Spontaneous chiral spin liquid on triangular lattice: a view by PEPS

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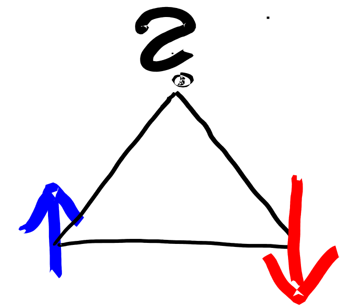
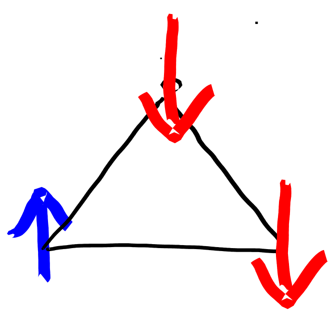
Triangular anti-ferromagnets

Ising anti-ferromagnet $J > 0$

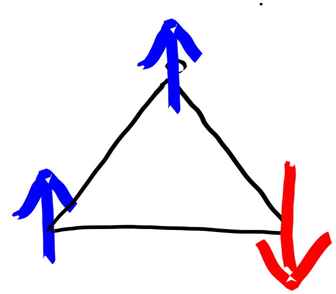
$$H = J\sum_{\langle i,j \rangle}(S_i^z S_j^z)$$



- Classical example of **geometrical** frustration
- **Macroscopic degeneracy**: All tilings from



or



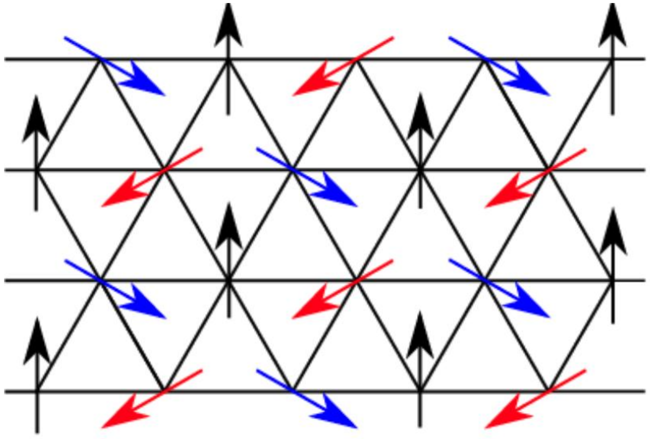
(and rotations)

Triangular anti-ferromagnets

Heisenberg spin-1/2 anti-ferromagnet $J > 0$

$$H = J \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)$$

- Classically / Mean-field gives 120^{o} **order**



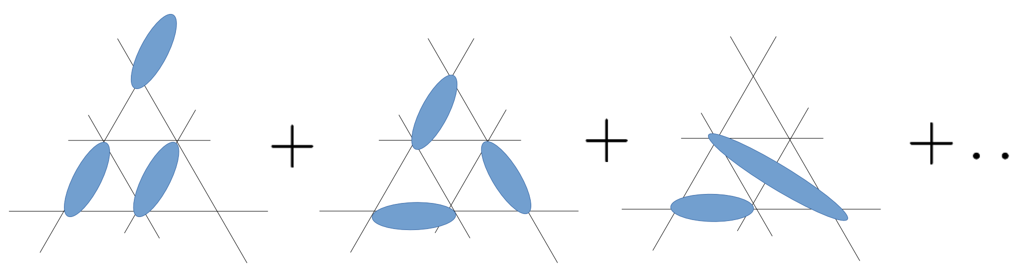
Triangular anti-ferromagnets

Heisenberg spin-1/2 anti-ferromagnet $J > 0$

$$H = J\sum_{\langle i,j\rangle}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)$$

- **Anderson**: Resonating Valence Bond (RVB) state

$$|\mathrm{RVB}\rangle = \sum_c \phi_c |c\rangle =$$



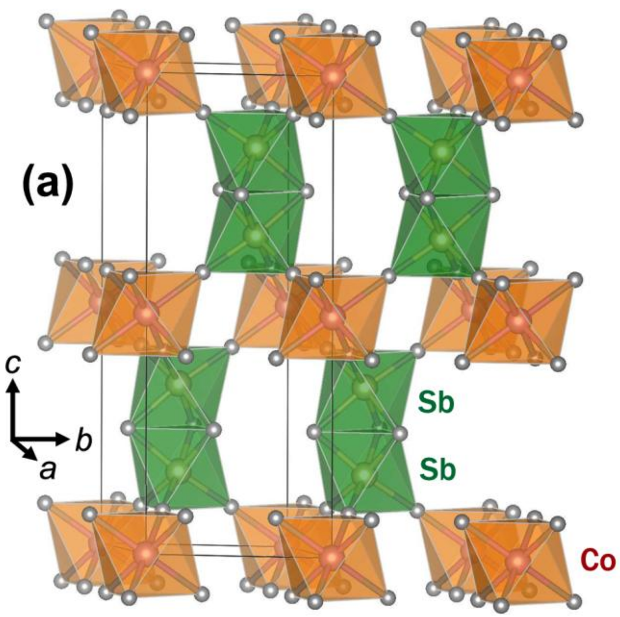
 $= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

- **(Spin) Liquid: All symmetries are preserved**

Triangular anti-ferromagnets: Gifts from Nature

Cobaltites: Co^{2+} in octahedral cage of Oxygens
"effective" spin-1/2

$Ba_3CoSb_2O_9$



- **ideal TL** and mostly J_1 (XXZ)
- no Dzyaloshinskii–Moriya (DM)
- no Jahn-Teller
- easy plane (XY) or easy-axis (Ising)

Chernyshev, Pollica 2024;
Li, Gegenwart, and Tsirlin, J. Phys.: Condens. Matter 32, 224004 (2020)

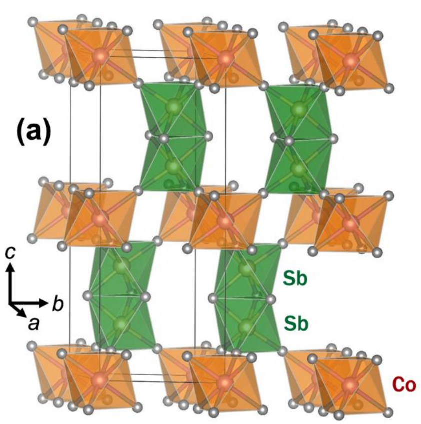
Triangular anti-ferromagnets: Gifts from Nature

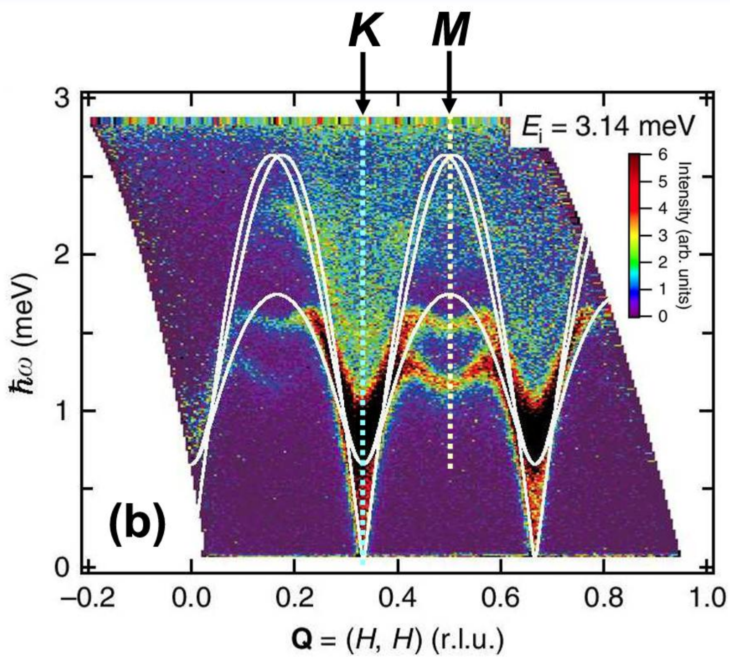
Cobaltites: Co^{2+} in octahedral cage of Oxygens
"effective" spin-1/2

$$H = J_1 \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) + \cdots$$

- **ideal TL** and mostly J_1 (XXZ)
- **120^o order**

$Ba_3CoSb_2O_9$





Chernyshev, Pollica 2024;
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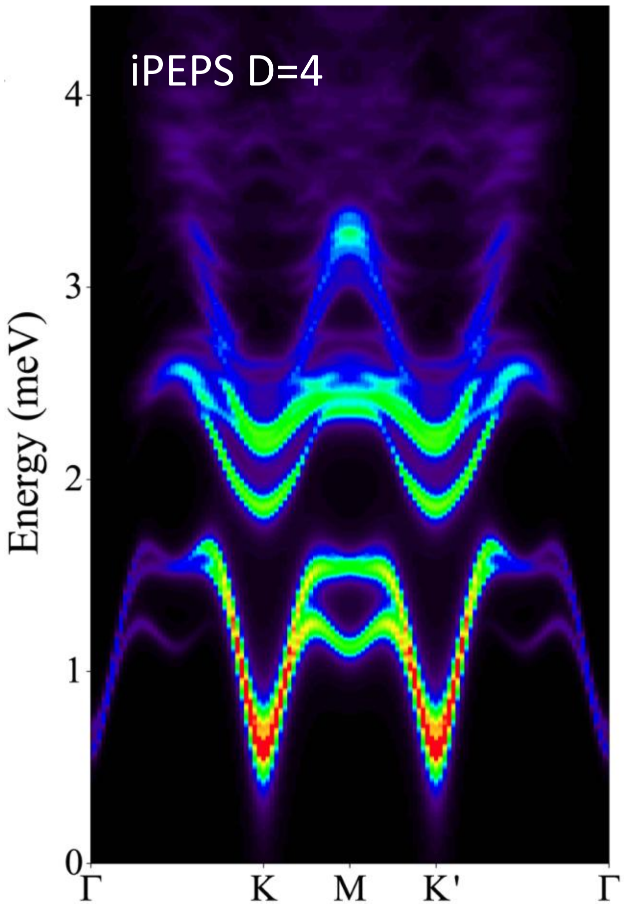
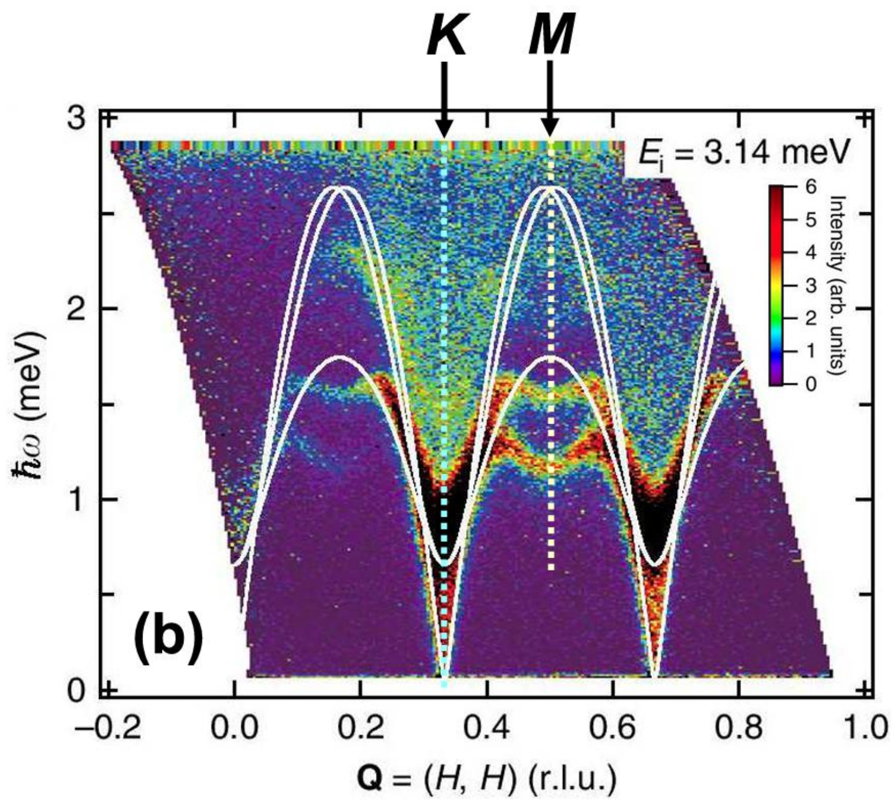
Triangular anti-ferromagnets: Gifts from Nature



$$H = J_1 \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) + \cdots$$

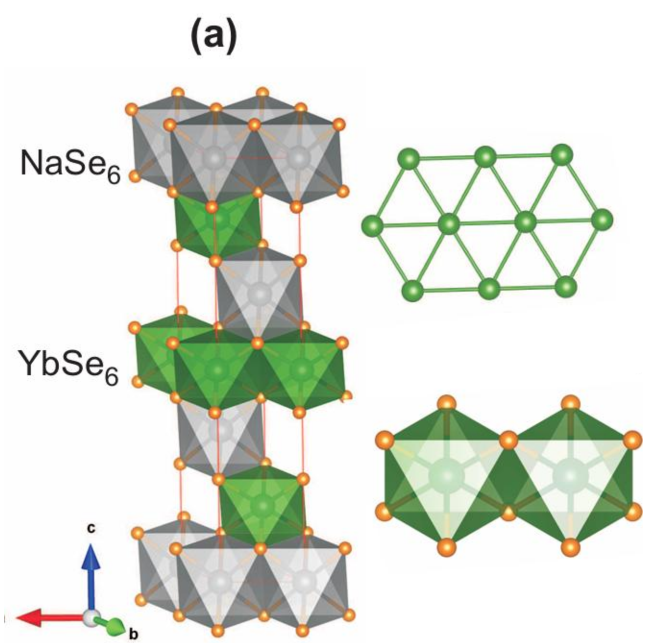


Chernyshev, Pollica 2024; Chi, Liu, Wan, Liao, and Xiang, PRL (2022)

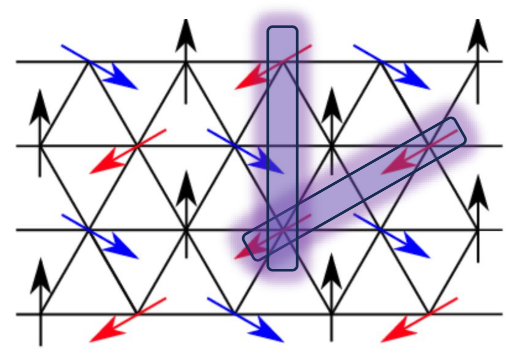
Triangular anti-ferromagnets: Gifts from Nature

Rare-earth: i.e. Yb^{3+} in octahedral cage of Oxygens or Selenia give **“effective” spin-1/2**

$NaYbSe_2$



- $J = 7/2$ + crystal-field splitting $\Rightarrow$ effective pseudo-spin $S = 1/2$
- **ideal TL** and also J_2 - **Frustration!**

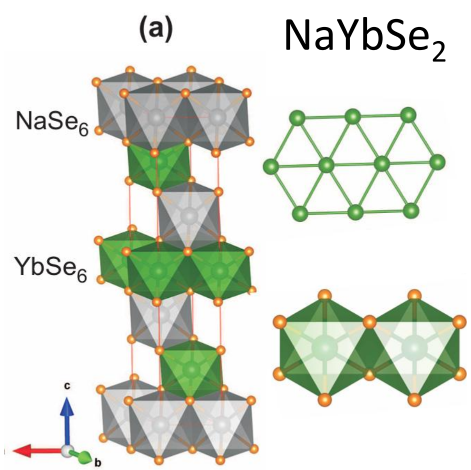


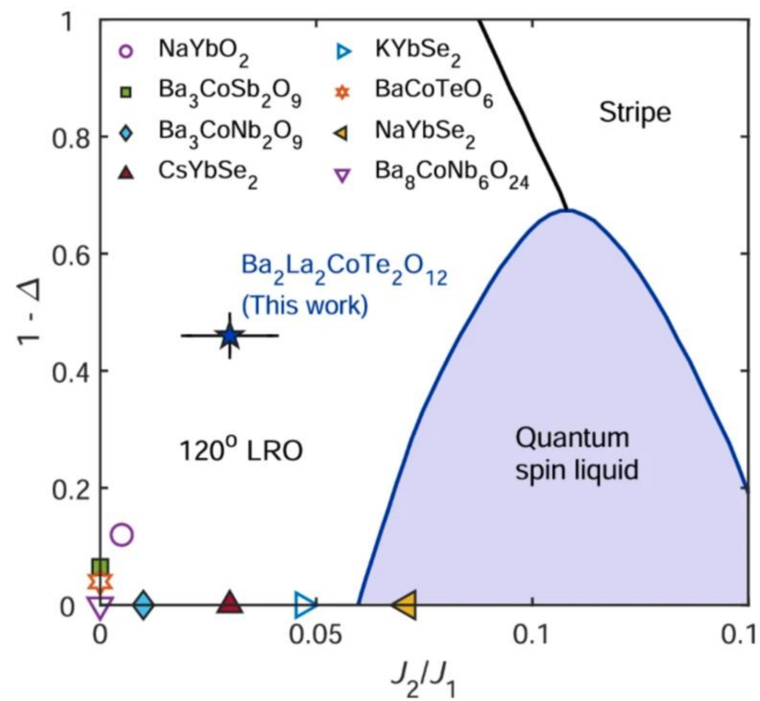
Ranjith et al. PRB 100, 224417 2019; Chernyshev, Pollica 2024;

Triangular anti-ferromagnets: Gifts from Nature

Rare-earth: i.e. Yb^{3+} in octahedral cage of Oxygens or Selenia give **"effective" spin-1/2**

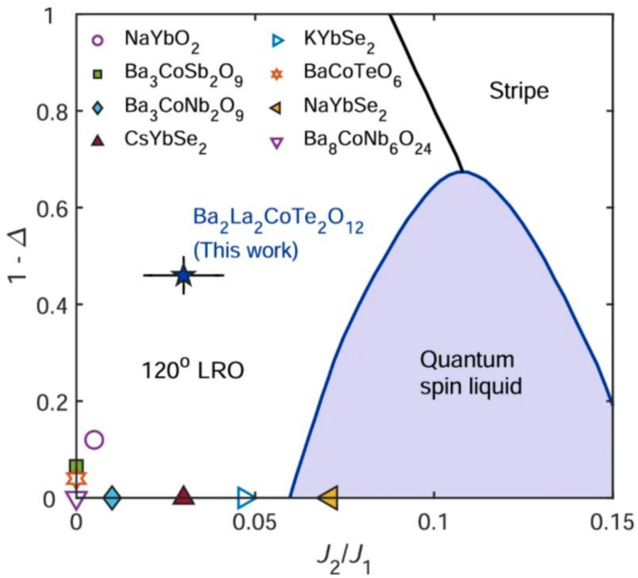
$$H = J_1 \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \cdots$$





Park et al., Nat. Comm. 15, 7264 (2024); Ranjith et al. PRB 100, 224417 2019; Chernyshev, Pollica 2024;

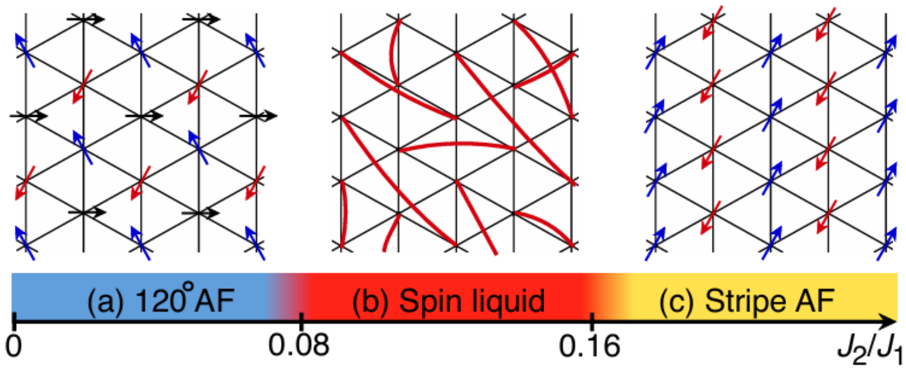
Triangular anti-ferromagnets: Gifts from Nature



$$H = J_1 \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \cdots$$

What is the **phase diagram** ?

- What is the **nature** of paramagnetic phase (QSL)?
- **Dynamics** ?

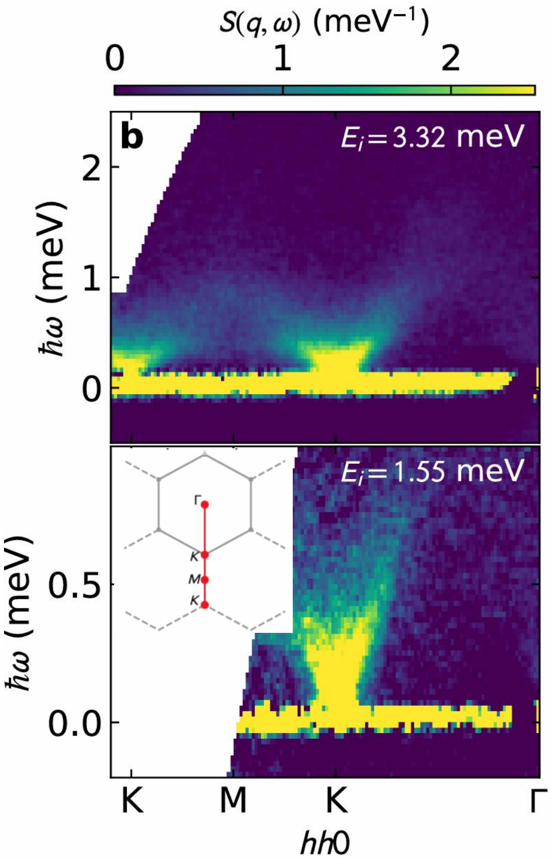


Anderson's RVB ?

Iqbal et al., PRB 93, 144411 (2016)

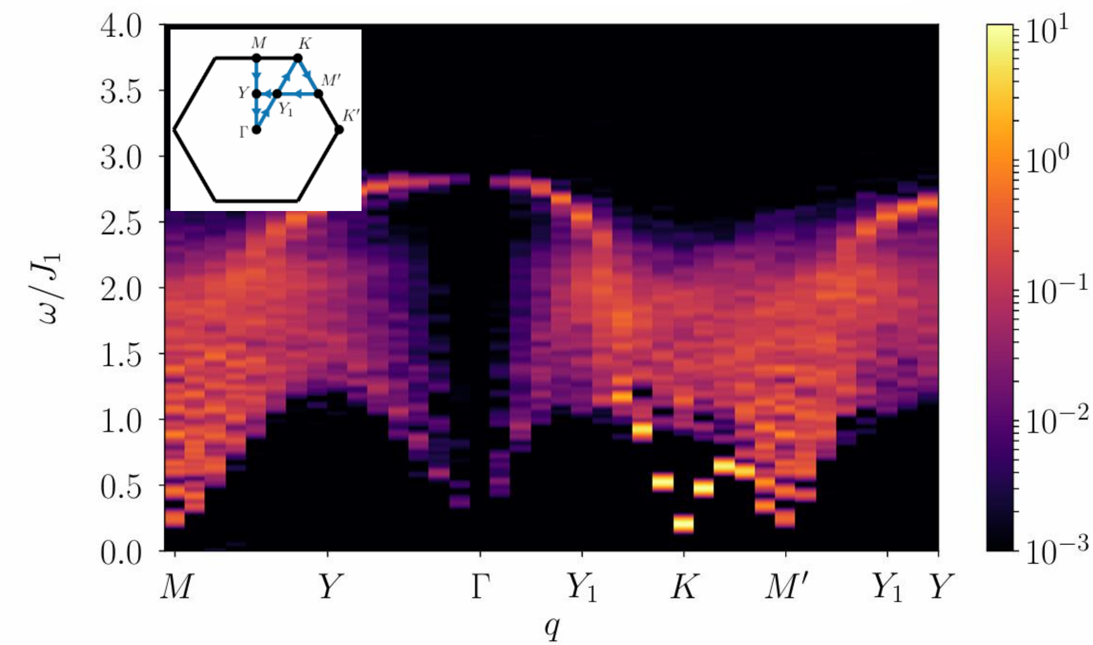
Triangular anti-ferromagnets: Gifts from Nature

$\mathrm{NaYbSe_2}$ $\mathbf{J_2/J_1 \approx 0.07}$



$$H = J_1 \sum_{\langle i,j \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_2 \sum_{\langle\langle i,j \rangle\rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + \cdots$$

$\boldsymbol{J_2/J_1 = 0.09}$ VMC of π-flux GPFW



Scheie et al. arXiv:2406.17773v1; Ferrari, Becca, PRX 9, 031026 (2019)

Abandoning $U \to \infty$ limit:

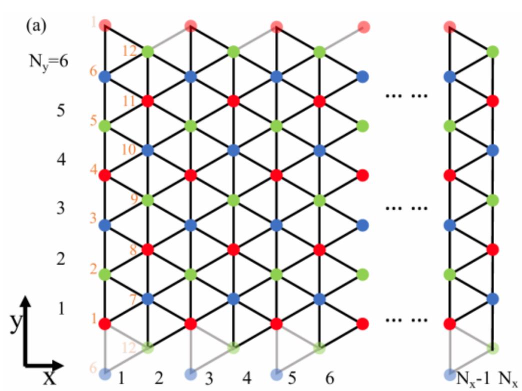
Spontaneous T-symmetry breaking

PHYSICAL REVIEW X **10**, 021042 (2020)

Chiral Spin Liquid Phase of the Triangular Lattice Hubbard Model: A Density Matrix Renormalization Group Study

Aaron Szasz,[1,2,3,*] Johannes Motruk,[1,2] Michael P. Zaletel,[1,2,4] and Joel E. Moore[1,2]

$$H = -t\sum_{\langle i,j\rangle\sigma}(\boldsymbol{c}_{i\sigma}^{\dagger}\boldsymbol{c}_{j\sigma} + \boldsymbol{c}_{j\sigma}^{\dagger}\boldsymbol{c}_{i\sigma}) + U\sum_i(\boldsymbol{n}_{i\uparrow}\boldsymbol{n}_{j\downarrow})$$



- DMRG simulations up to YC6 (width 6) cylinders
- **Spontaneous emergence of CSL**
  - **CSL: gapped with broken P, T but conserved PT**

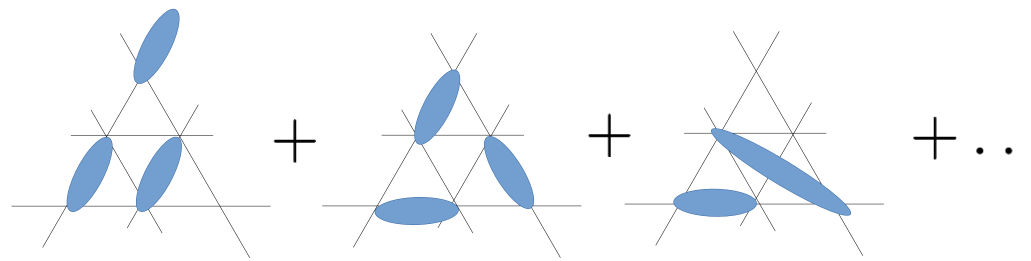
See also Chen et al. PRB 106, 094420, 2022

Abandoning $U \to \infty$ limit:

Spontaneous T-symmetry breaking

- Realization of Anderson's RVB / Kalmeyer-Laughlin $\nu = 1/2$ CSL

$$|\mathrm{RVB}\rangle = \sum_c \phi_c |c\rangle =$$



 $= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

$$\Updownarrow$$

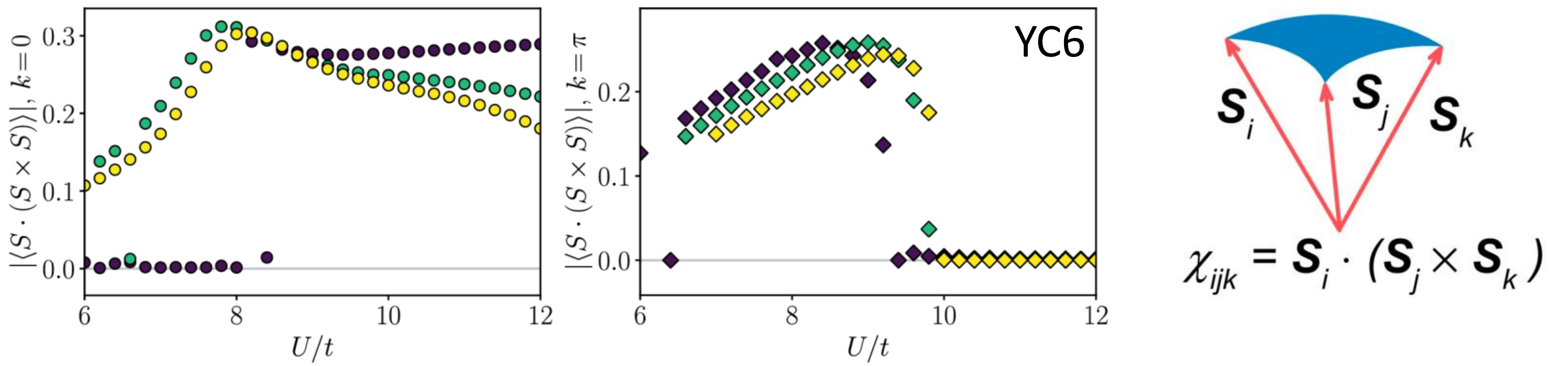
$$\psi_{KL}(z_1, ..., z_N) = \prod_{j<k} (z_j - z_k)^2 exp(-\frac{1}{4l_0^2} \sum_i^N |z_i|)$$

Kalmeyer, Laughlin, PRL (1987)
Zou, Doucot, Shastry, PRL (1989)

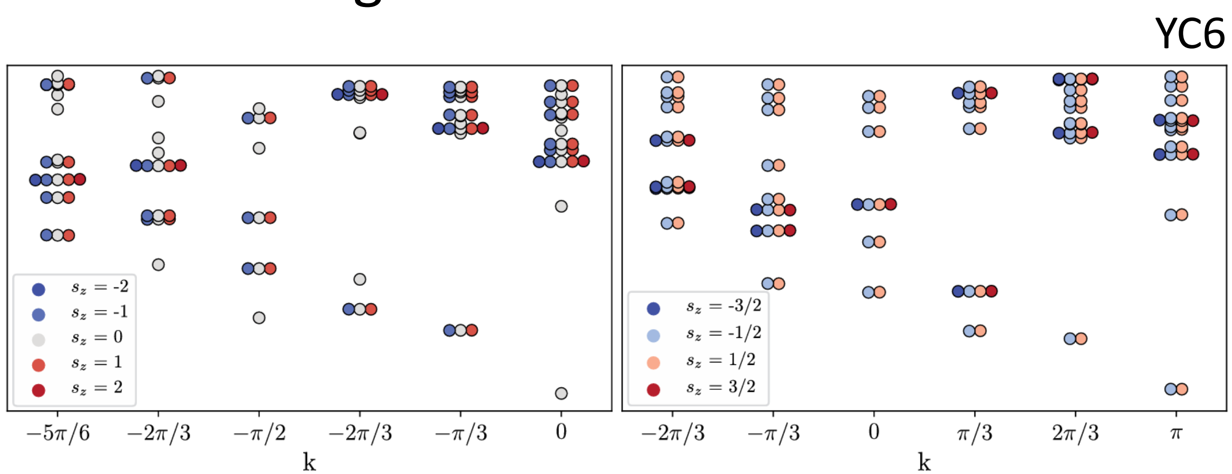
Abandoning $U \to \infty$ limit:

Spontaneous T-symmetry breaking

- Scalar spin chirality



- $SU(2)_1$ WZW counting

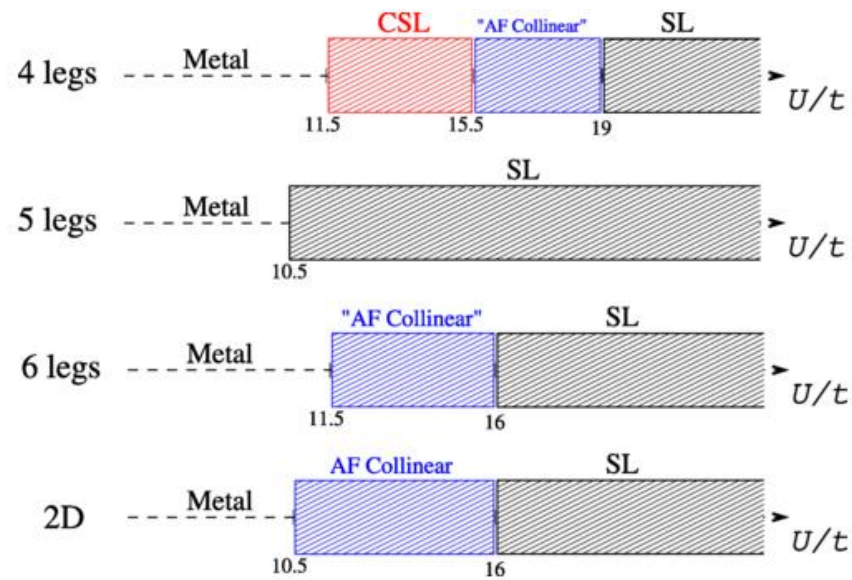


Abandoning $U \to \infty$ limit:

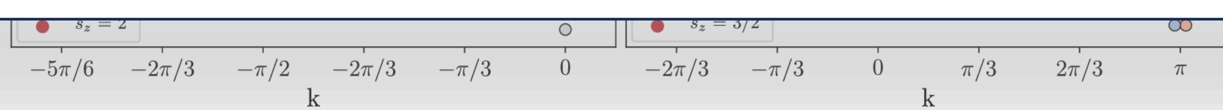
Spontaneous T-symmetry breaking

- Scalar spin chirality
- SU

- Further investigation into 2D-limit is desirable



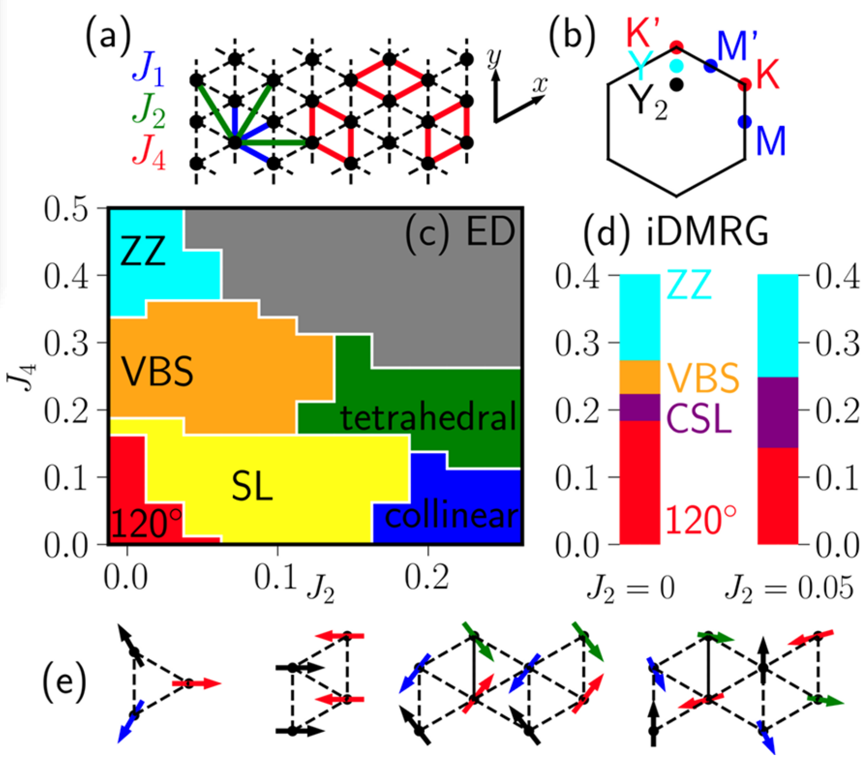
VMC by L. Tocchio, A. Montorsi, F. Becca, PRR (2021)



Abandoning $U \to \infty$ limit:
Spontaneous T-symmetry breaking

- Larger cylinders: **Effective spin-1/2 model** by Cookmeyer, Motruk, Moore, PRL 127, 087201 (2021)

$$
\begin{aligned}
H &= J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + H_4 \\
H_4 &= J_4 \sum_{\langle ijkl \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) \\
&\quad -(\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)
\end{aligned}
$$

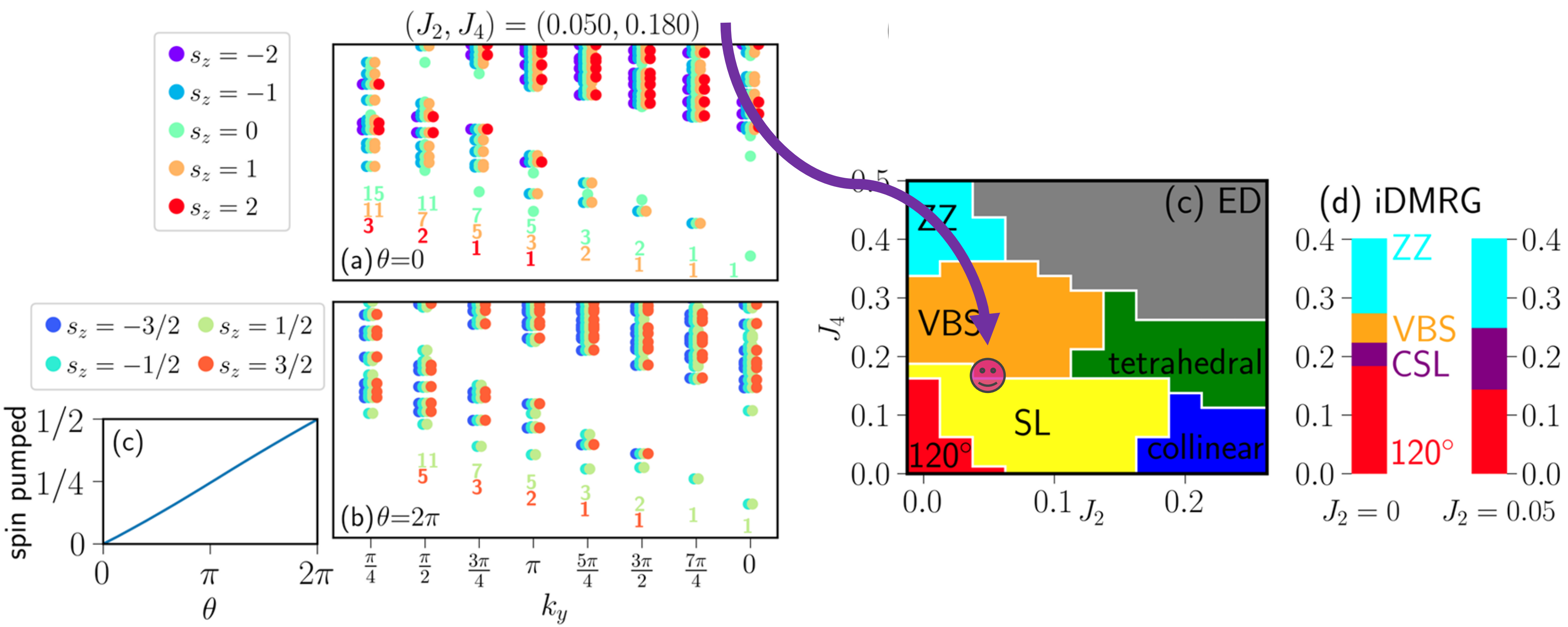


- H_4 appears at t^4/U^3 order in expansion of Hubbard model
- Mean-field decoupling on chiral background $H_4 \propto S.(S \times S)$

Abandoning $U \to \infty$ limit:
Spontaneous T-symmetry breaking

- Larger cylinders: **Effective spin-1/2 model** by Cookmeyer, Motruk, Moore, PRL 127, 087201 (2021)

SU(2)$_1$ WZW counting on iDMRG on **YC8** Cylinders

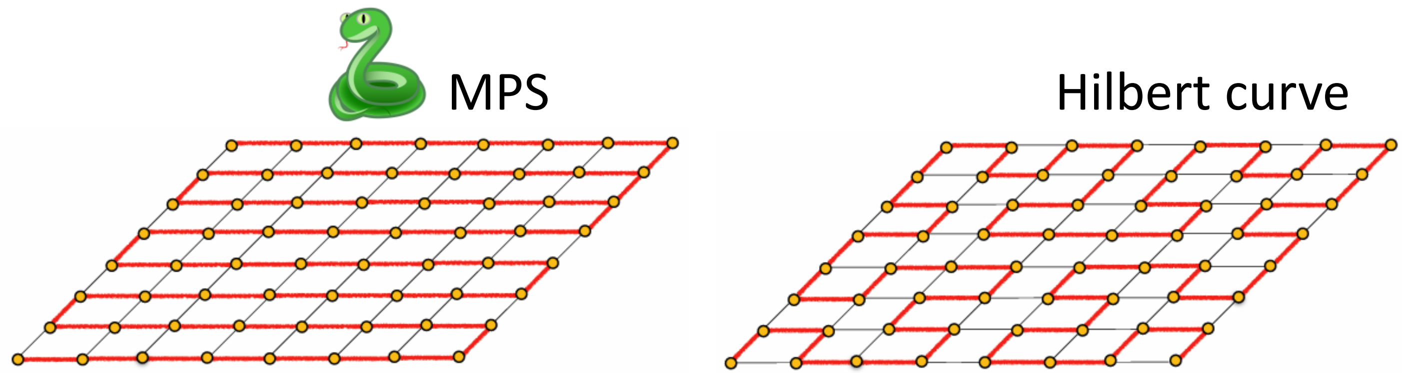


Triangular anti-ferromagnets

- Dynamics in ordered phases
  - In presence of additional interactions beyond pure isotropic Heisenberg exchange
- Phase diagrams in presence of frustration
  - Nature of paramagnetic states
- Spontaneous time-reversal symmetry breaking and Chiral spin liquids
- … much more

In two dimensions – Matrix product states

Let's keep doing what worked in 1D …



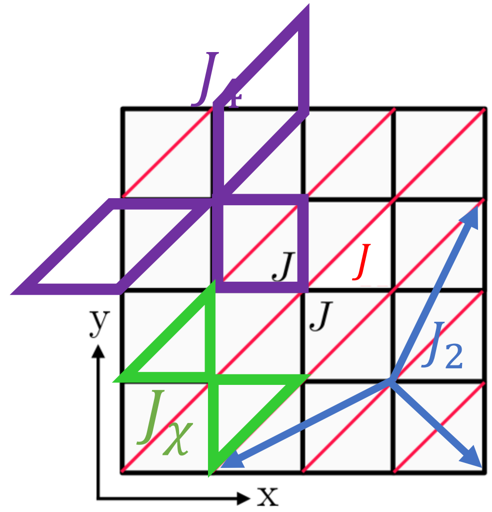
… except, the cost is exponential even for a gapped system !

picture from Cataldi et al., Quantum 5, 556 (2021)

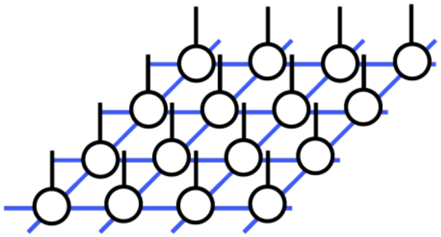
iPEPS

- **Extended spin-1/2 model on a triangular lattice**
  - Also consider scalar spin chirality

$$
\begin{aligned}
H &= J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\
&+ J_\chi \sum_{i,j,k \in \triangle} \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k) + H_4 \\
H_4 &= \sum_{\langle ijkl \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_k \cdot \mathbf{S}_l) + (\mathbf{S}_i \cdot \mathbf{S}_l)(\mathbf{S}_j \cdot \mathbf{S}_k) \\
&- (\mathbf{S}_i \cdot \mathbf{S}_k)(\mathbf{S}_j \cdot \mathbf{S}_l)
\end{aligned}
$$



- Gradient optimization of iPEPS up D=6

$$|\psi\rangle = \sum_{s_1 s_2 \dots s_N} (\quad$$  $$\quad) |s_1 s_2 \dots s_N\rangle$$

iPEPS:

Different orders, different ansätze

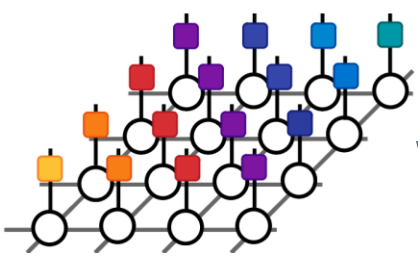
2x2 (and shift)

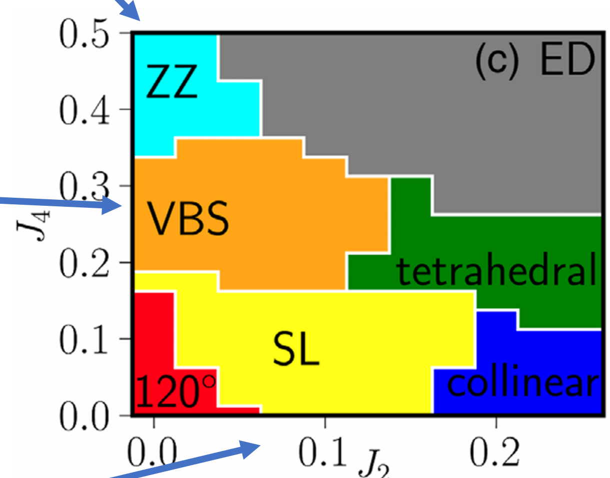
A	B	C	D
C	D	A	B
A	B	C	D
C	D	A	B

1x2

A	B	A	B
A	B	A	B

Spiral iPEPS





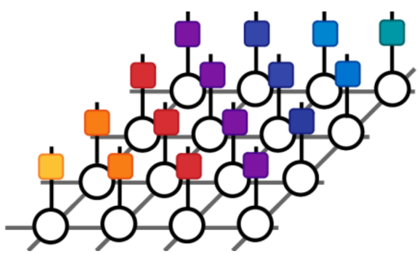
2x2

A	B	A	B
C	D	C	D
A	B	A	B
C	D	C	D

iPEPS:

Warm-up at $J_1 = 1$ only point

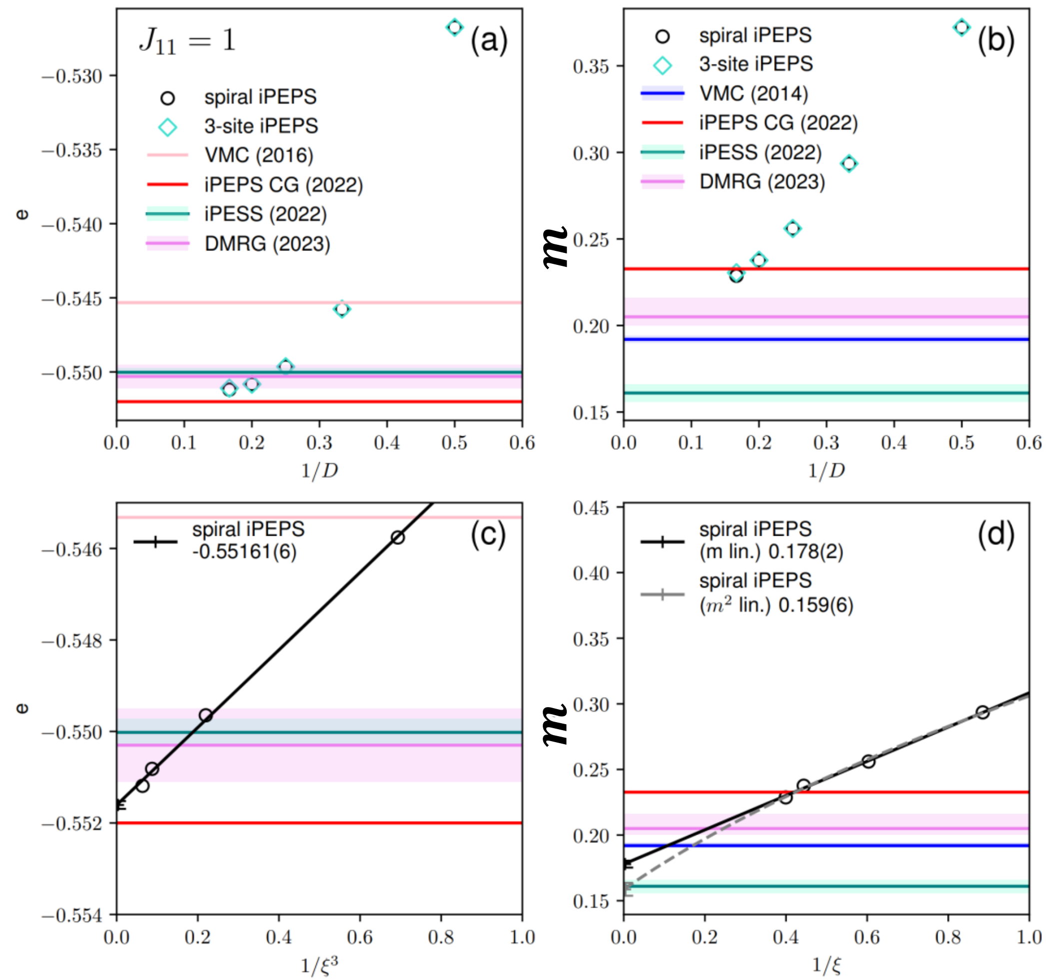
- Cross-check 3-site and spiral ansatz with $\boldsymbol{q} = (2\pi/3, 2\pi/3)$



$$|\psi(a, \boldsymbol{q})\rangle \; = \; U(\boldsymbol{q})|iPEPS(a)\rangle$$

$$U(\boldsymbol{q}) = \prod_{\boldsymbol{r}} u_{\boldsymbol{r}}(\boldsymbol{q}, \boldsymbol{r})$$

with $u_{\boldsymbol{r}}(\boldsymbol{q}, \boldsymbol{r}') = \exp[i\pi(\boldsymbol{q}.\boldsymbol{r}')S_{\boldsymbol{r}}^{y}]$

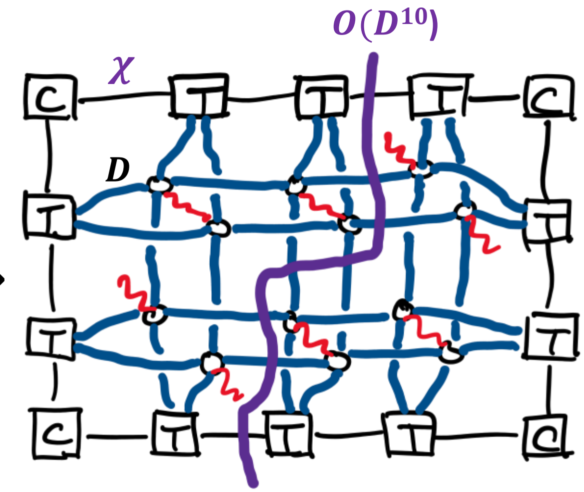


iPEPS:

Treating longer-range interactions

```
# C1------(1)1 1(0)----T1----(3)44 44(0)----T1_x----(3)39 39(0)---T1_2x---(3)24 24(0)--C2_2x
# 0(0)             (1,2)                 (1,2)                  (1,2)                 25(1)
# 0(0)         100  2  5             102 40 42              104 26 28                 25(0)
# |                \ 2  5                \ |  |                 \ |  |                  |
# T4-------(2)3 3-----a--|------45 45----a_x--6(1)----41  41-------a_2x-------27 27(1)--T2_2x
# |                   |  |                 |  |                   |  |                  |
# |        (3)6 6-------a*------46 46--------a*_x-----43  43----------a*_2x---29 29(2)  |
# 15(1)               16 17 \101            47 48 \103              37 38 \105           36(3)
# 15(0)         106  16 17              108 47 48                  37 38                36(0)
# |                \ |   |                 \ |  |              110\ |  |                  |
# T4_y--(2)9 9--------a_y-------20 20-----a_xy--------49 49(1)----a_2xy-------33 33(1)--T2_2xy
# |                   |   |                |  |                   |  |                  |
# |     (3)12 12---------a*_y---22 22------- a*_xy----50 50(2)--------a*_2xy--35 35(2)  |
# |                   10 13 \107            21 23 \109             32 34 \111           |
# 8(1)                10 13                 21 23                  32 34                 31(3)
# 8(0)                (0,1)                 (0,1)                  (0,1)                 31(0)
# C4_y---(1)7 7(2)-----T3_y--(3)19 19(2)----T3_xy---(3)51 51(2)---T3_2xy--(3)30 30(1)---C3_2xy
```

⟺

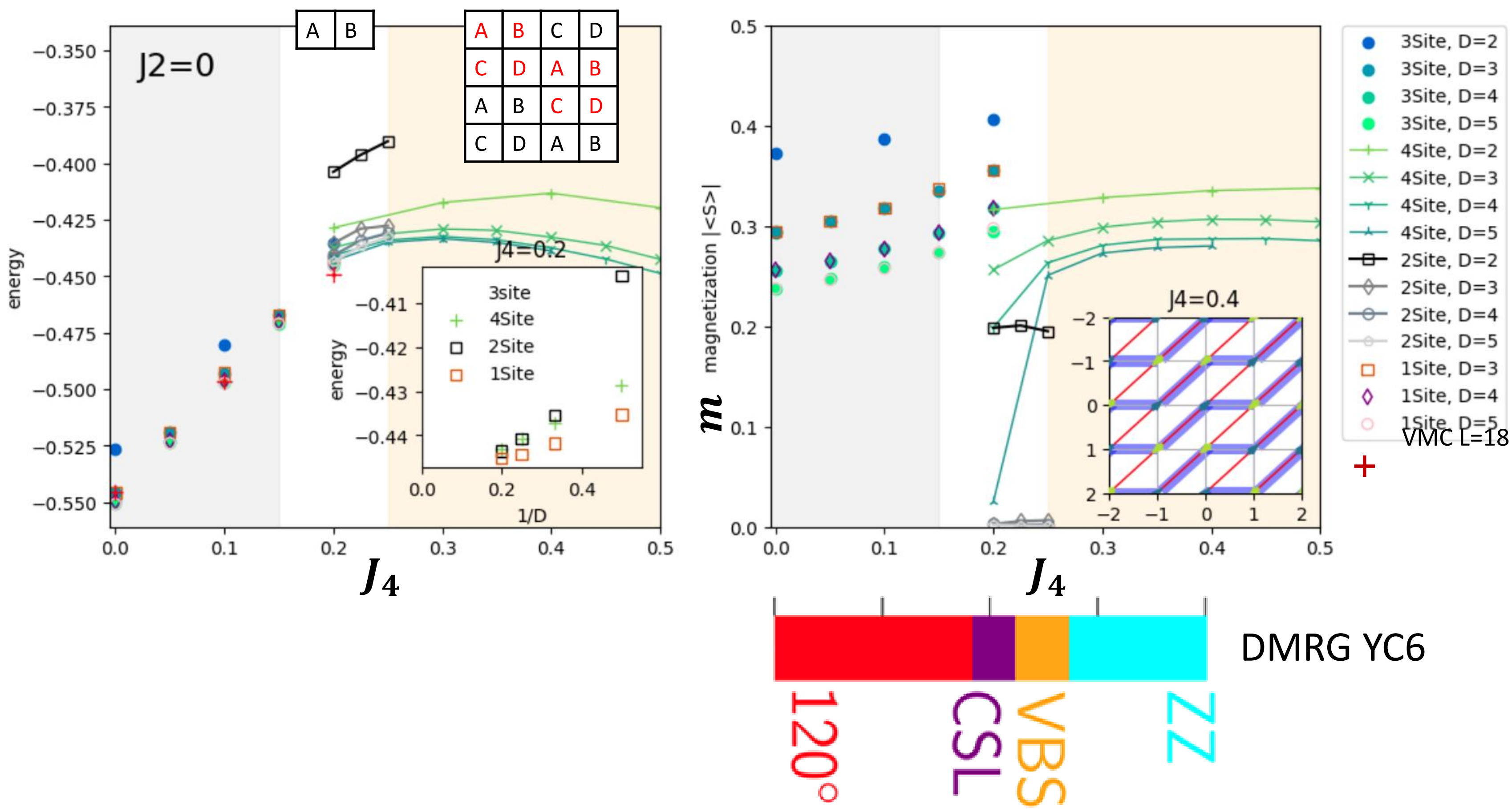



```
contract_tn= C1,[0,1],T1,[1,2,5,44],T4,[0,15,3,6],a,[I[0],2,3,16,45],a.conj(),[I[1],5,6,17,46],\
    T4_y,[15,8,9,12],C4_y,[8,7],T3_y,[10,13,7,19],a_y,[I[6],16,9,10,20],a_y.conj(),[I[7],17,12,13,22],\
    T3_xy,[21,23,19,51],a_xy,[I[8],47,20,21,49],a_xy.conj(),[I[9],48,22,23,50],\
    T1_2x,[39,26,28,24],C2_2x,[24,25],T2_2x,[25,27,29,36],a_2x,[I[4],26,41,37,27],a_2x.conj(),[I[5],28,43,38,29],\
    T2_2xy,[36,33,35,31],C3_2xy,[31,30],T3_2xy,[32,34,51,30],a_2xy,[I[10],37,49,32,33],a_2xy.conj(),[I[11],38,50,34,35],\
    T1_x,[44,40,42,39],a_x,[I[2],40,45,47,41],a_x.conj(),[I[3],42,46,48,43],I_out
path, path_info= get_contraction_path(*contract_tn,unroll=unroll if unroll else [],\
    names=names,path=None,memory_limit=mem_limit if unroll else None,optimizer="default")
R= contract_with_unroll(*contract_tn,optimize=path,backend='torch',\
    unroll=unroll if unroll else [],checkpoint_unrolled=checkpoint_unrolled,
    checkpoint_on_device=checkpoint_on_device,who=who,verbosity=verbosity)
```

… runs on extension of **opt_einsum**
(**custom unrolling with checkpointing** for AD)

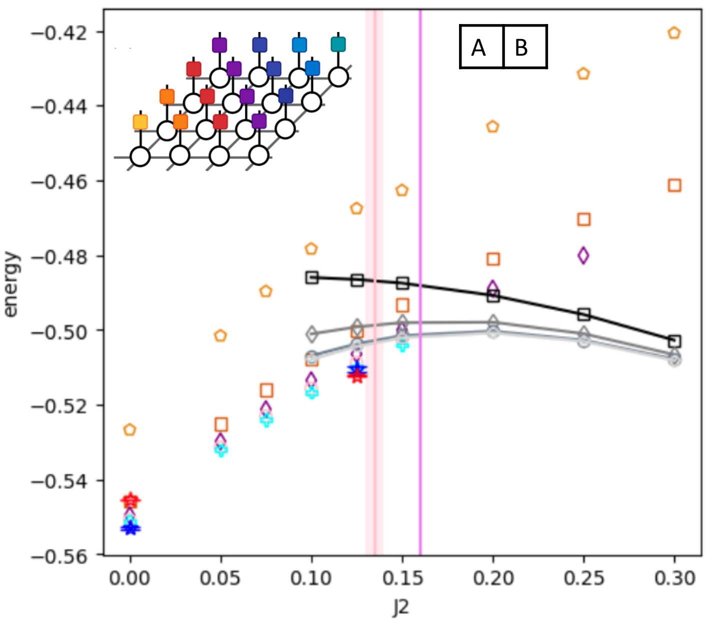
iPEPS $J_2 = 0$

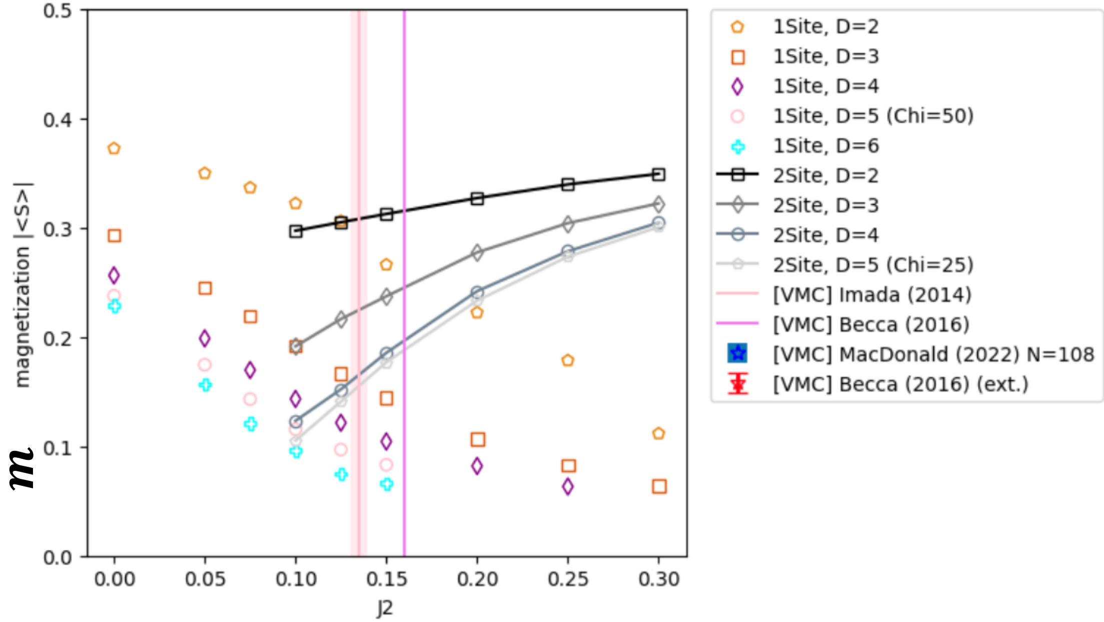
- Possible scenario:
  120⁰ order transitions into **VBS** via **1st order** transition

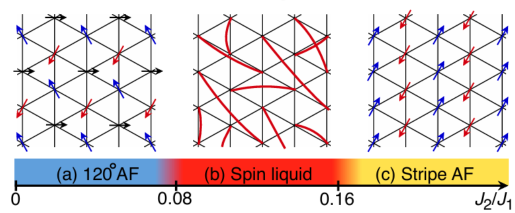


iPEPS $J_2 > 0$

- No clear paramagnet up to D=6. Order parameter scaling ?



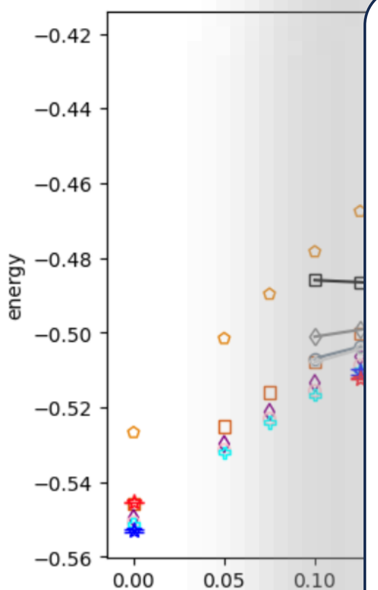




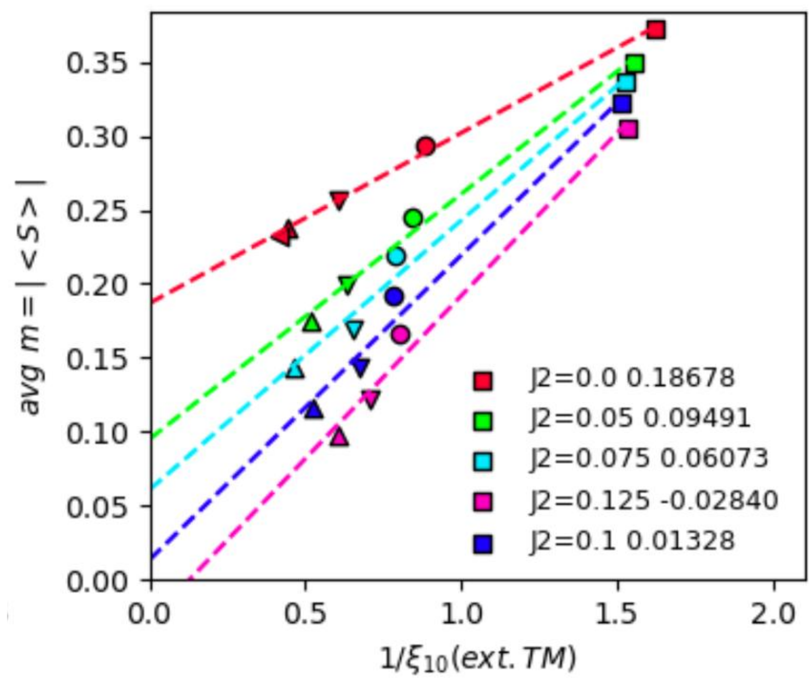
- Optimization is **problematic**. High environment bond dimensions χ are crucial

iPEPS $J_2 > 0$

- No clear paramagnet up to D=6. Order parameter scaling ?



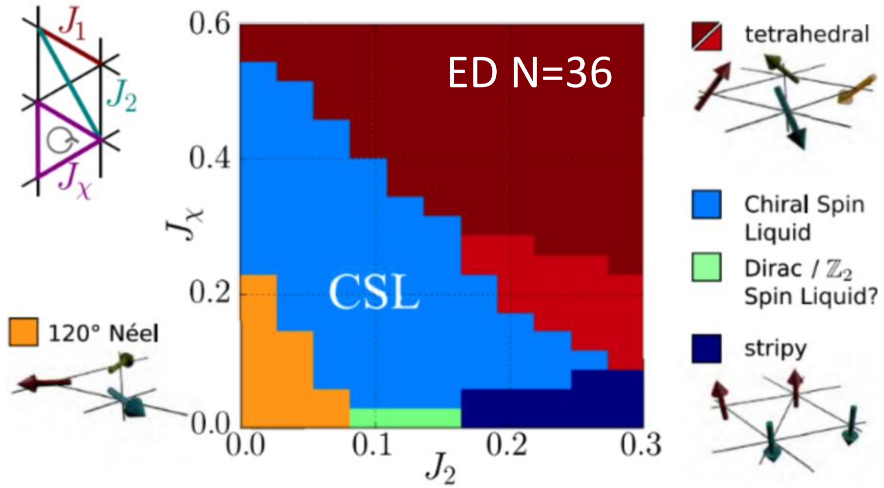
FCLS: Higher bond dimension data are needed



- Optimizat
High envir
dimension

iPEPS: Strategy for CSL

- What works ? Perturb the (gapless) spin liquid by explicitly breaking time-reversal symmetry
  - **D=3 -** Square lattice $J_1 - J_2 - \lambda$
  - **D=8 -** Kagome $J_1 - J_\chi$
  - **D=??? –** Triangular lattice $J_1 - J_2 - J_\chi$

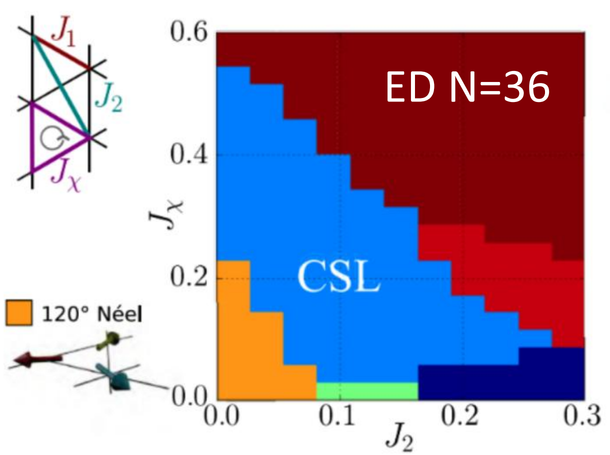


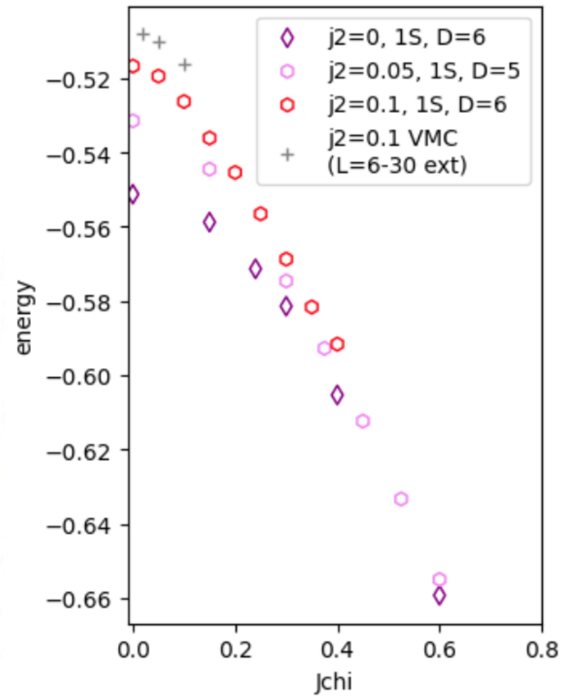
Wietek, Läuchli, PRB 95, 035141(2017)
Niu, Hasik, Chen, Poilblanc, PRB 106, 245119, (2022)
Hasik, Van Damme, Poilblanc, Vanderstraeten, PRL 129, 177201 (2022)

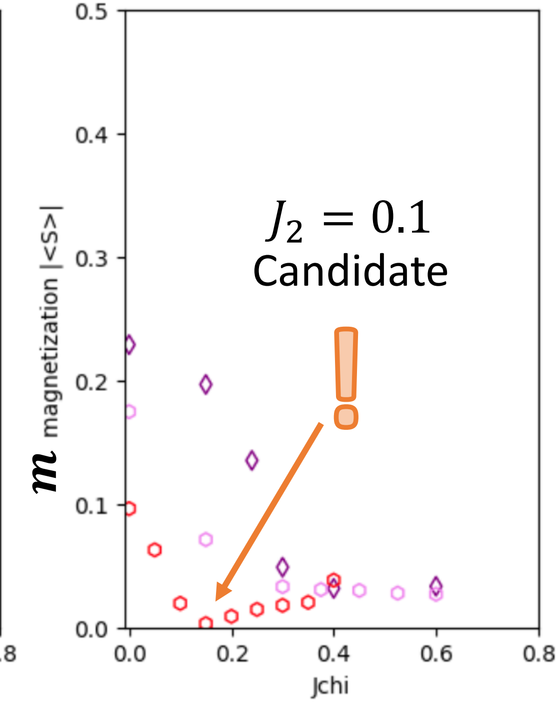
iPEPS: Strategy for CSL I

- What works ? Perturb the (gapless) spin liquid by explicitly breaking time-reversal symmetry

- **D=3 -** Square
- **D=8 -** Kagome
- **D=??? –** Triangular



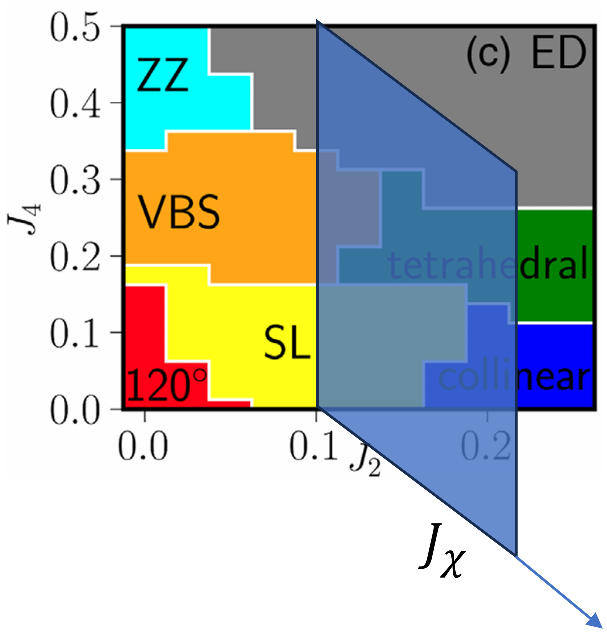




iPEPS: Strategy for CSL II

- Adiabatically continue towards $J_\chi = 0, J_4 > 0$ plane

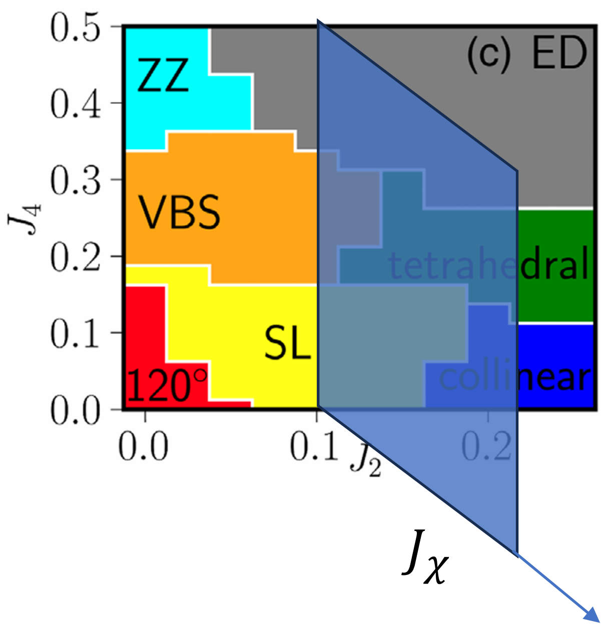
- **D=3 -** Square
- **D=8 -** Kagome
- **D=??? –** Triangular

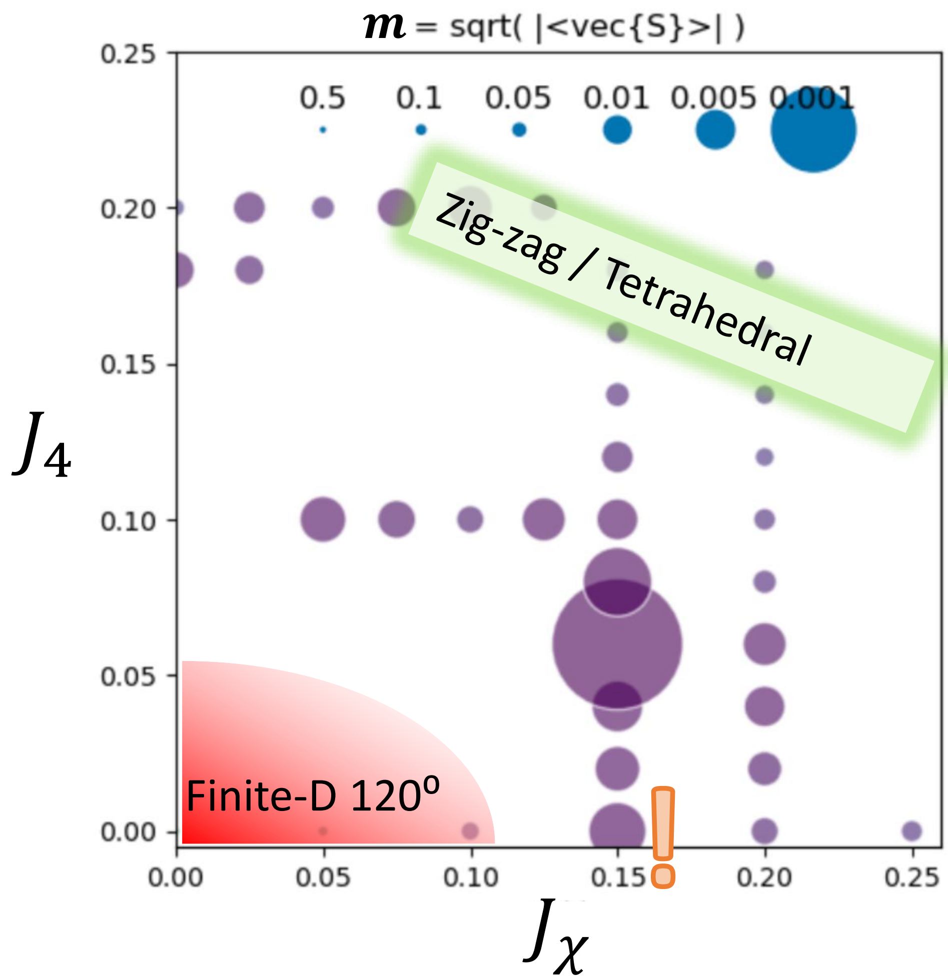


iPEPS: Strategy for CSL II

- Adiabatically continue towards $J_\chi = 0, J_4 > 0$ plane at $J_2 = 0.1$

- **D=3 -** Square
- **D=8 -** Kagome
- **D=??? –** Triangular





Summary I

- Ongoing effort to characterize triangular lattice antiferromagnets via **iPEPS**
  - Global picture looks good
  - Needs push to higher **D**
    & **symmetries** where applicable
  - Promising J_4 region for **CSL**
    in the thermodynamic limit (D=8?)

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Laurens Vanderstraeten (ULB)
Yi Xu (Rice)
Francesco Ferrari (Industry)

Summary II

Mature software

github.com/jurajHasik/peps-torch

github.com/yastn/yastn

- ➢ **AD + abelian symmetries + fermions**
- ➢ YASTN power PEPS simulations in D-wave's recent:

"Computational supremacy in quantum simulation"
by King et al (D-wave and collaborators)
arXiv:2403.00910



with Marek M. Rams, Gabriela Wójtowicz, and Aritra Sinha

JAGIELLONIAN UNIVERSITY IN KRAKÓW

And others

- 1D: ITensor, TenPy, MpsKit.jl, many more …
- 2D: PepsKit.jl, variPEPS, and not many more