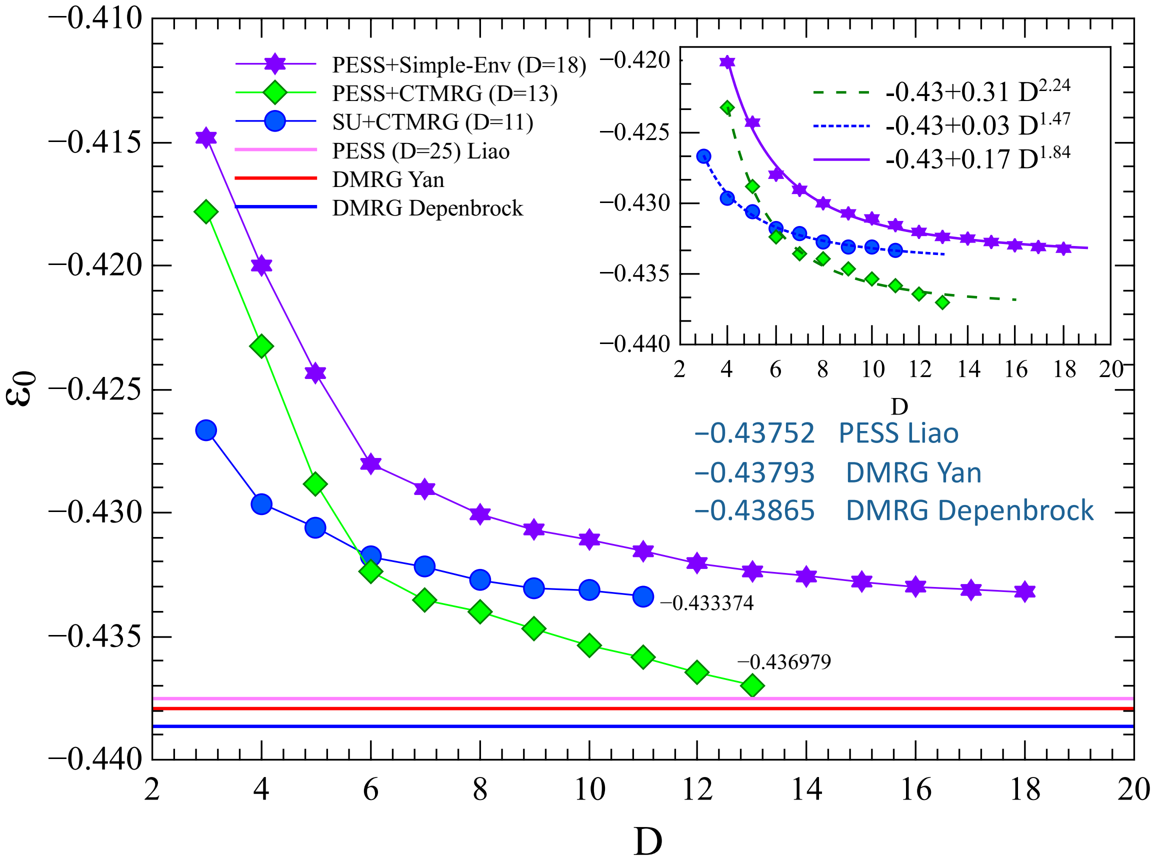


Triangle PESS Update

Xie et al, PRX (2014)
Liao et al, PRL (2017)

Small Breathing Limit

Isotropic Point: $J_\bigtriangledown / J_\vartriangle = 1$



Gapless U(1) QSL (DMRG)
- Y.C.He et al, PRX (2017)
- Repellin et al, PRB (2017)

Gapless U(1) QSL (PEPS)
- Xie et al, PRX (2014)
- Picot et al, PRb (2016)
- Liao et al, PRL (2017)

Gapless U(1) QSL (VMC)
- Ran et al, PRL (2007)
- Y. Iqbal et al, PRB (2013)
- Y. Iqbal et al, PRB (2014)
- Y. Iqbal et al, PRB (2015)

Gapped Z_2 QSL (PEPS)
- Poilblanc et al, PRB (2012)
- Schuch et al, PRB (2012)
- Poilblanc et al, PRB (2013)

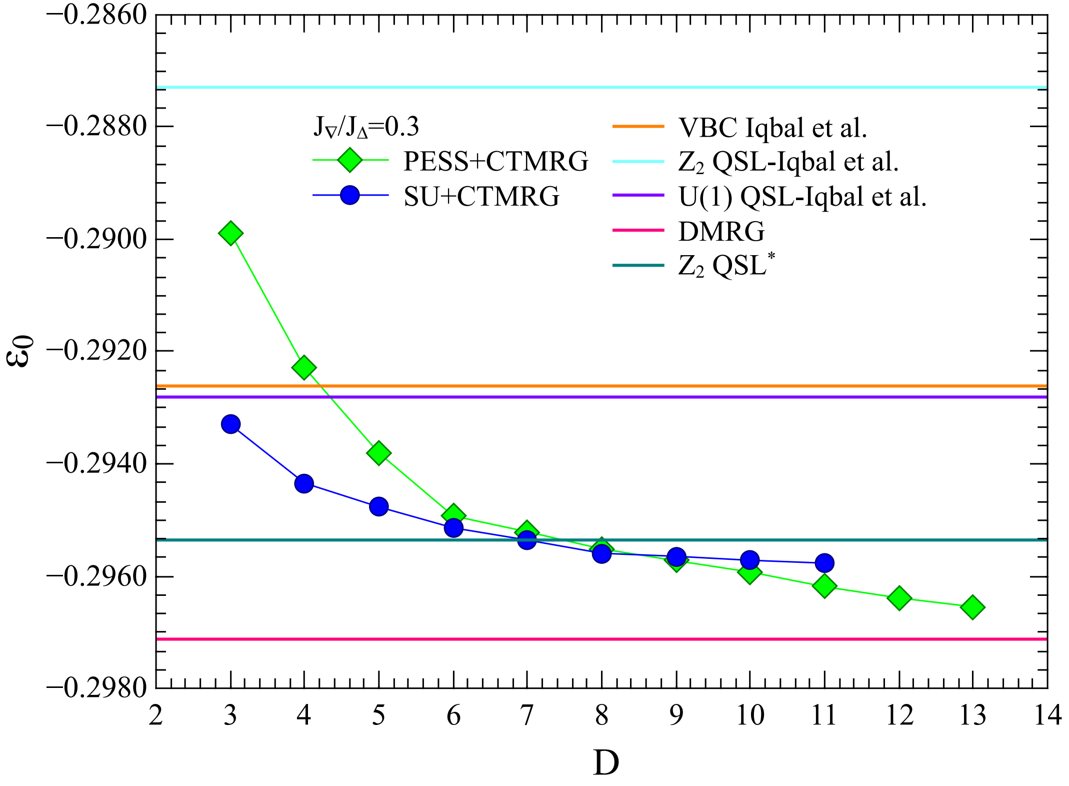
Gapped Z_2 QSL (DMRG)
- Jiang et al, Science (2008)
- Yan et al, Science (2011)
- Depenbrock et al, PRL (2012)

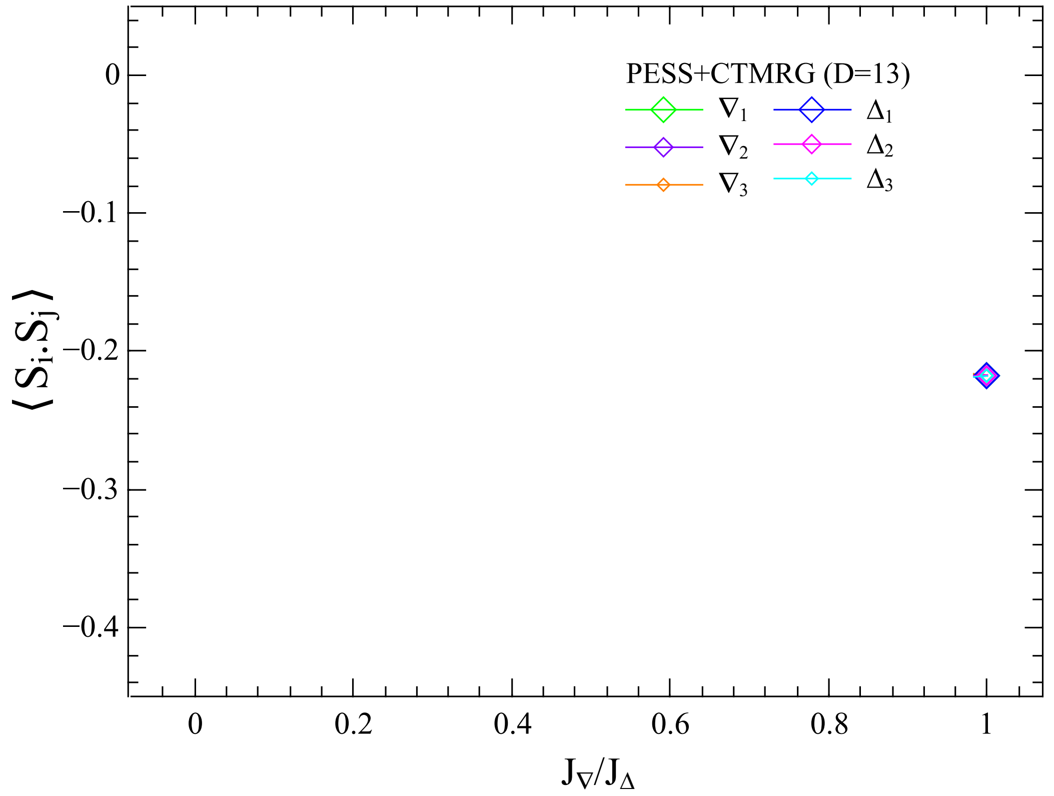
$J_\bigtriangledown / J_\vartriangle \ll 1$ $J_\bigtriangledown / J_\vartriangle = 1$

Small Breathing Limit

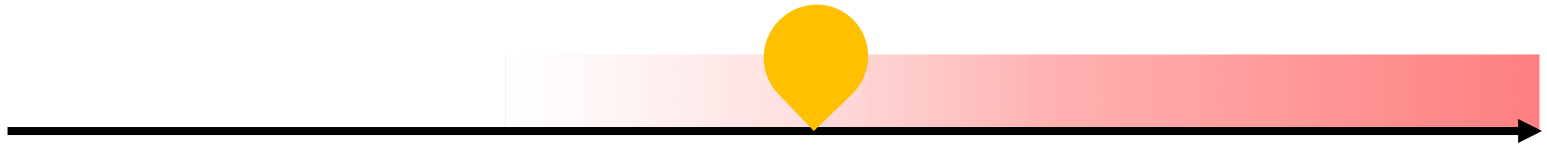
$$H = J_{\triangle} \sum_{\langle ij \rangle \in \triangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_{\triangledown} \sum_{\langle ij \rangle \in \triangledown} \mathbf{S}_i \cdot \mathbf{S}_j$$

$J_{\triangledown}/J_{\triangle}=0.3$





Experiment



$J_{\triangledown}/J_{\triangle} \ll 1$

$J_{\triangledown}/J_{\triangle} \approx 0.55$

Orian et al, PRL, (2017)

$J_{\triangledown}/J_{\triangle} = 1$

Large Breathing Limit

$J_{\bigtriangledown} / J_{\triangle} = 0.01$

VBC (VMC+PEPS)

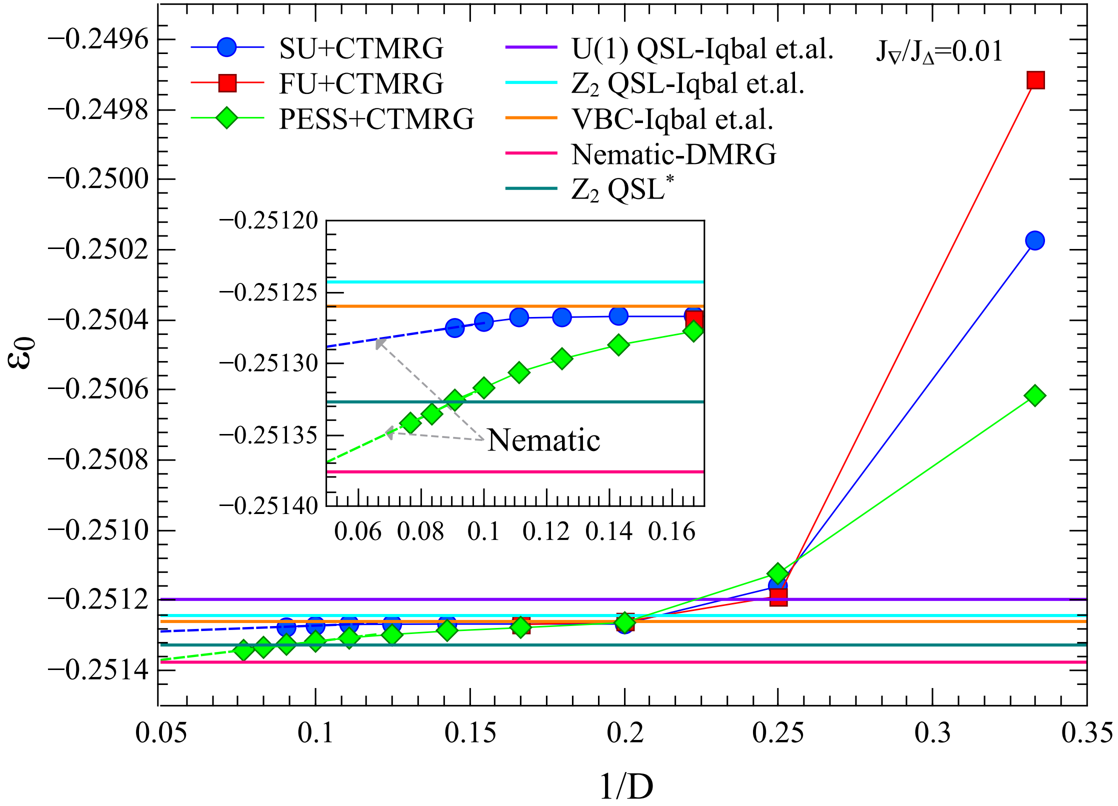
Y. Iqbal et al, PRB (2018)

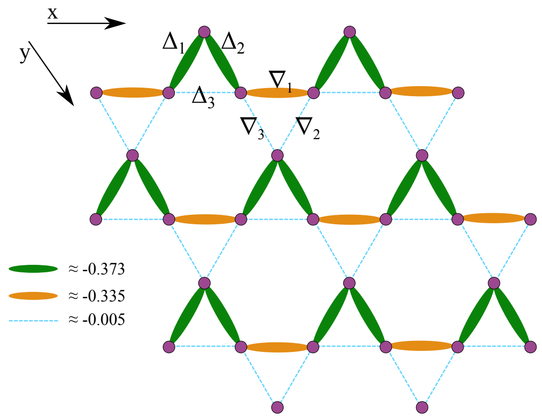
Gapped Z_2 QSL (PEPS)

M. Iqbal et al, arXiv:1912.08284 (2019)

Nematic (DMRG)

Repellin et al, PRB (2017)





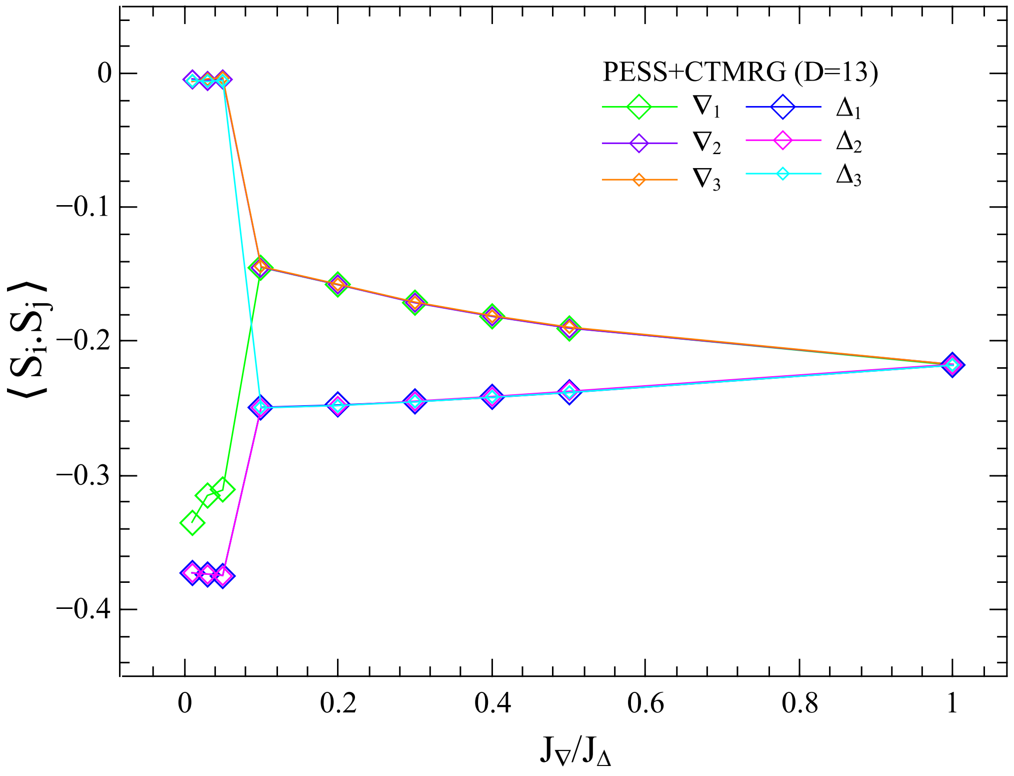
Lattice Nematic state:

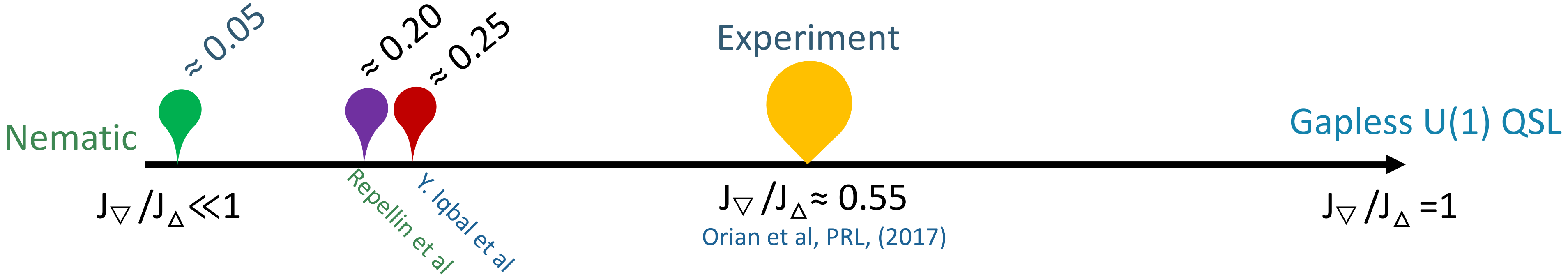
Preserves Translational Symmetry

Breaks Rotational Symmetry

$J_{\bigtriangledown} / J_{\triangle} \ll 1$ $J_{\bigtriangledown} / J_{\triangle} = 1$

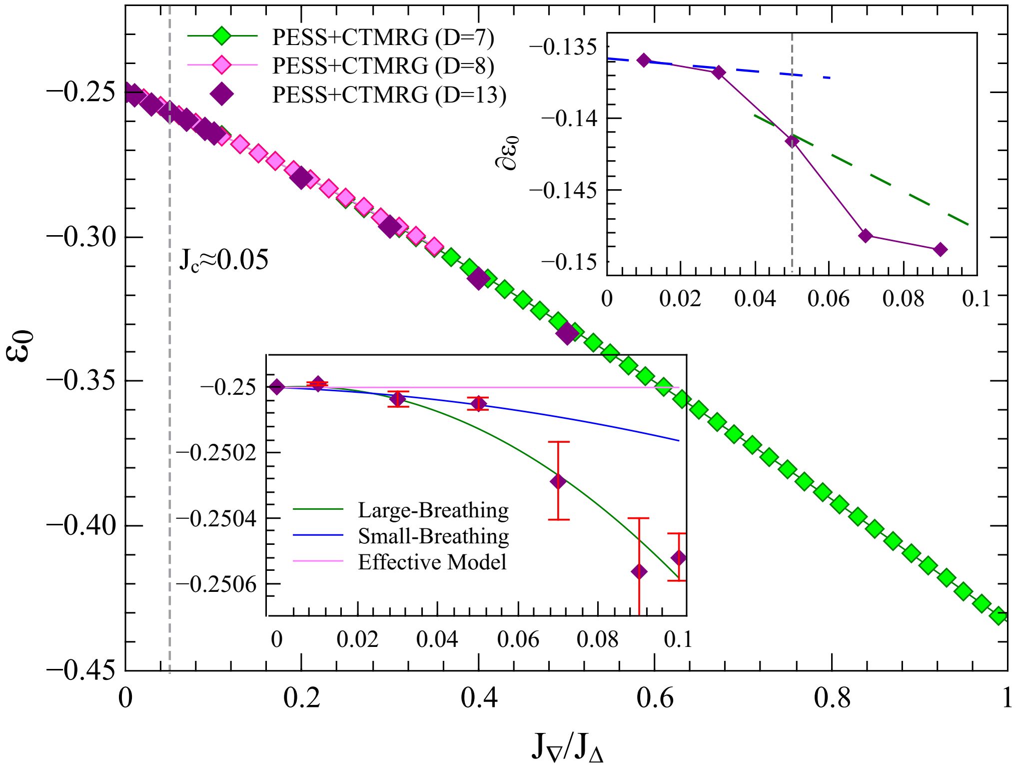
Quantum Phase Transition





Quantum Phase Transition

The QPT is First-Order



$$\frac{\varepsilon_0}{J_\triangle} = -0.25 + c_1 \frac{J_\triangledown}{J_\triangle} + c_2 \left(\frac{J_\triangledown}{J_\triangle}\right)^2 + \ldots.$$

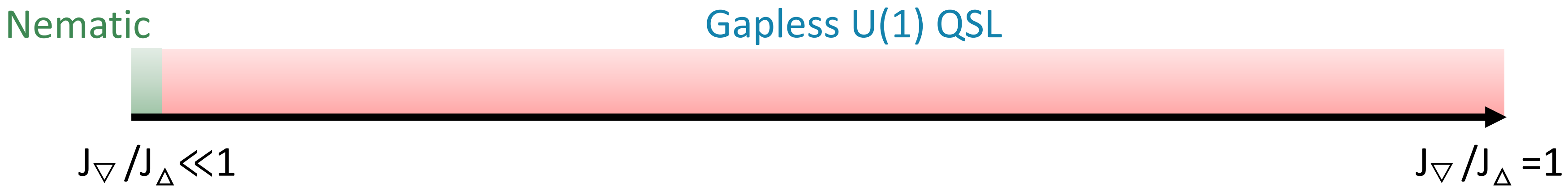
Wave Function	c_1	c_2
nematic (PESS)	-0.1358	-0.0113
U(1) QSL (PESS)	-0.1345	-0.0663
U(1) QSL (Iqbal et al.)	-0.1190	-0.079
$\mathbb{Z}_2$ QSL (Iqbal et al.)	-0.1245	0
VBC (Iqbal et al.)	-0.1255	-0.055
$\mathbb{Z}_2$ QSL*	-0.1323	-0.0628
Effective Model	-0.1353	0

Y. Iqbal et al, PRB (2018)

M. Iqbal et al, arXiv:1912.08284 (2019)

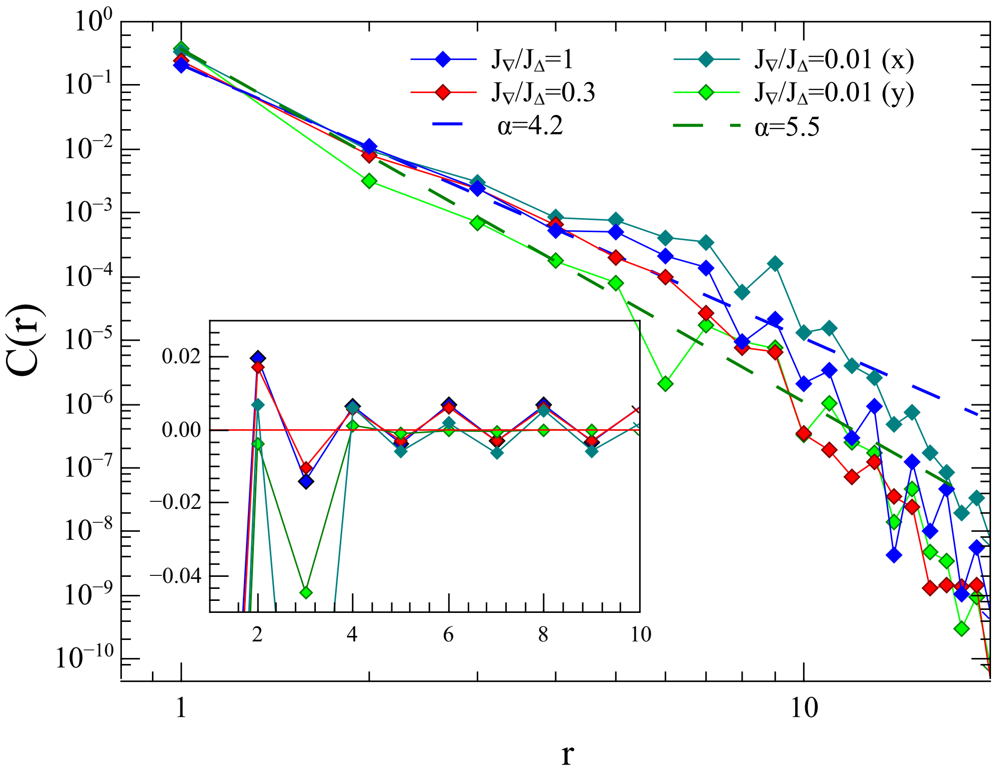
Repellin et al, PRB (2017)

F Mila, PRL (1998)



Quantum Phase Transition

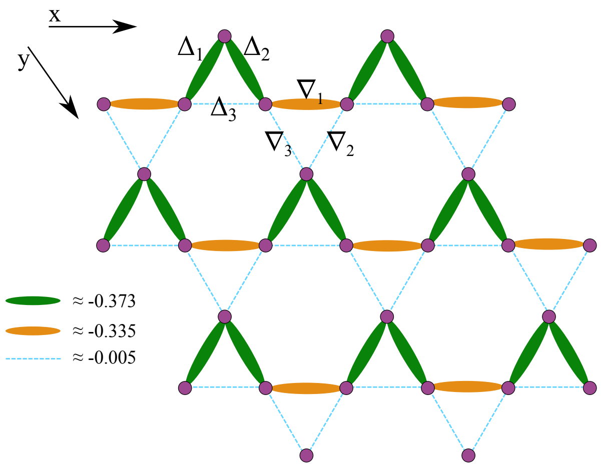
The Lattice Nematic Phase is also a Critical Gapless phase

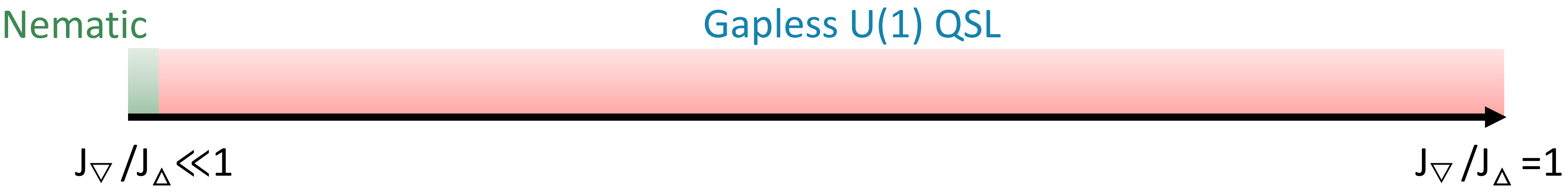


$$C(r) = \langle \mathbf{S}_{(x,y)} . \mathbf{S}_{(x+r,y)} \rangle - \langle \mathbf{S}_{(x,y)} \rangle . \langle \mathbf{S}_{(x+r,y)} \rangle$$

Log-log plot of the long range spin-spin correlations show an approximate power-law decay given by:

$$C(r) \sim C_0 r^{-\alpha}$$





Conclusion and Outlook

- Breathing anisotropy arises naturally in materials with impurity or under perturbation
- The spin-½ Breathing Kagome antiferromagnetic model is a suitable play ground to understand the effects of breathing anisotropy
- Tensor Network methods are powerful techniques for studying frustrated systems
- Gapless U(1) Spin Liquid of the BKH model persists to very large breathing anisotropies
- Lattice Nematic phase at very large breathing limit
- First-order QPT between the U(1) QSL and the Nematic phase at $J_{\triangledown}/J_{\vartriangle} \approx 0.05$
- The Nematic phase is a critical gapless phase
- Our results is also in agreement with current experiment on Vanadium Oxyfluoride compound