Frustrated Magnetism on the Stuffed Honeycomb Lattice

Florida State University

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with Dmitrii Kochkov, Jyotisman Sahoo, and Rebecca Flint

[PRB 98, 134419 Sahoo, Kochkov, Clark, Flint]

[in preparation, Kochkov, Sahoo, Flint, Clark]

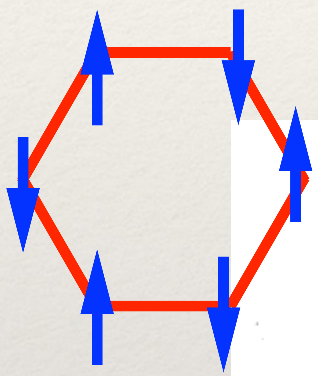
A History of (Frustrated) Magnetism

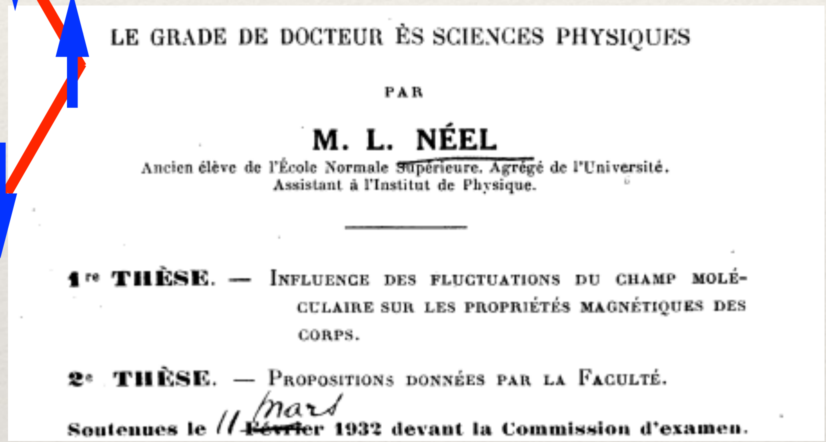
(abridged)

Ancient Greece - 6'th century BC first use of term `lodestone' in writings of Thales of Miletus

Louis Neel **1932 -** *ferromagnet* All spins aligned

anti-ferromagnet anti-aligned moments





LE GRADE DE DOCTEUR ÈS SCIENCES PHYSIQUES

PAR

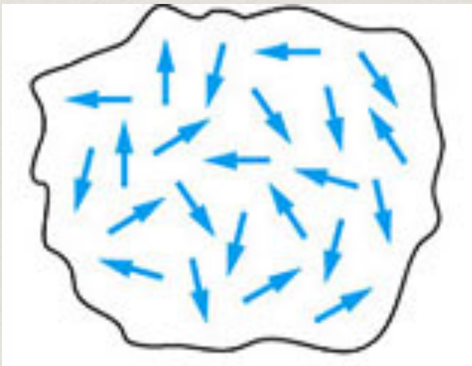
M. L. NÉEL

Ancien élève de l'École Normale Supérieure. Agrégé de l'Université. Assistant à l'Institut de Physique.

1re THÈSE. — INFLUENCE DES FLUCTUATIONS DU CHAMP MOLÉCULAIRE SUR LES PROPRIÉTÉS MAGNÉTIQUES DES CORPS.

2e THÈSE. — PROPOSITIONS DONNÉES PAR LA FACULTÉ.

Soutenues le 11 ~~Février~~ mars 1932 devant la Commission d'examen.



Onsager **1944 -** *solution to 2d Ising model* Rigorous proof that the paramagnet (spin gas) phase exists

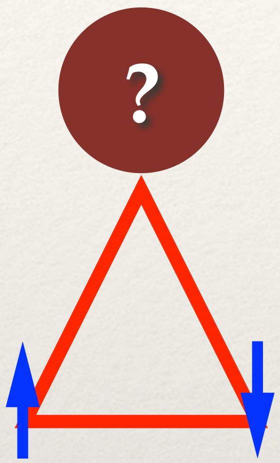
Louis Neel **1948 -** *ferri-magnet* spontaneous moments

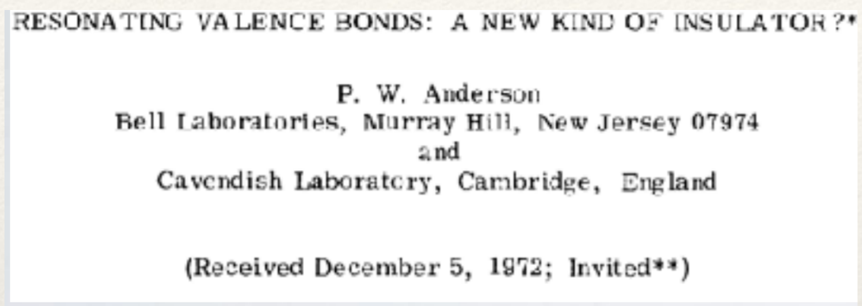
A History of (Frustrated) Magnetism

(abridged)

Phil Anderson - 1973 *spin-liquid*

triangular lattice can't be an anti-ferromagnet





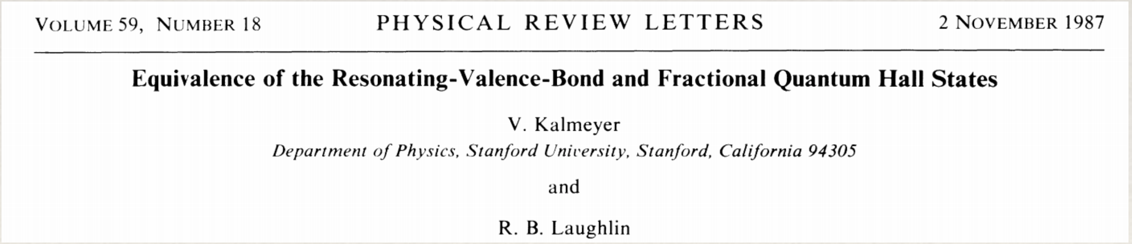
RESONATING VALENCE BONDS: A NEW KIND OF INSULATOR?*

P. W. Anderson
Bell Laboratories, Murray Hill, New Jersey 07974
and
Cavendish Laboratory, Cambridge, England

(Received December 5, 1972; Invited**)

so maybe it's a *spin-liquid*

Kalmeyer - Laughlin ~ 1987 Triangular lattices is a chiral spin liquid wave-function



VOLUME 59, NUMBER 18 PHYSICAL REVIEW LETTERS 2 NOVEMBER 1987

Equivalence of the Resonating-Valence-Bond and Fractional Quantum Hall States

V. Kalmeyer
Department of Physics, Stanford University, Stanford, California 94305
and
R. B. Laughlin

Numerics ~ 1988-1999 triangular lattice is 120 degree

History - Summarized

Lodestone (ferromagnet)

Anti-ferromagnet

Ferri-magnet

Paramagnet

Spin-liquid

Chiral Spin Liquid

What’s a spin-liquid?

an ancient view

Literally… a liquid of spins.

- no symmetry breaking
- no order

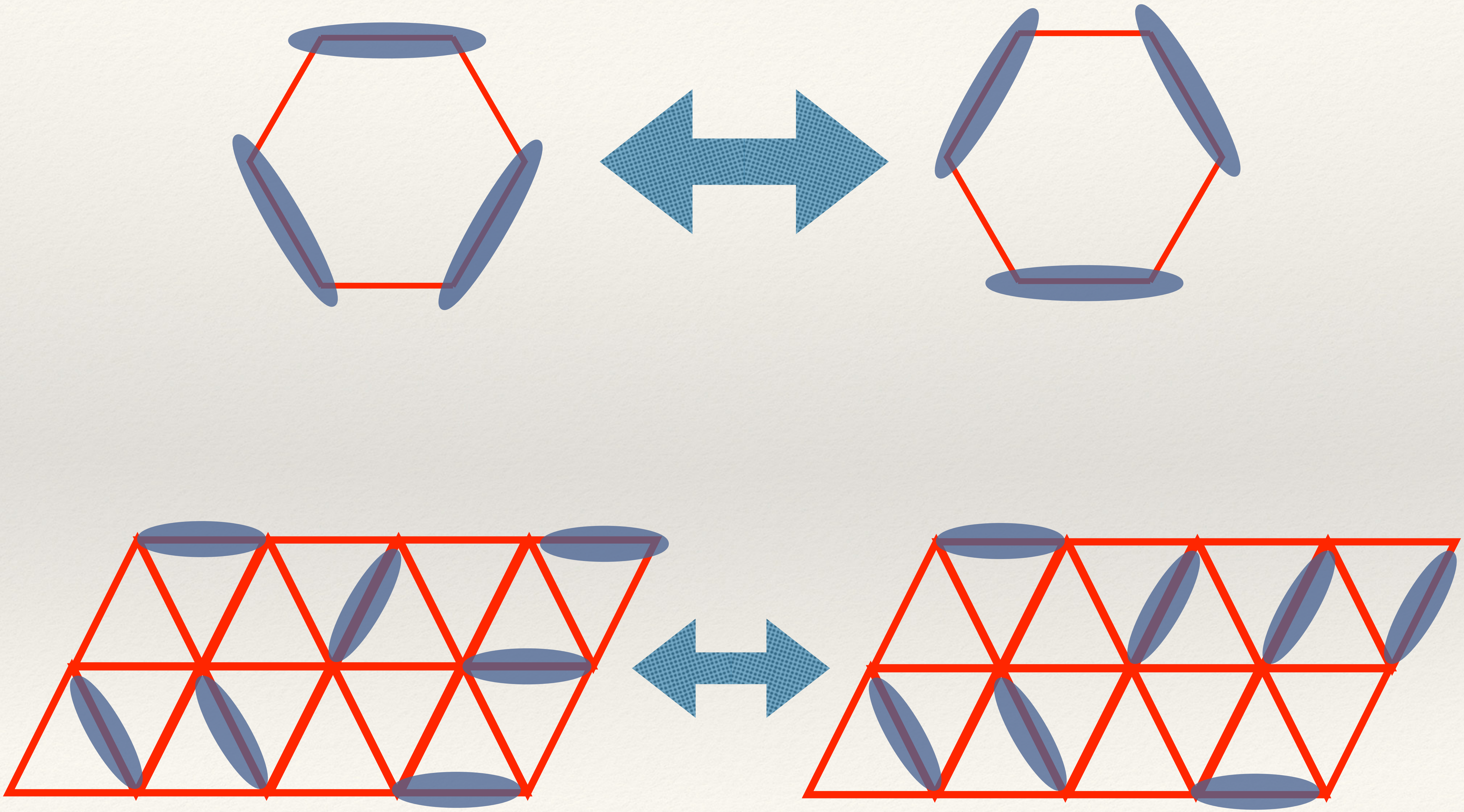
Exception: Chiral Spin-Liquid has chiral edge modes.

Q: Isn’t this just a quantum version of the paramagnet?

What's a spin-liquid?

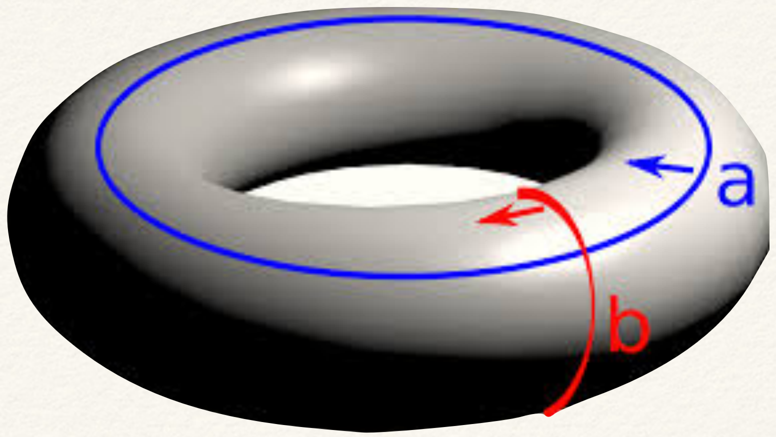
Resonating Valence Bonds (Anderson)

$= |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ **(EPR singlet)**



What’s a spin-liquid?

a modern view

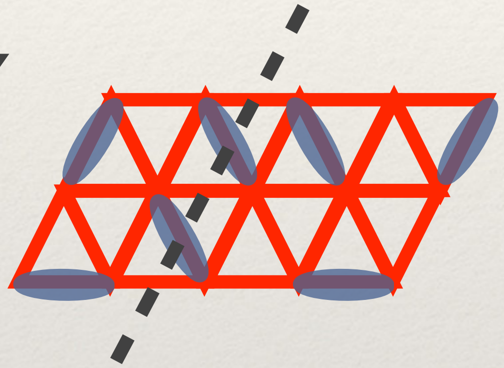


Topologically degenerate

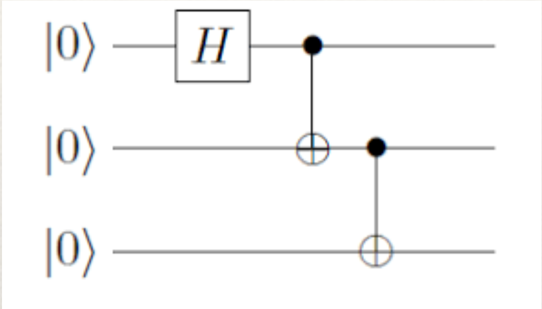
> On a torous there are four degenerate states.
>
> On a cylinder there are two degenerate states.
>
> On a plane there is one ground state.

Universal Subleading Entanglement

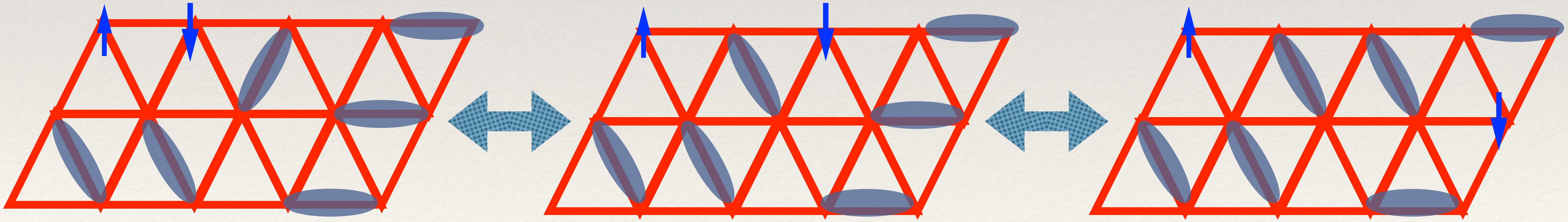
$$S = \alpha L - \gamma$$
$$\gamma = \log(2)$$



Long Range Entanglement



Fractionalized Excitations



neutral spinons with s=1/2

(compare to s=1 magnons)

Much about spin-liquids are understood and there are a few exemplars known.

This talk is about the next step of finding large more robust regimes of spin-liquid behavior. This is the key property of this talk.

The vanilla triangular lattice wasn't a spin-liquid.

Q: Where are the spin-liquids?

Theory		Experiment
Triangular:	120 degree order	organics
Square:	Neel state	
Honeycomb:	Neel state	
✓ **Kagome:**	spin liquid (probably)	✓ Herbertsmithite

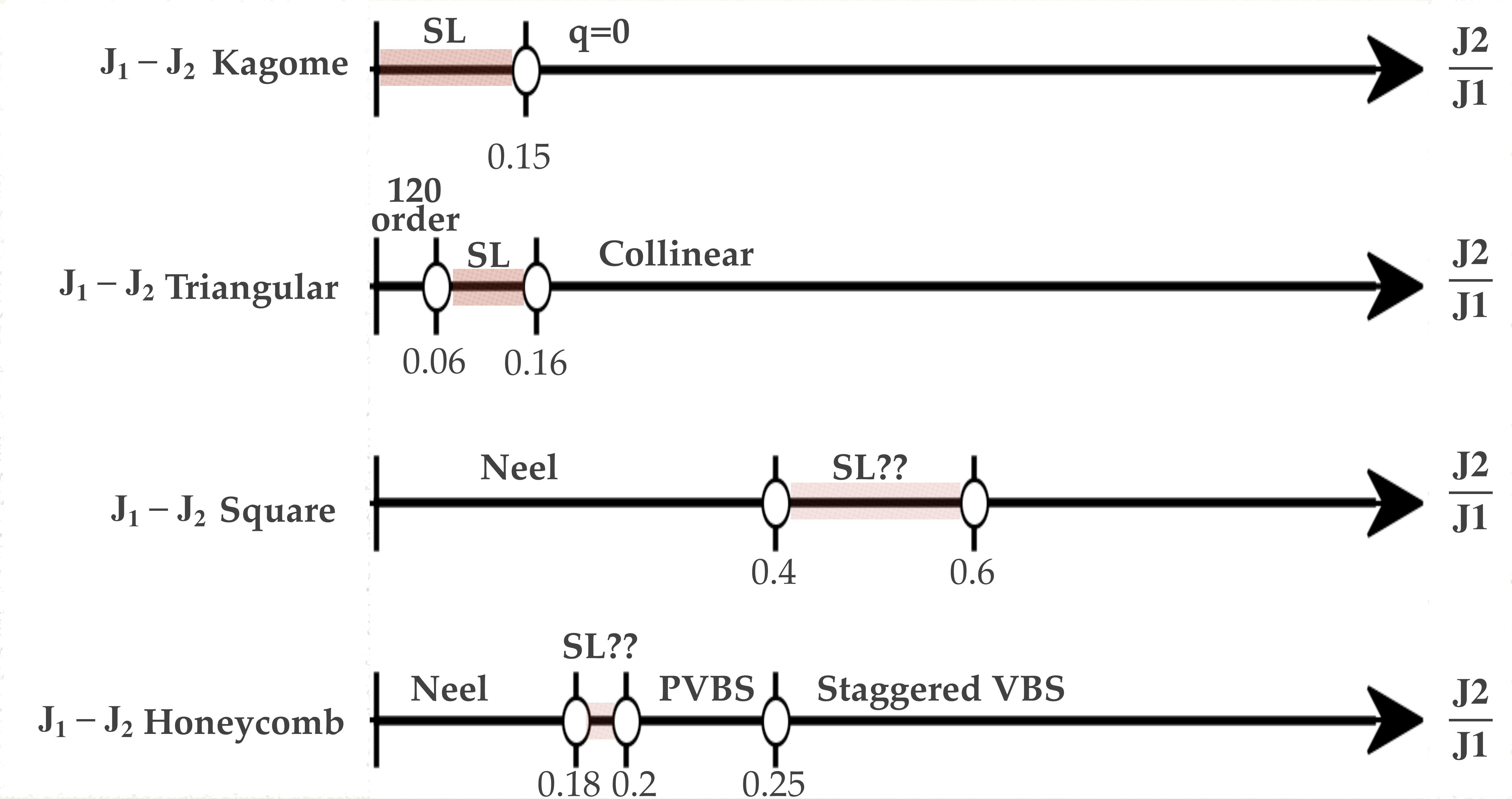
Ignoring 3-d and chiral spin liquids

[Fu; Imai; Han; Lee - Science (2015)]

[Yan;White;Huse - Science 332, 1173-1176 (2011)]

The vanilla triangular lattice wasn't a spin-liquid.

Q: Where are the spin-liquids?



[Zhu, White - PRB 92, 041105]

[Albuquerque, et. al -Phys. Rev. B **84**, 024406]

[Gong; Sheng; Motrunich; Fisher - https://arxiv.org/abs/1306.6067]

Q: Can we extend regimes of spin-liquid?

Q: Can we extend regimes of spin-liquid?

Q: How does one find a new spin liquid?

Q: Can we extend regimes of spin-liquid?

Q: How does one find a new spin liquid?

Try a Hamiltonian and …

solve the classical model.

`Easy' but classical $\neq$ quantum

Phases `similar'

solve the quantum model.

Hard

- **Exact Diagonalization**
- **Density Matrix Renormalization Group**
- **Quantum Monte Carlo**

A new alternative: Inverse Methods

A new alternative: Inverse Methods *(tangeant)*

Guess a Hamiltonian

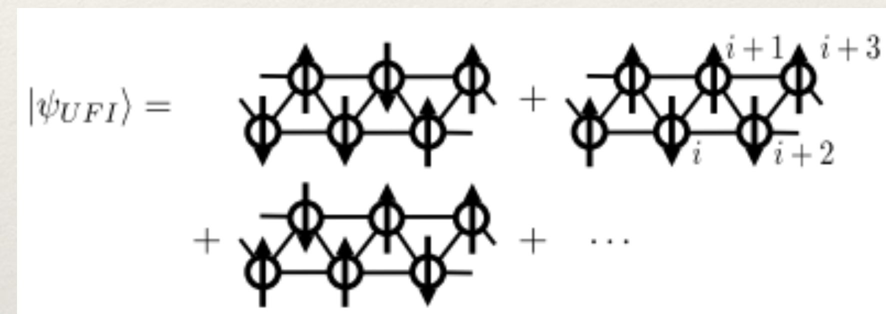
Find the wave-function

Measure properties

EHC

Generate a Hamiltonian

Write down a wave-function



Pick desired properties

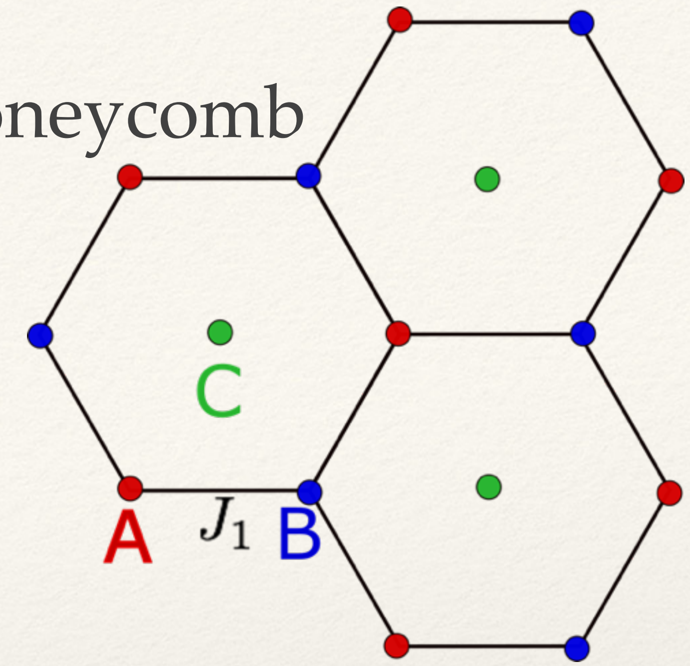
no order

[PRX 8, 031029 Cherktov and Clark]

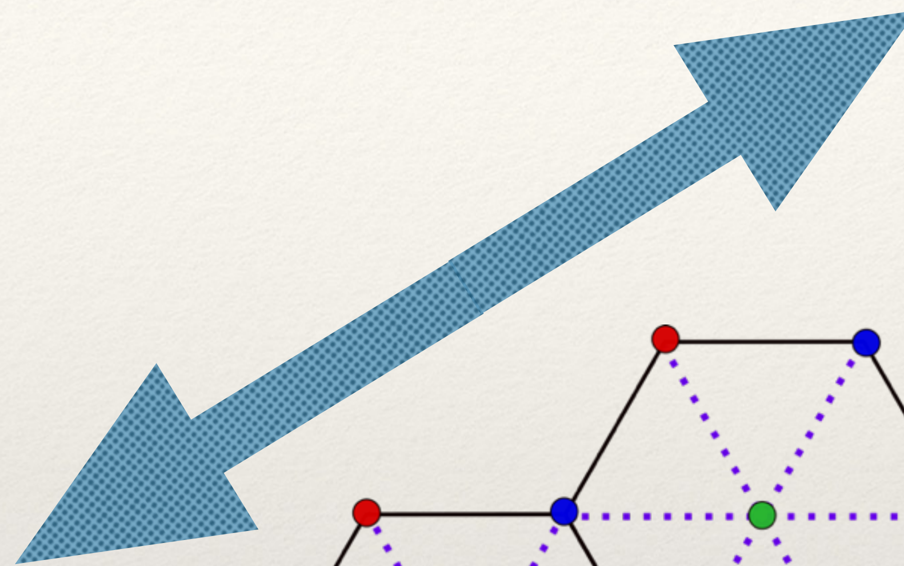
Try a Hamiltonian…

Q: Which Hamiltonian?

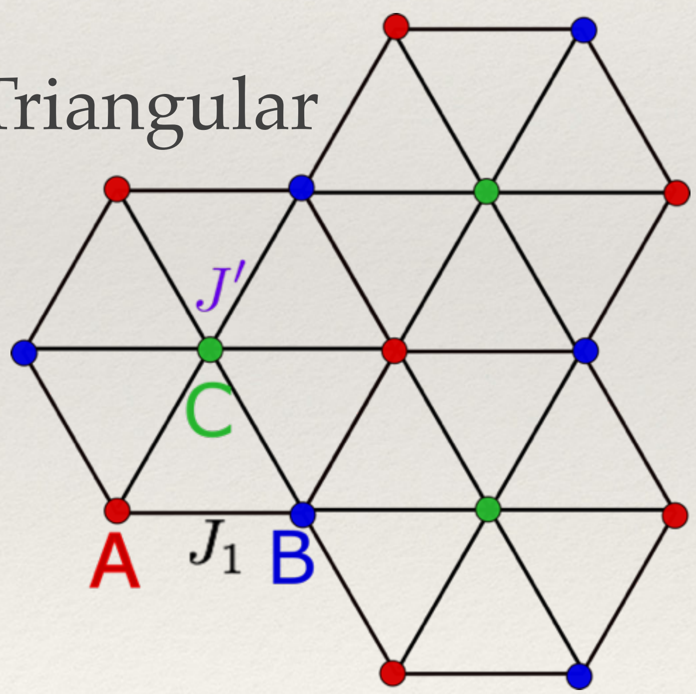
Honeycomb

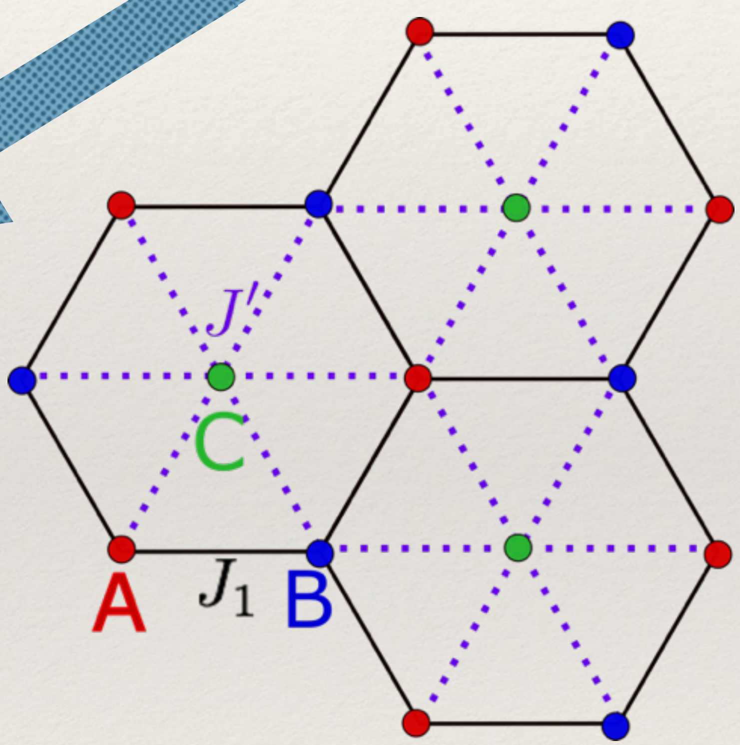


$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i^{A} \cdot \mathbf{S}_j^{B}$$



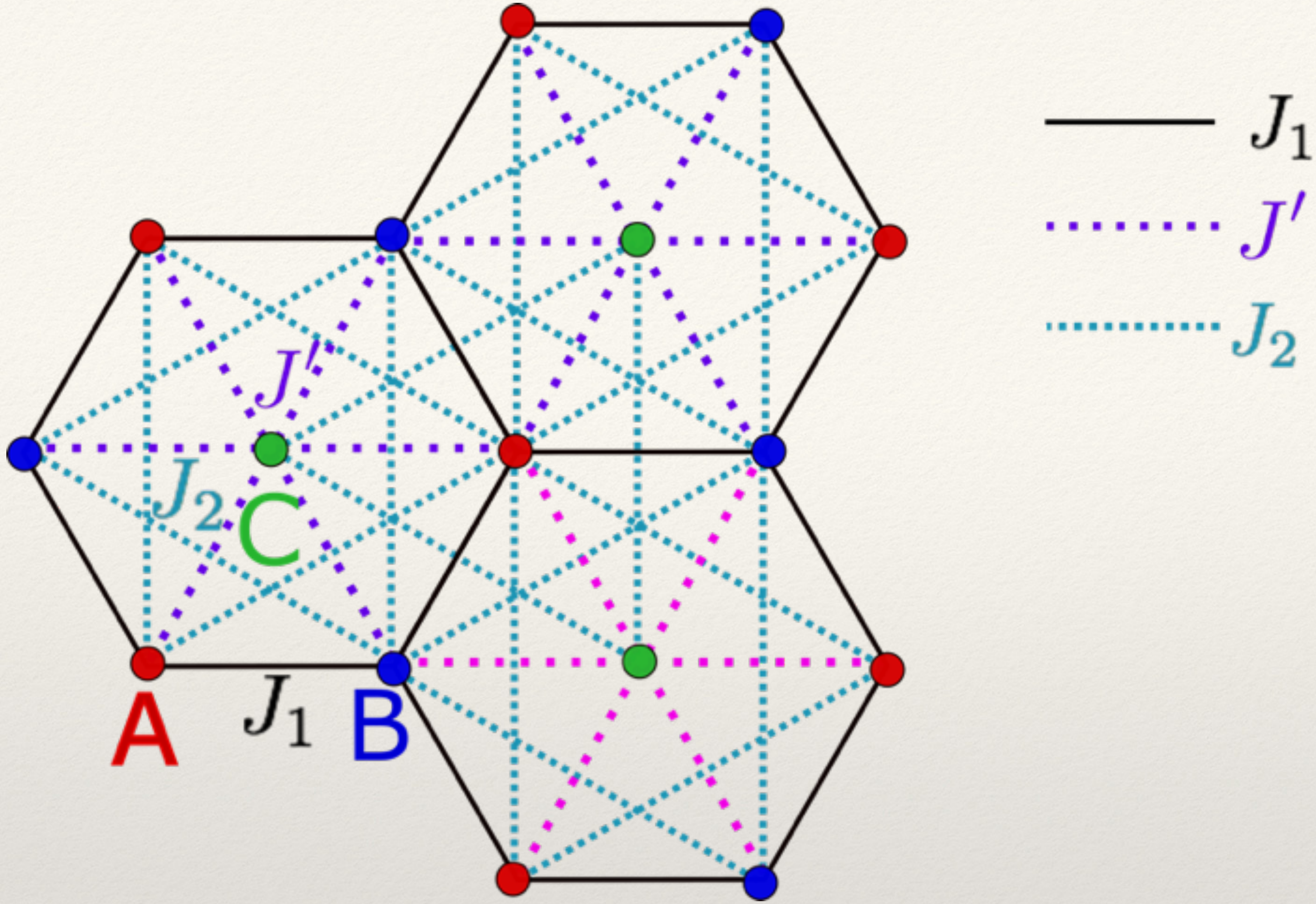
Triangular





Stuffed Honeycomb

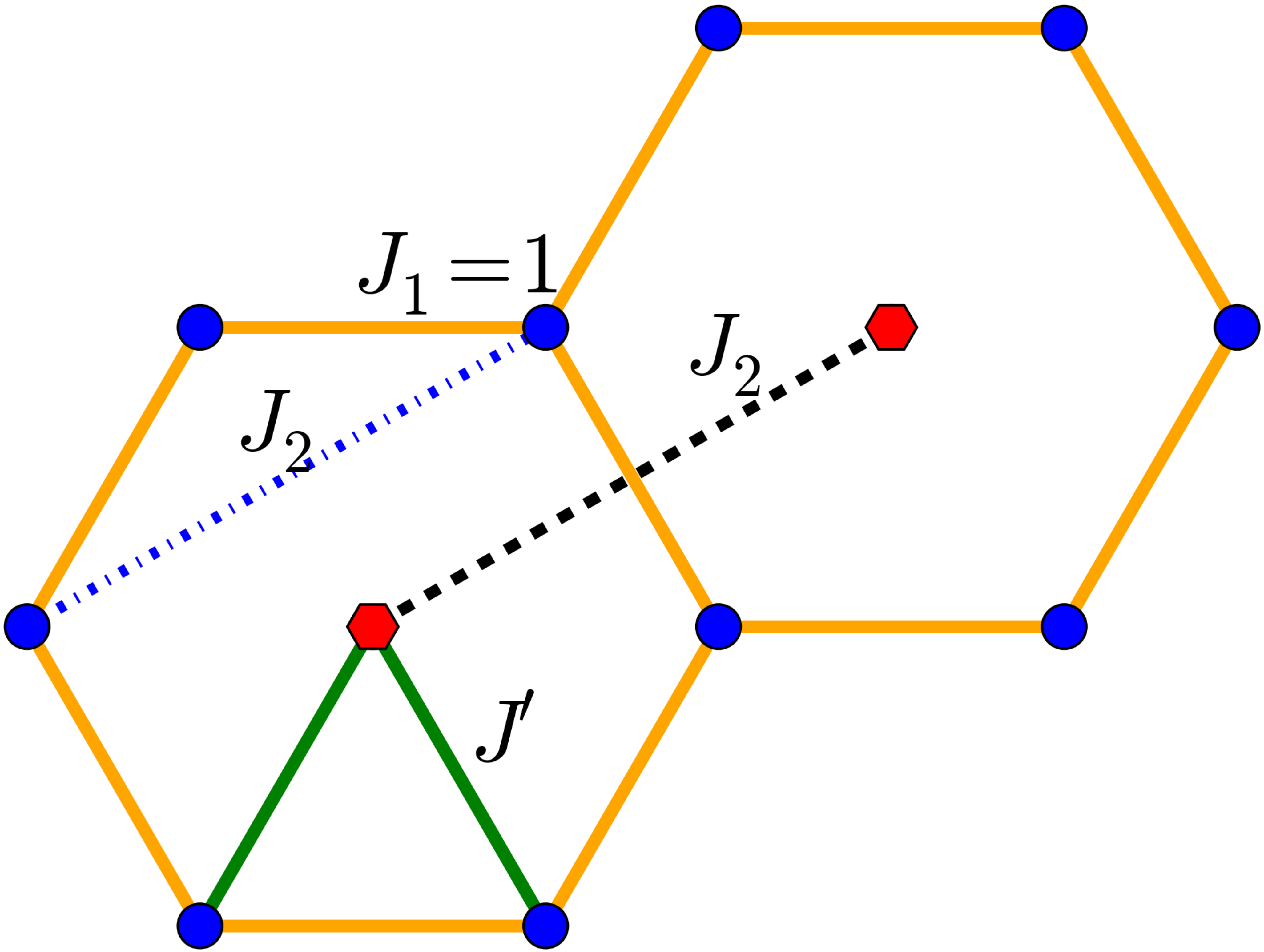
$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i^{A} \cdot \mathbf{S}_j^{B} + J' \sum_{\substack{\langle i,j \rangle \\ \eta = A,B}} \mathbf{S}_i^{\eta} \cdot \mathbf{S}_j^{C}$$



$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i^A \cdot \mathbf{S}_j^B + J_2 \sum_{\substack{\langle\langle i,j \rangle\rangle \\ \eta=A,B,C}} \mathbf{S}_i^\eta \cdot \mathbf{S}_j^\eta + J' \sum_{\substack{\langle i,j \rangle \\ \eta=A,B}} \mathbf{S}_i^\eta \cdot \mathbf{S}_j^C$$

Stuffed Honeycomb

$$\hat{H} = \sum_{\langle i_1, j_1\rangle} \vec{S_{i_1}} \vec{S_{j_1}} + J_2 \sum_{\langle i_2, j_2\rangle} \vec{S_{i_2}} \vec{S_{j_2}} + J' \sum_{\langle i_3, j_3\rangle} \vec{S_{i_3}} \vec{S_{j_3}} + J_2 \sum_{\langle i_4, j_4\rangle} \vec{S_{i_4}} \vec{S_{j_4}} + J_\chi \sum_{i,j,k\in\Delta} \vec{S_i}(\vec{S_j} \times \vec{S_k})$$

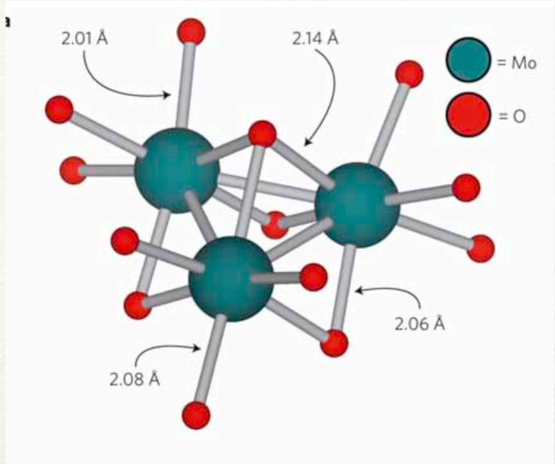


Motivation for this model…

Project started from experimental motivation concerning $LiZn_2Mo_3O_8$

Interpolates between triangular and honeycomb

Engineer from triangular trilayer.



solve the classical model.

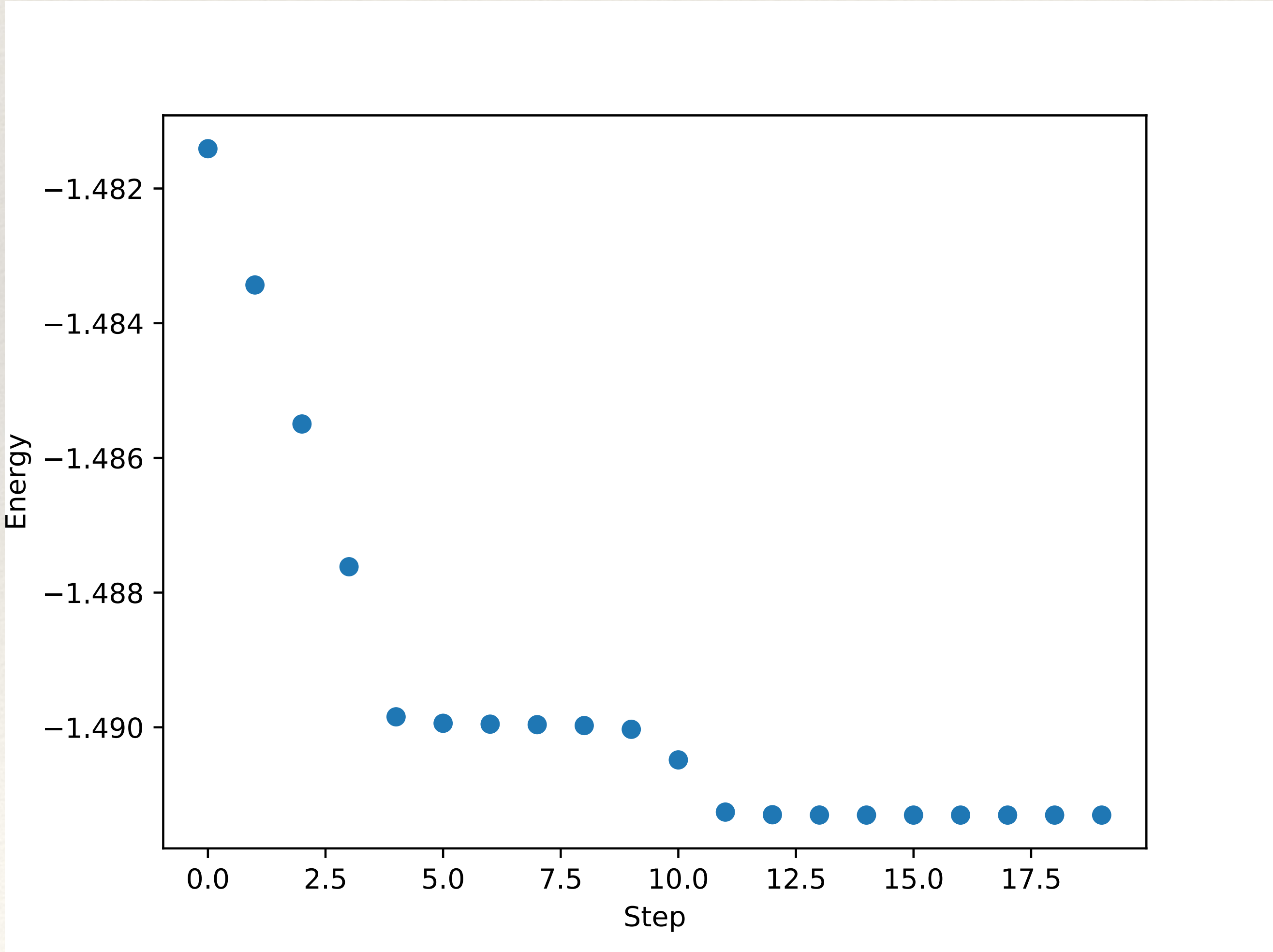
Q: How?

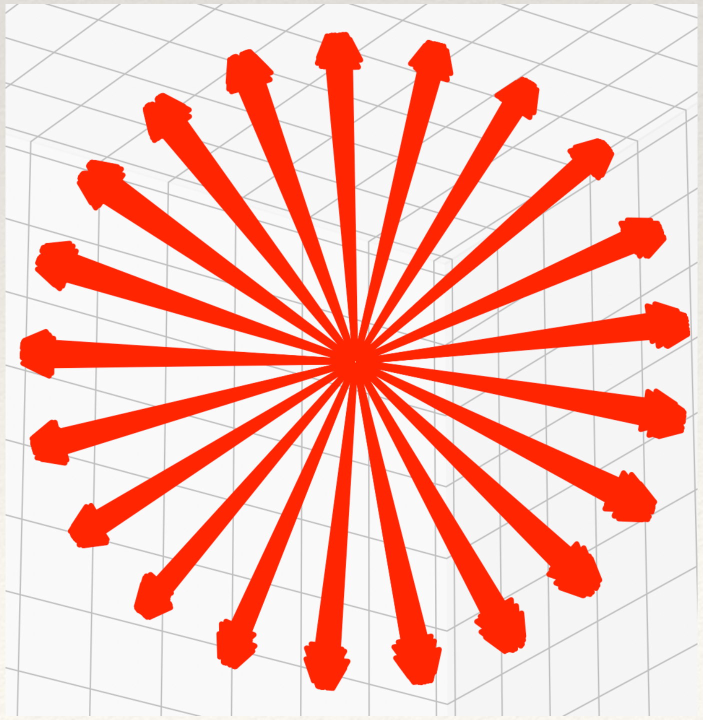
Iterative minimization; variational ansatz.

Pick a random spin.

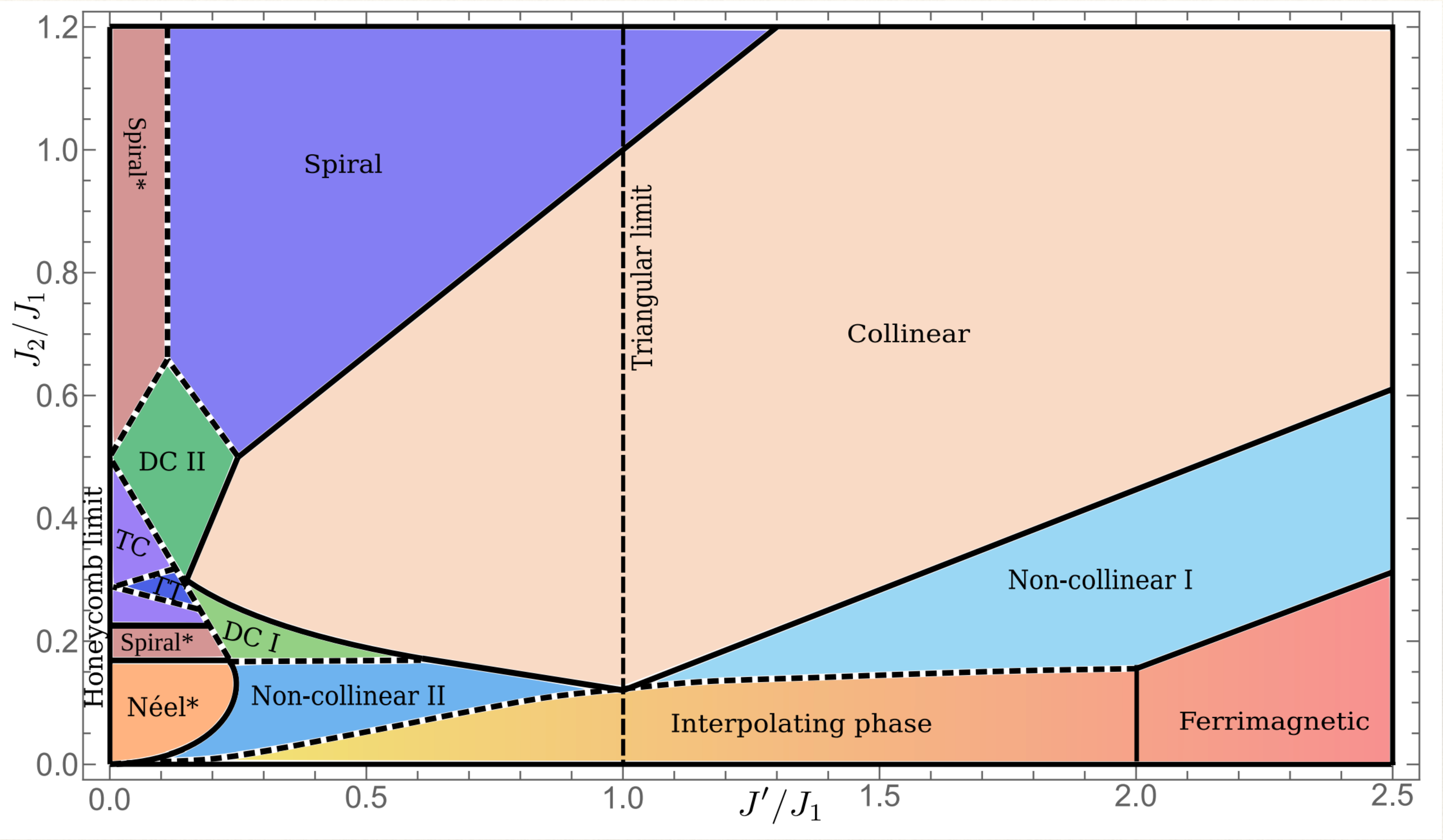
Change it so the energy goes down.

Iterate…





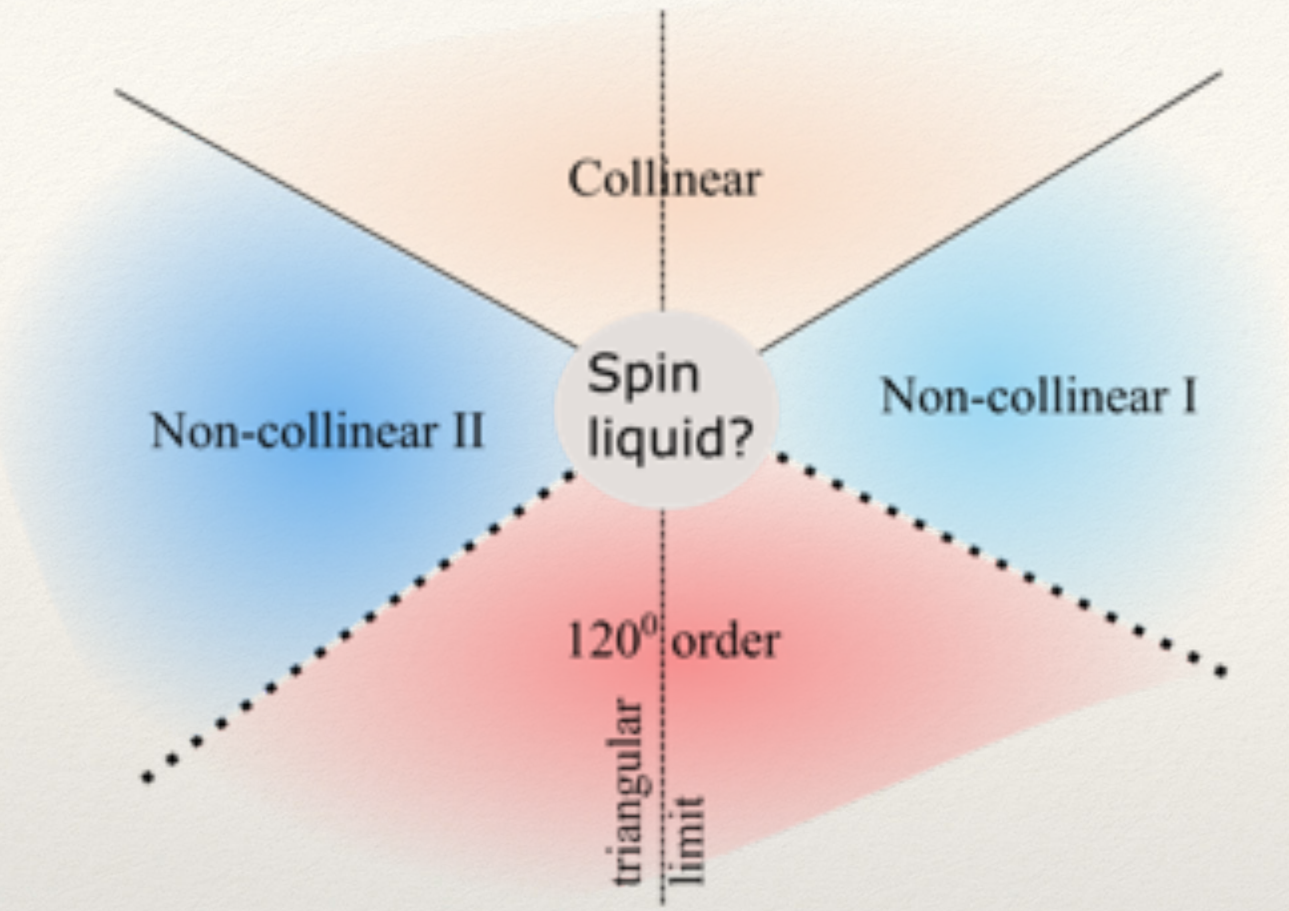
Classical phase diagram



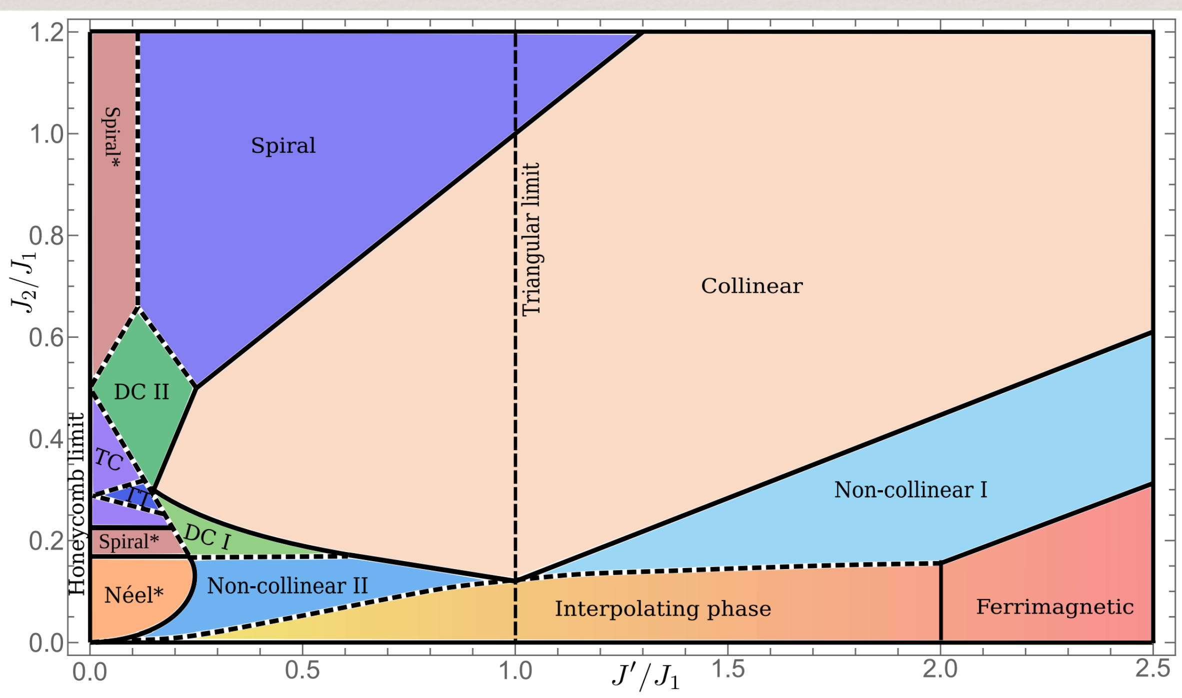
Q: What should we look for to find a spin-liquid?

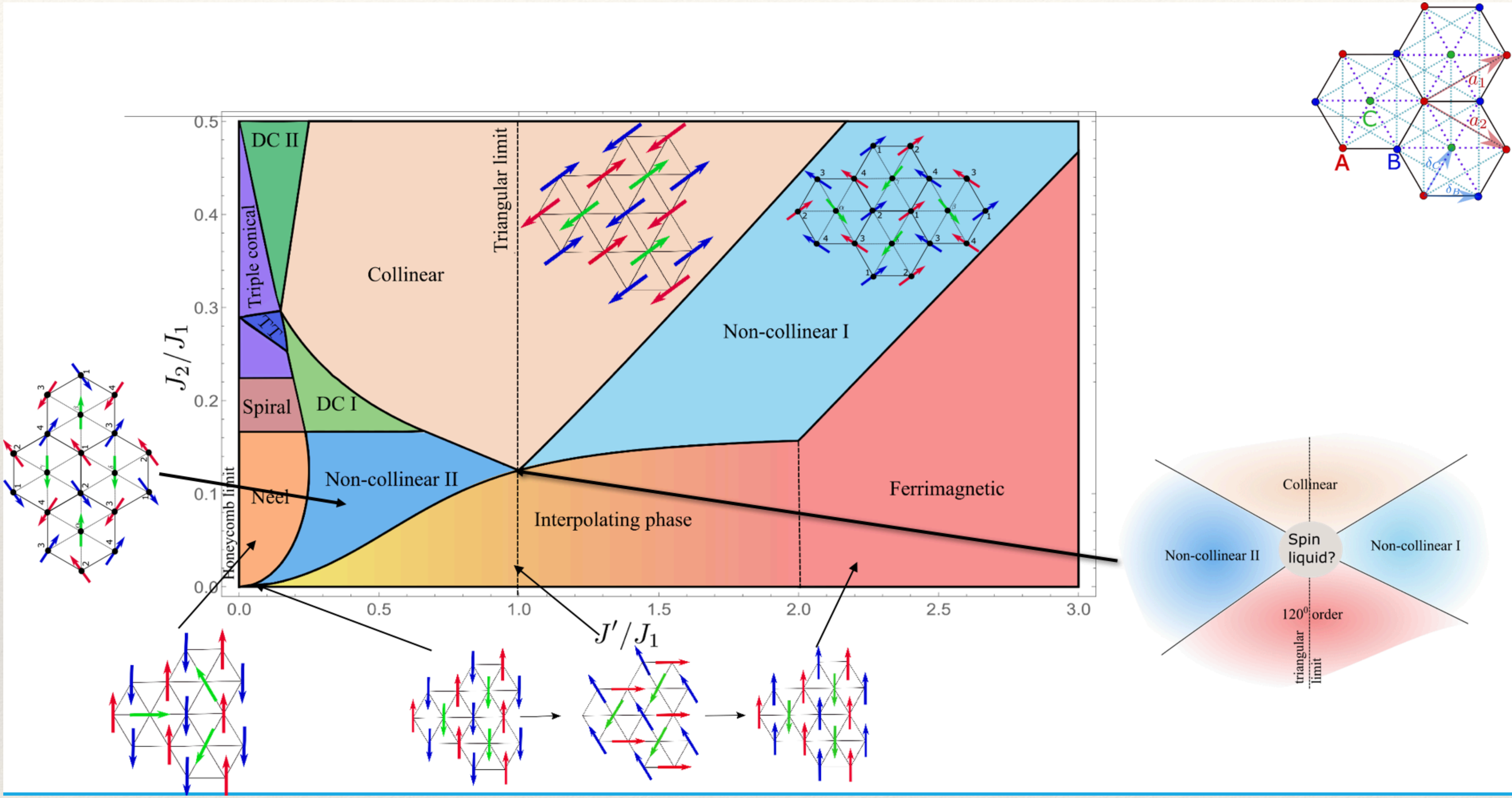
paramagnet?

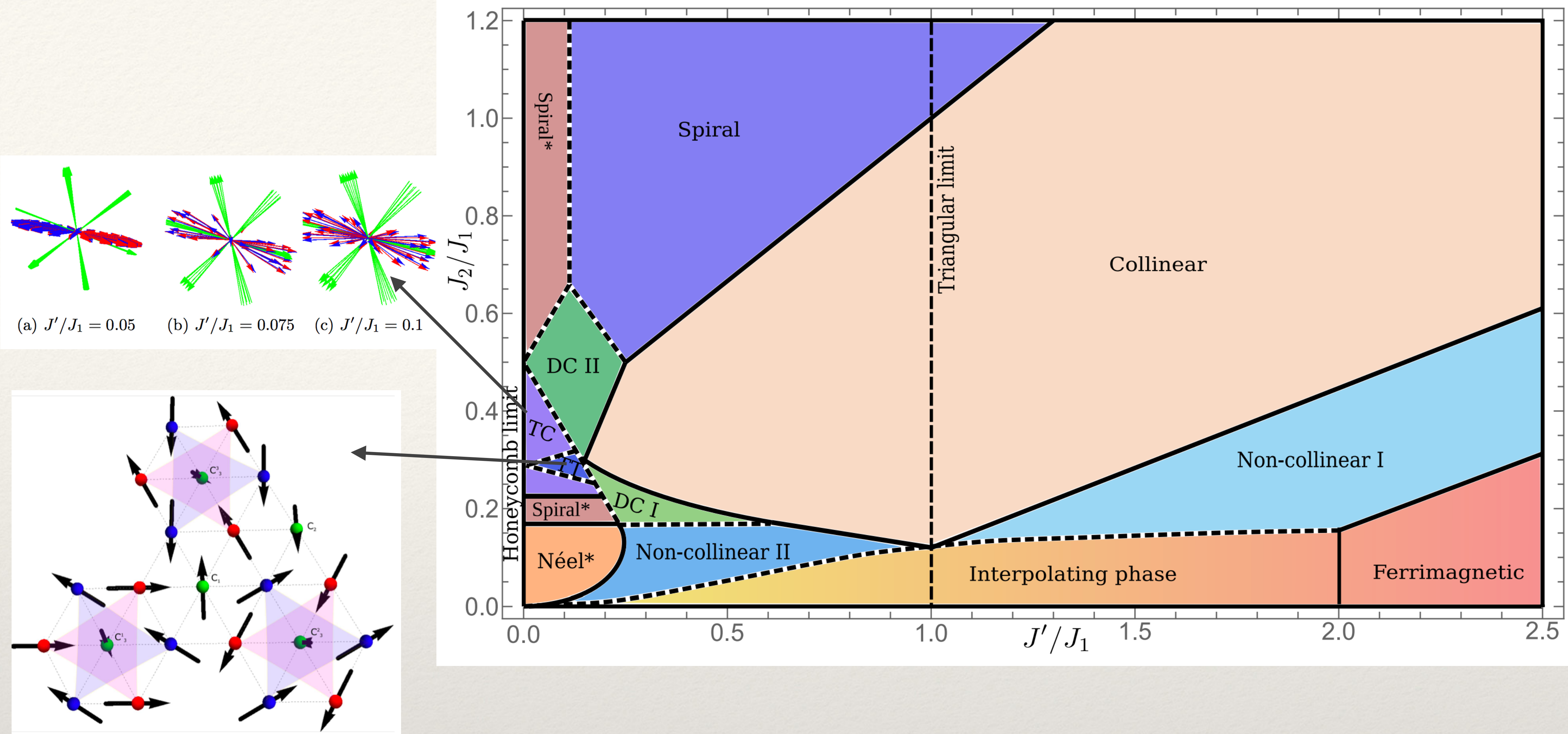
Q: What should we look for to find a spin-liquid?



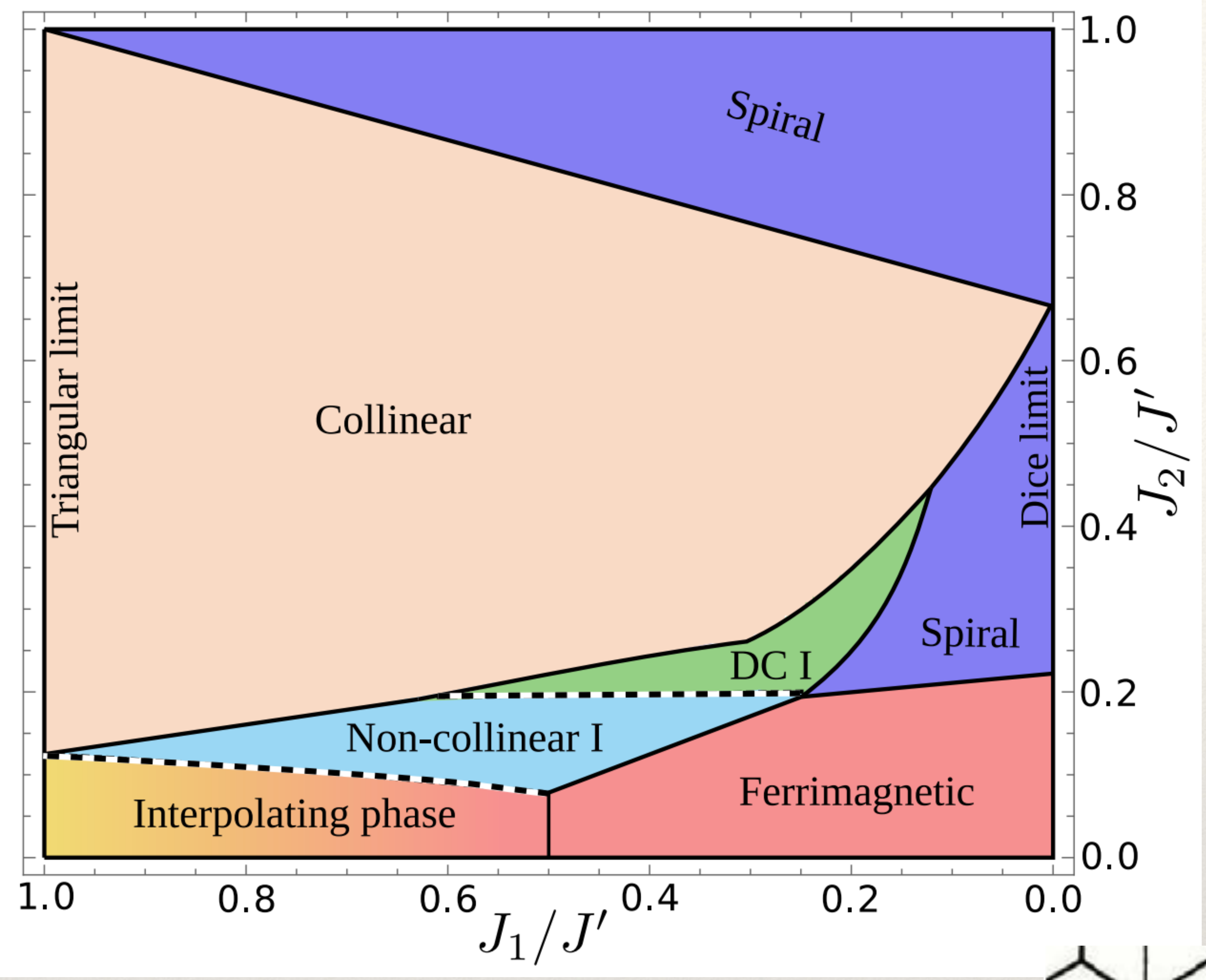
Fluctuations around a classical multi-critical point are apt to give spin-liquids.



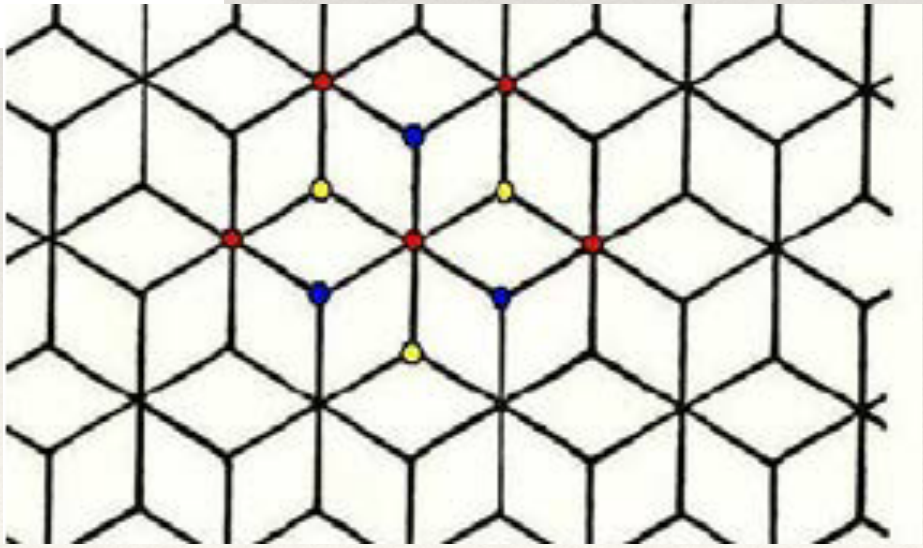

DC II
Triple conical
TT
Spiral
DC I
Collinear
Triangular limit
Non-collinear I
Non-collinear II
Néel
Honeycomb limit
Interpolating phase
Ferrimagnetic
J_2/J_1
J'/J_1
0.0
0.1
0.2
0.3
0.4
0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Collinear
Spin liquid?
Non-collinear II
Non-collinear I
120^0 order
triangular limit
A
B
C
a_1
a_2
δ_C
δ_B



(a) $J'/J_1 = 0.05$
(b) $J'/J_1 = 0.075$
(c) $J'/J_1 = 0.1$
Spiral*
Spiral
DC II
TC
TT
DC I
Spiral*
Néel*
Non-collinear II
Collinear
Triangular limit
Honeycomb limit
Non-collinear I
Interpolating phase
Ferrimagnetic
J_2/J_1
J'/J_1
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.0
0.5
1.0
1.5
2.0
2.5

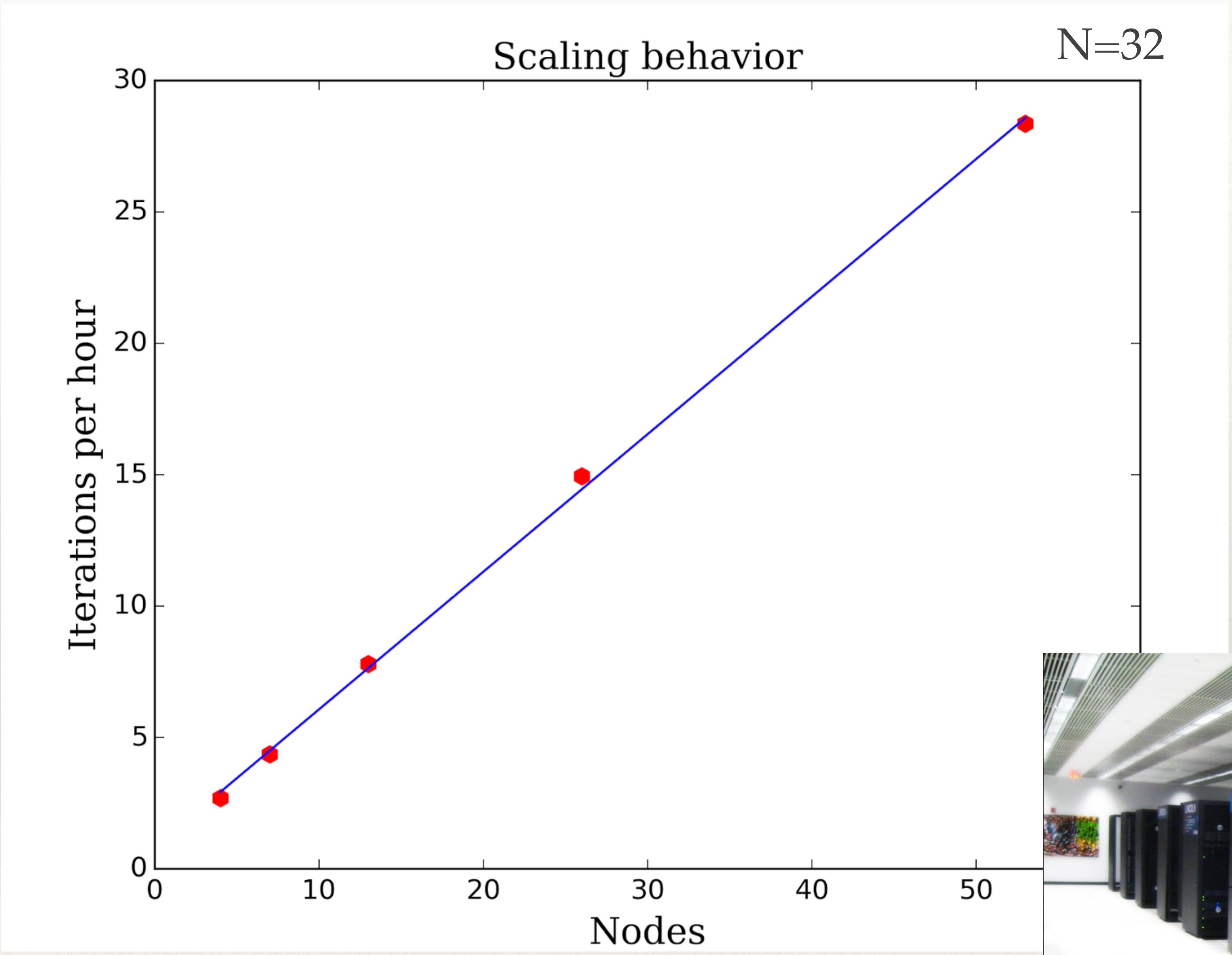


Spiral
Collinear
Triangular limit
Dice limit
Spiral
DC I
Non-collinear I
Ferrimagnetic
Interpolating phase
1.0
0.8
0.6
0.4
0.2
0.0
J_2/J'
J_1/J'



solve the quantum model.

exact diagonalization



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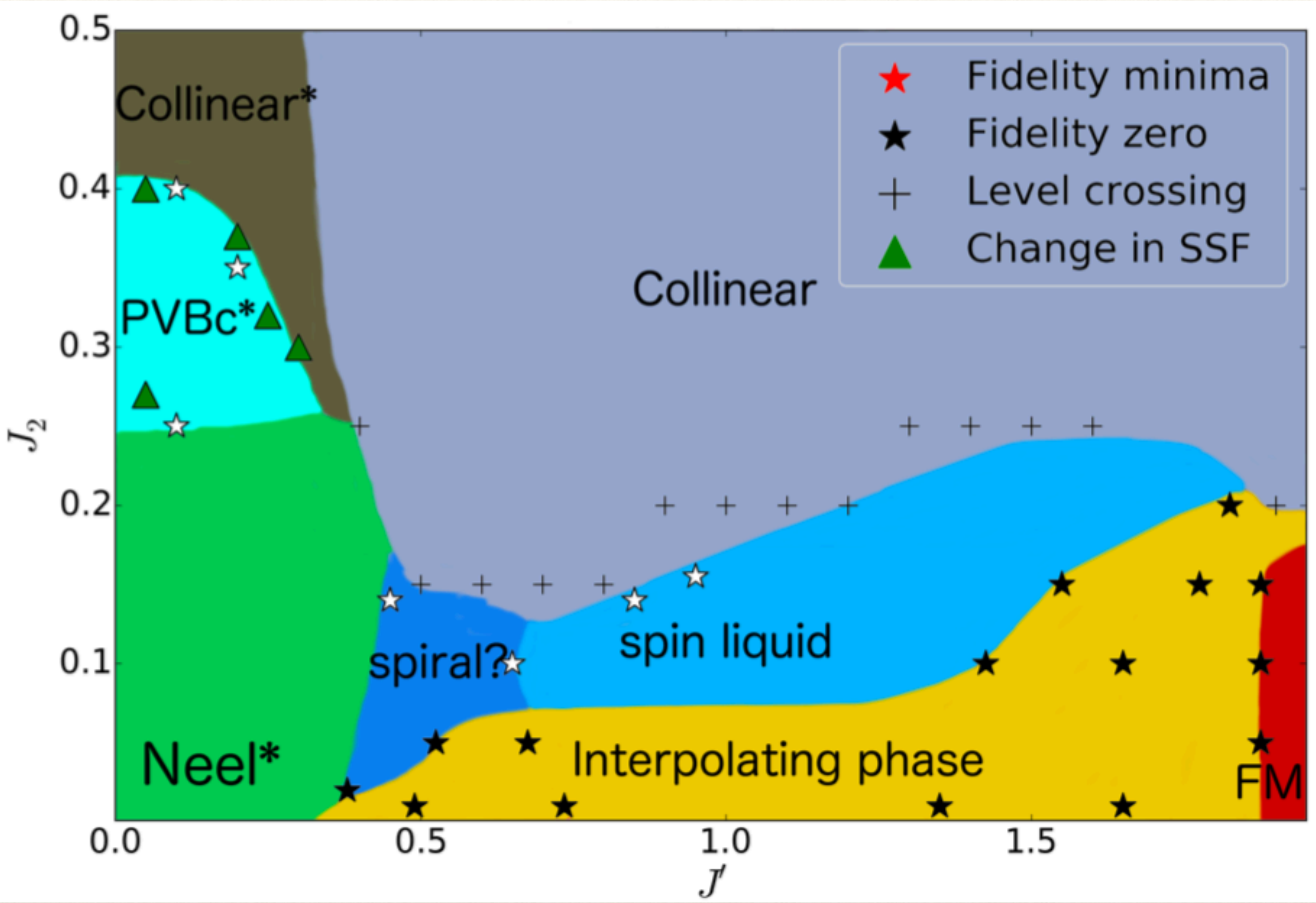
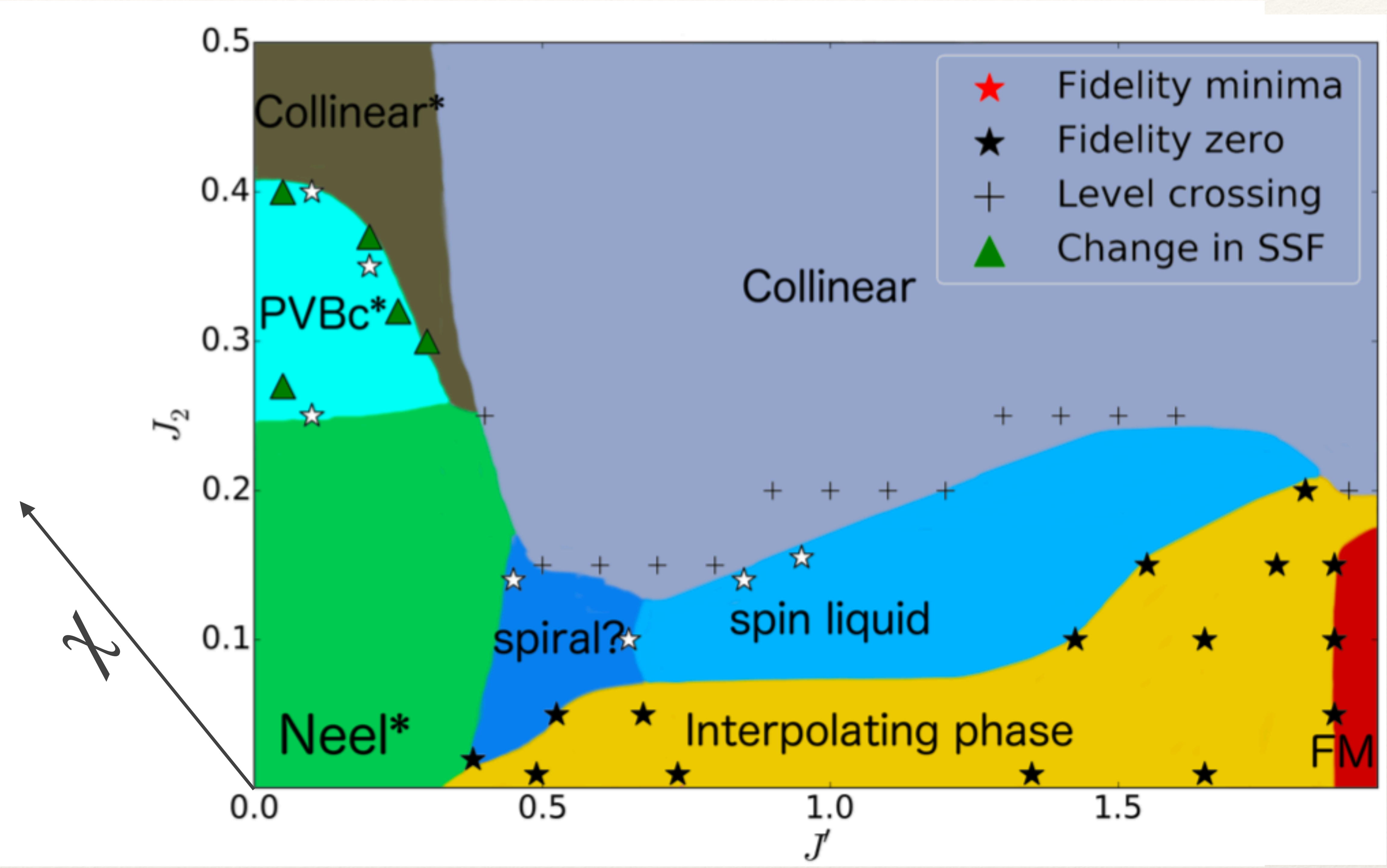


Also a rich phase diagram

Another axis: Chirality $H_{\text{Heisenberg}} + \chi \sum_{ijk \in \Delta} s_i \cdot (s_j \times s_k)$



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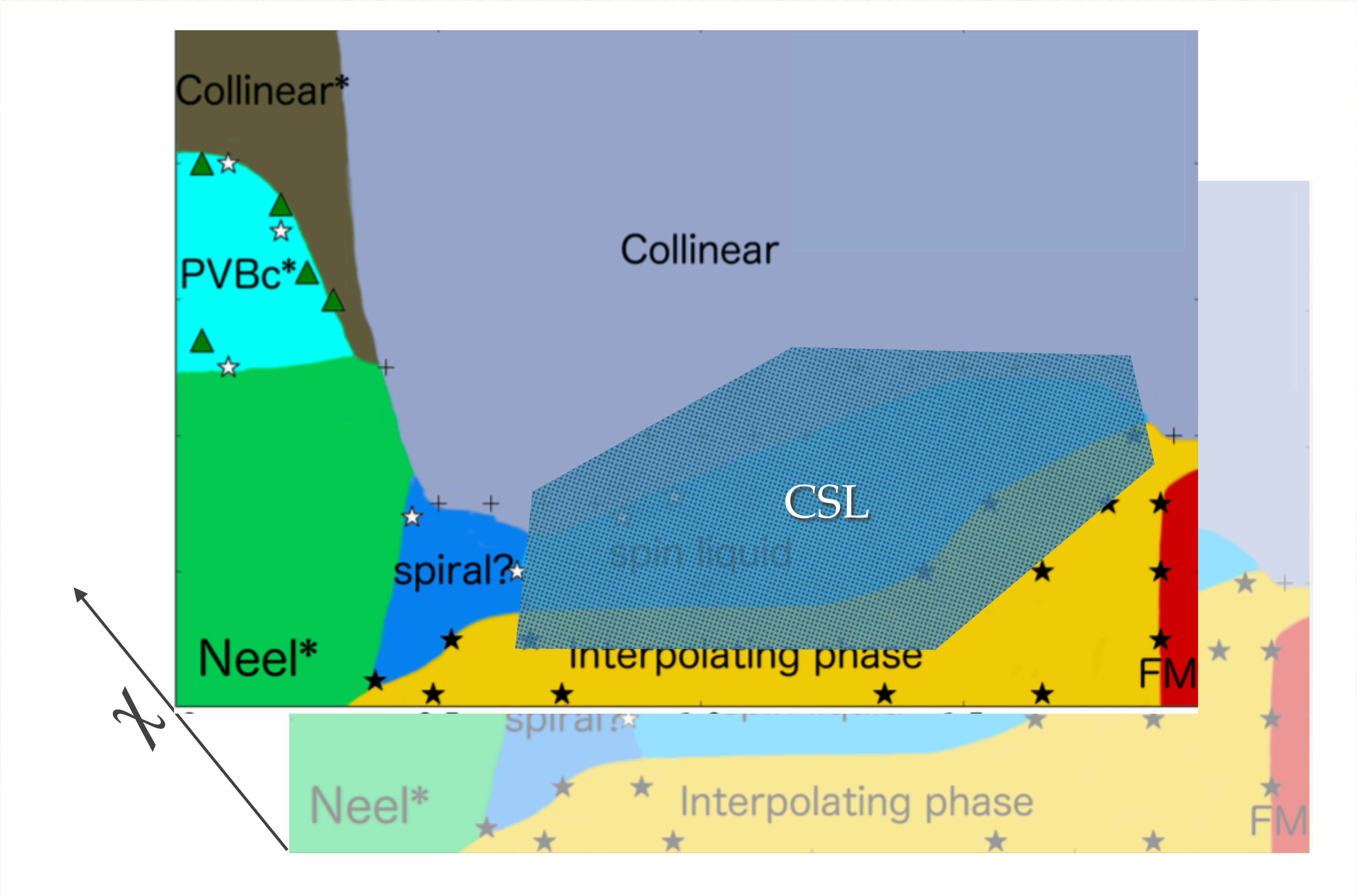

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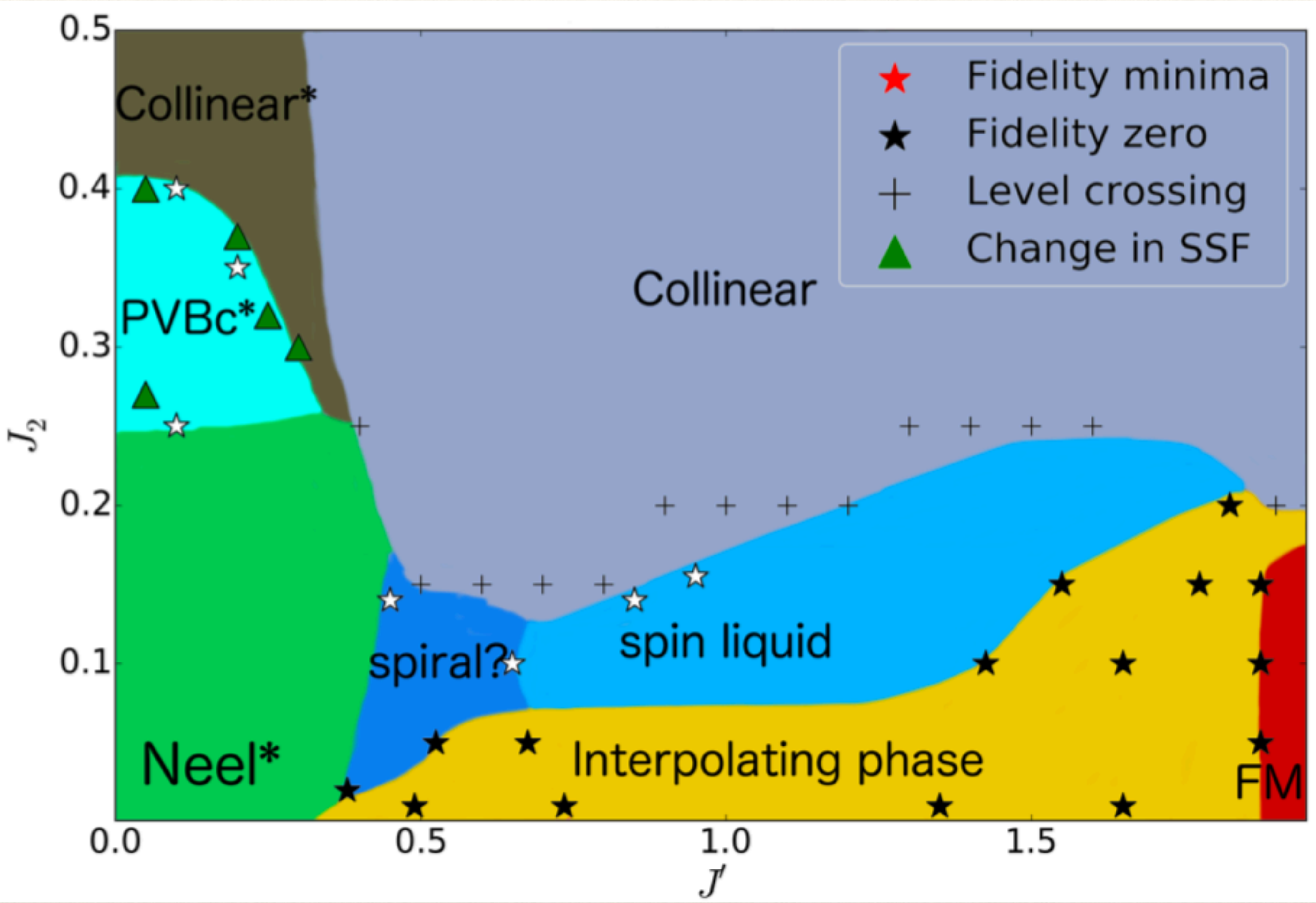
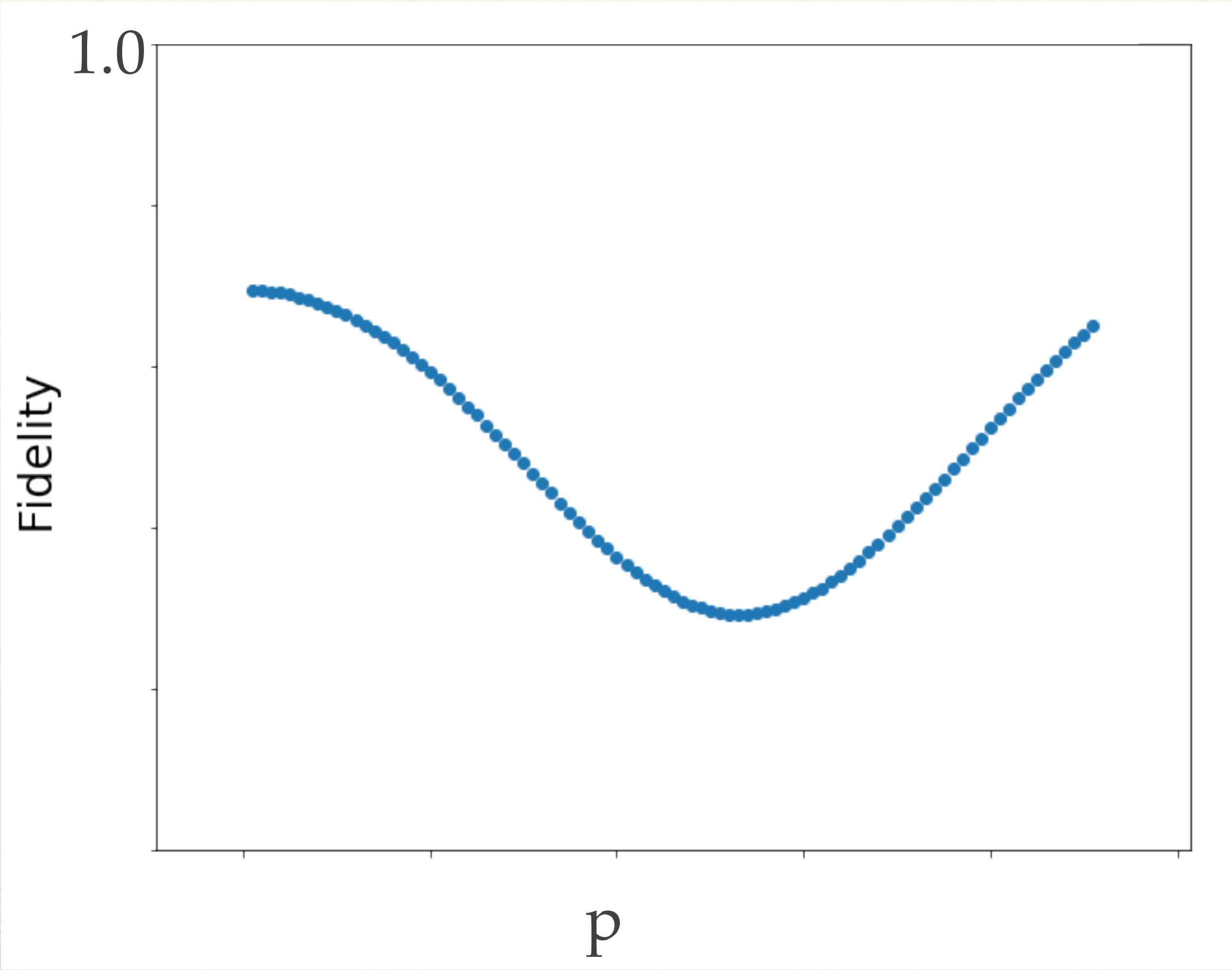


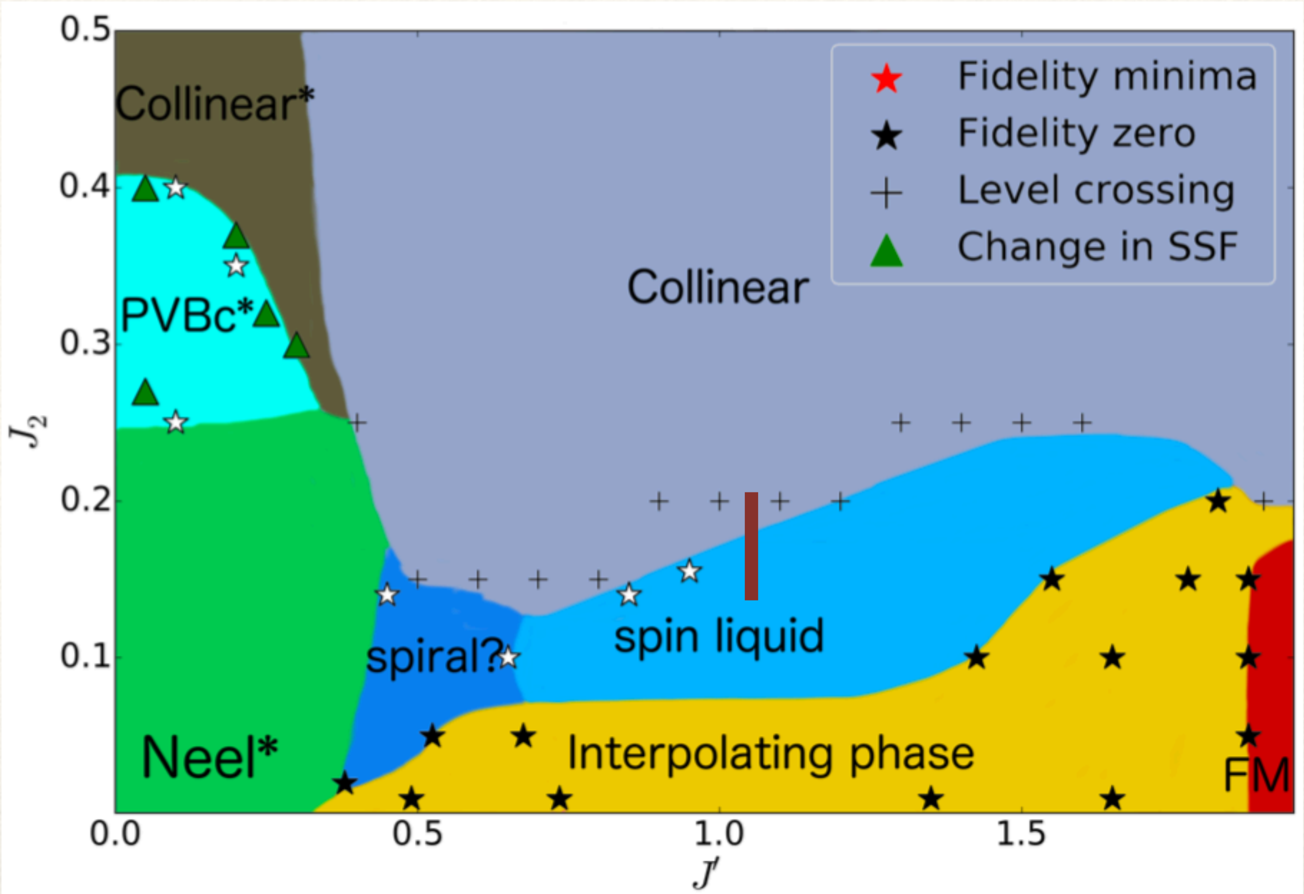
Also a rich phase diagram…how do we know where all the phases are?

Need an approach which doesn't need to know the list of possible phases a priori

Why? *(measure, an order parameter at each point and extrapolating is very painful)*

Fidelity to find phases.



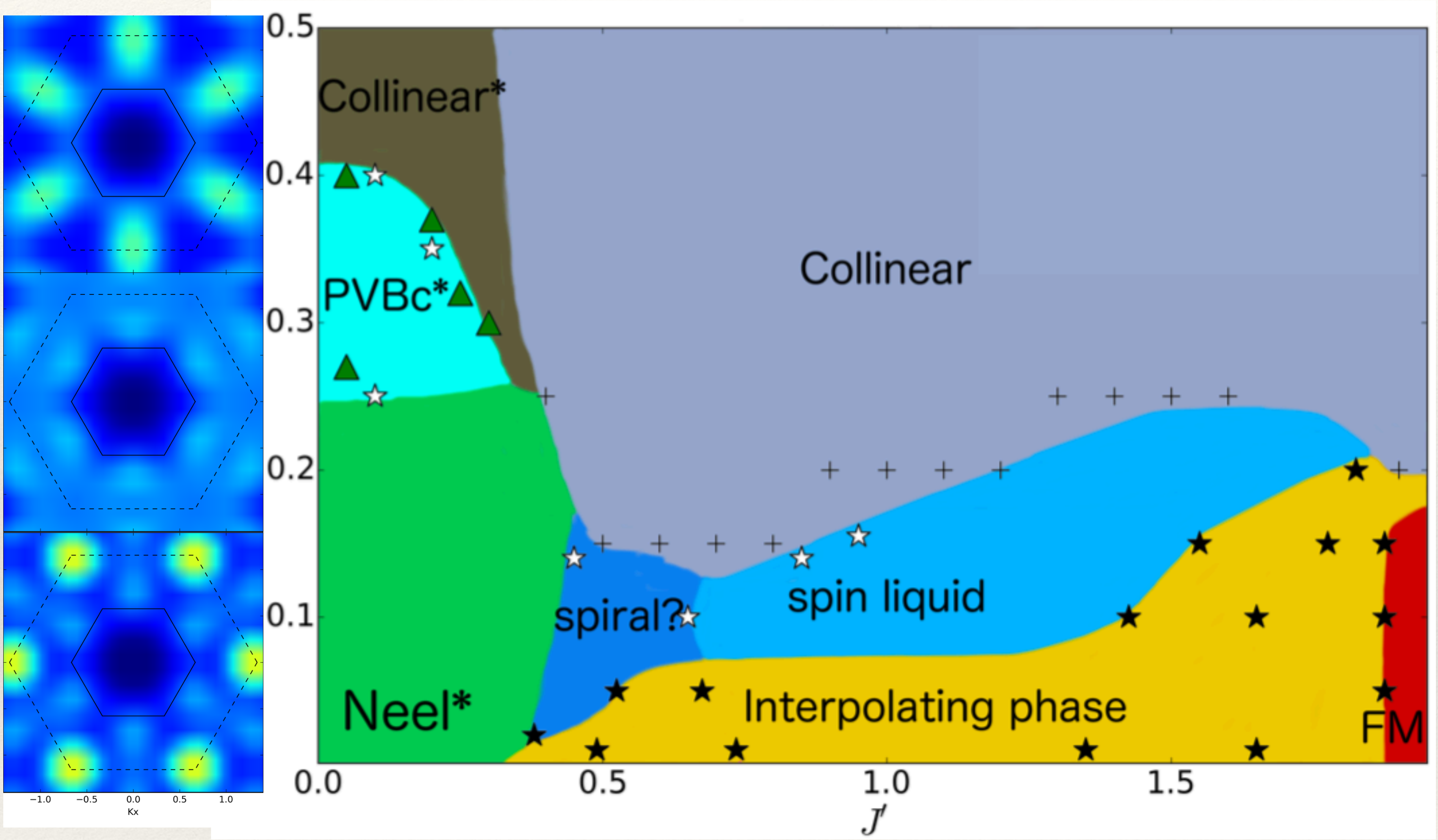


Allows us to map out the entire phase diagram.

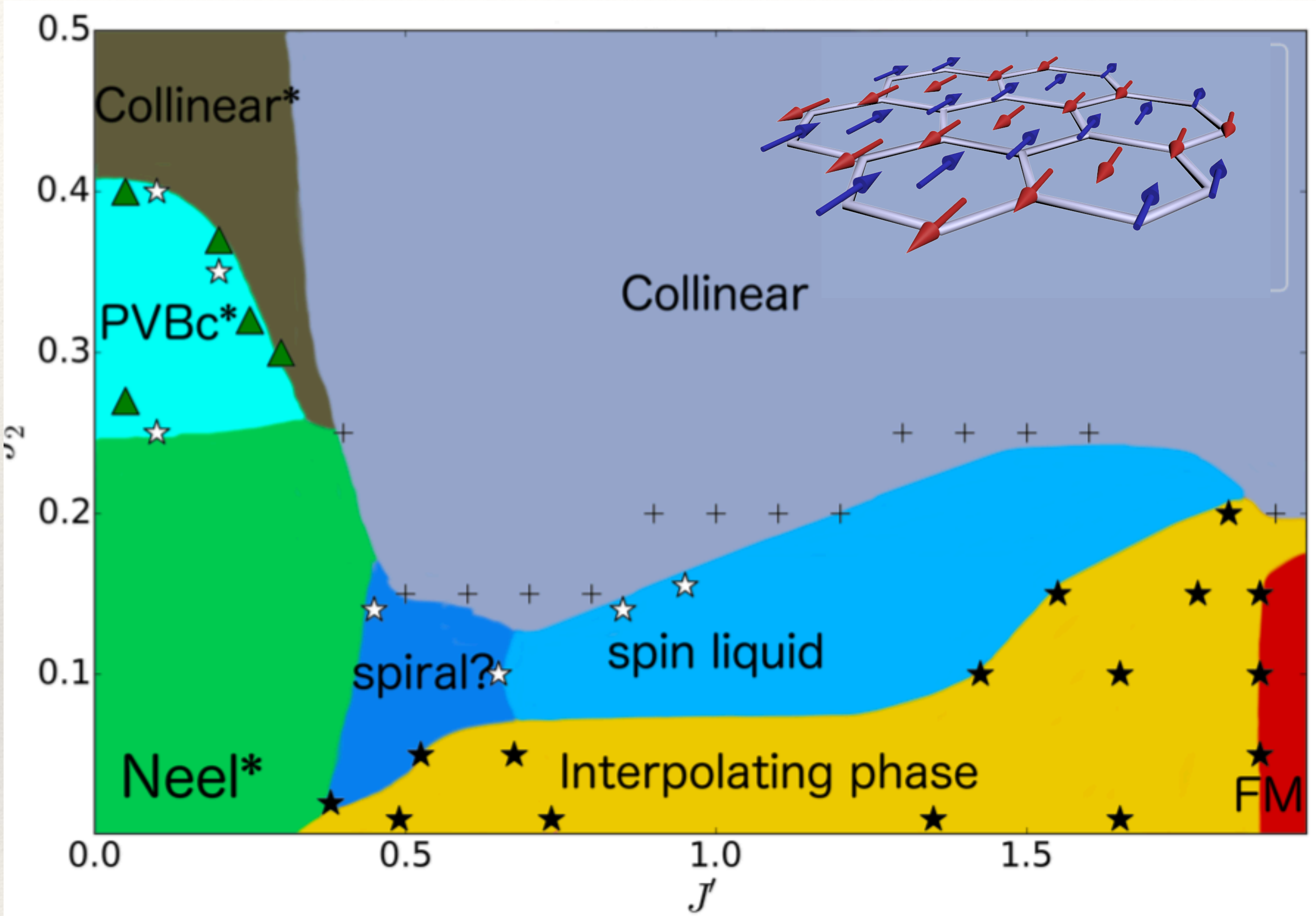
(subtle but cool detail where this breaks down in the interpolating phase - ask me later)

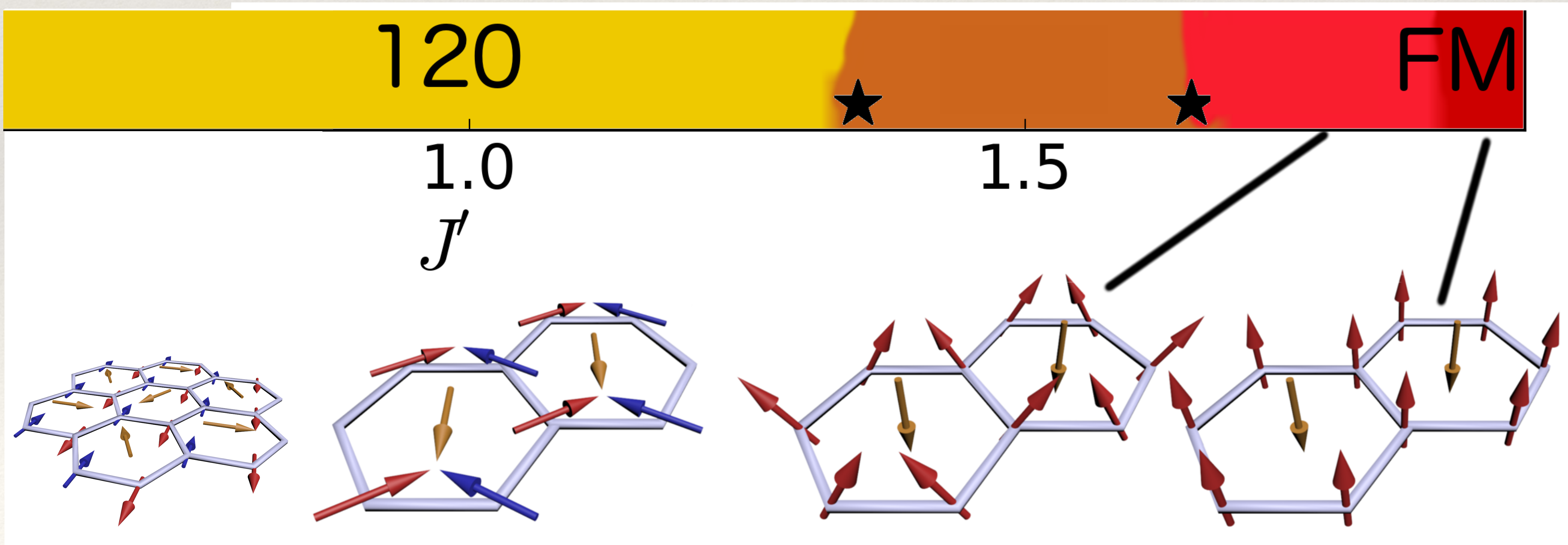
Once you know where the phases are you can measure properties to determine them.

Structure Factors

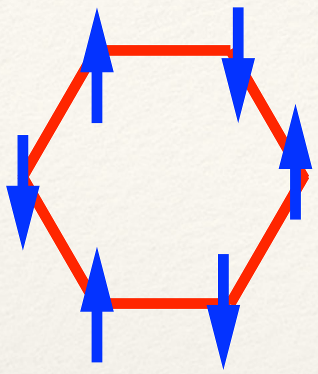


Once you know where the phases are you can measure properties to determine them.

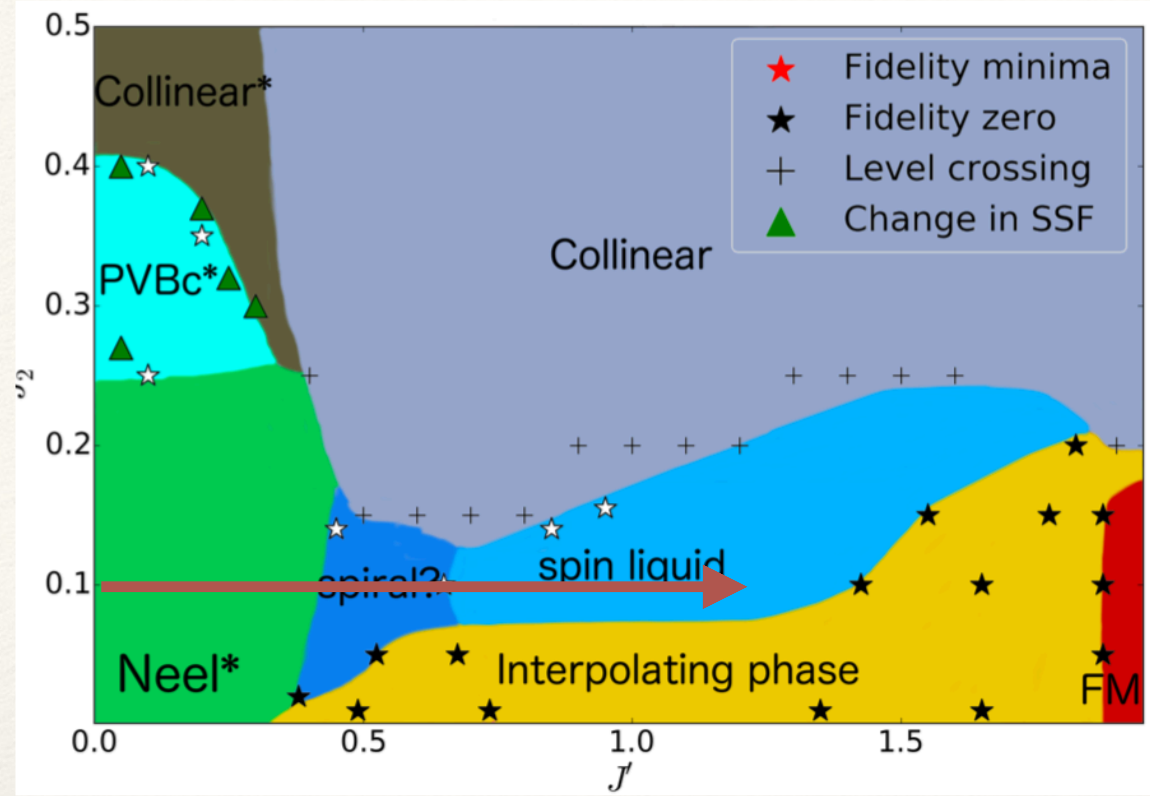



120
FM
1.0
1.5
J'

Spiral Phase

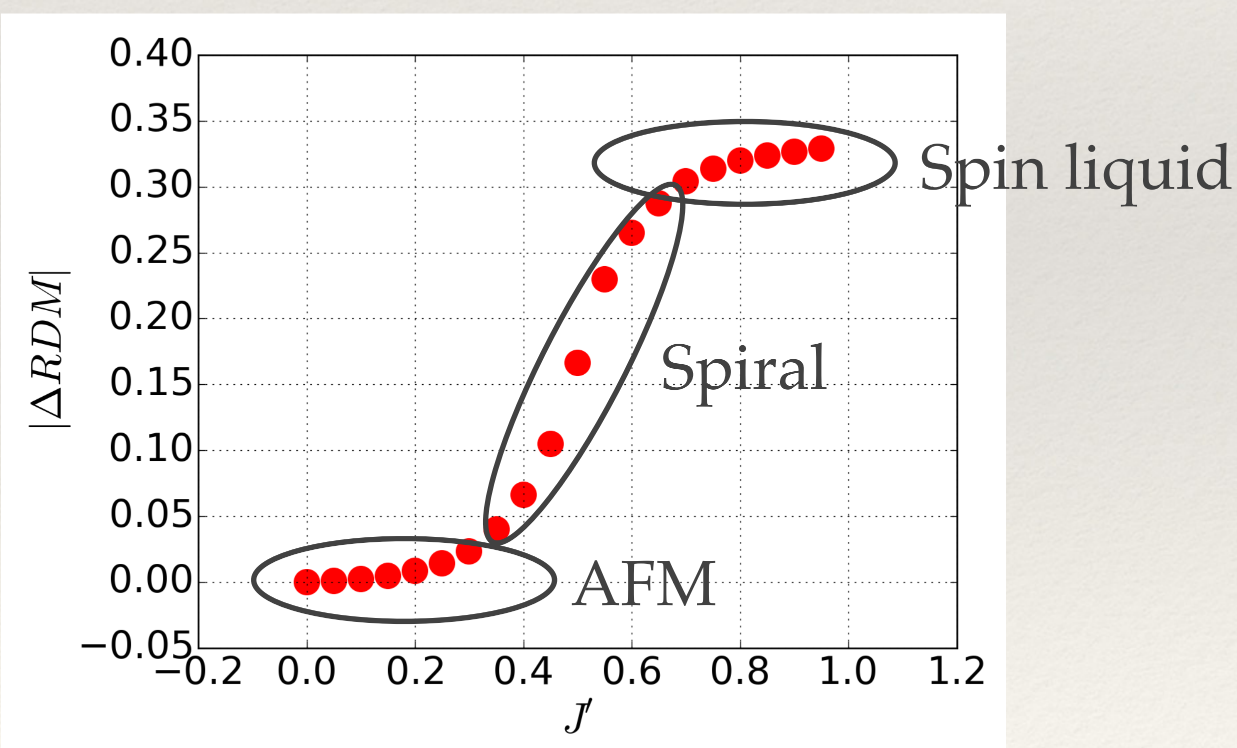


$$\rho_{hex} = Tr_{nothex}\rho = \sum_{|\beta\rangle} \langle\beta|\rho|\beta\rangle$$



Compute the reduced density matrix on a hexagon.

Measure how quickly it changes.

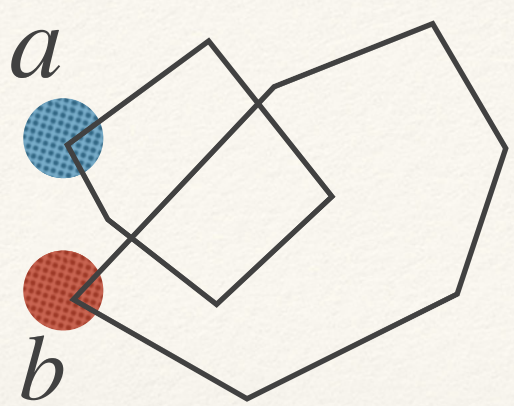


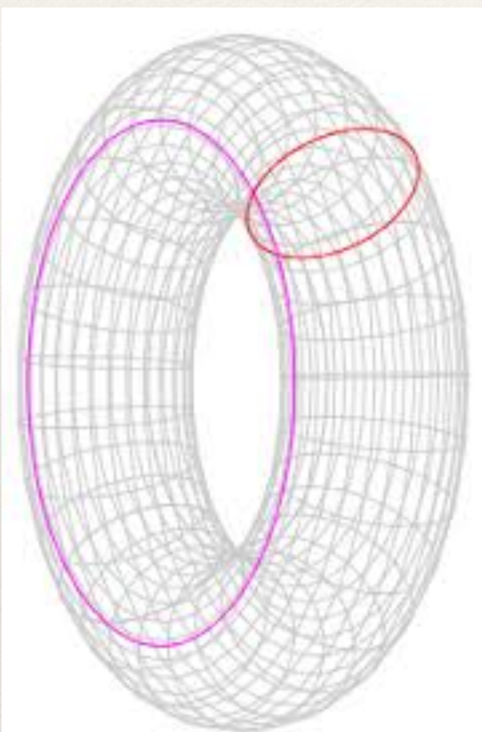
Q: What type of spin liquid(s)?

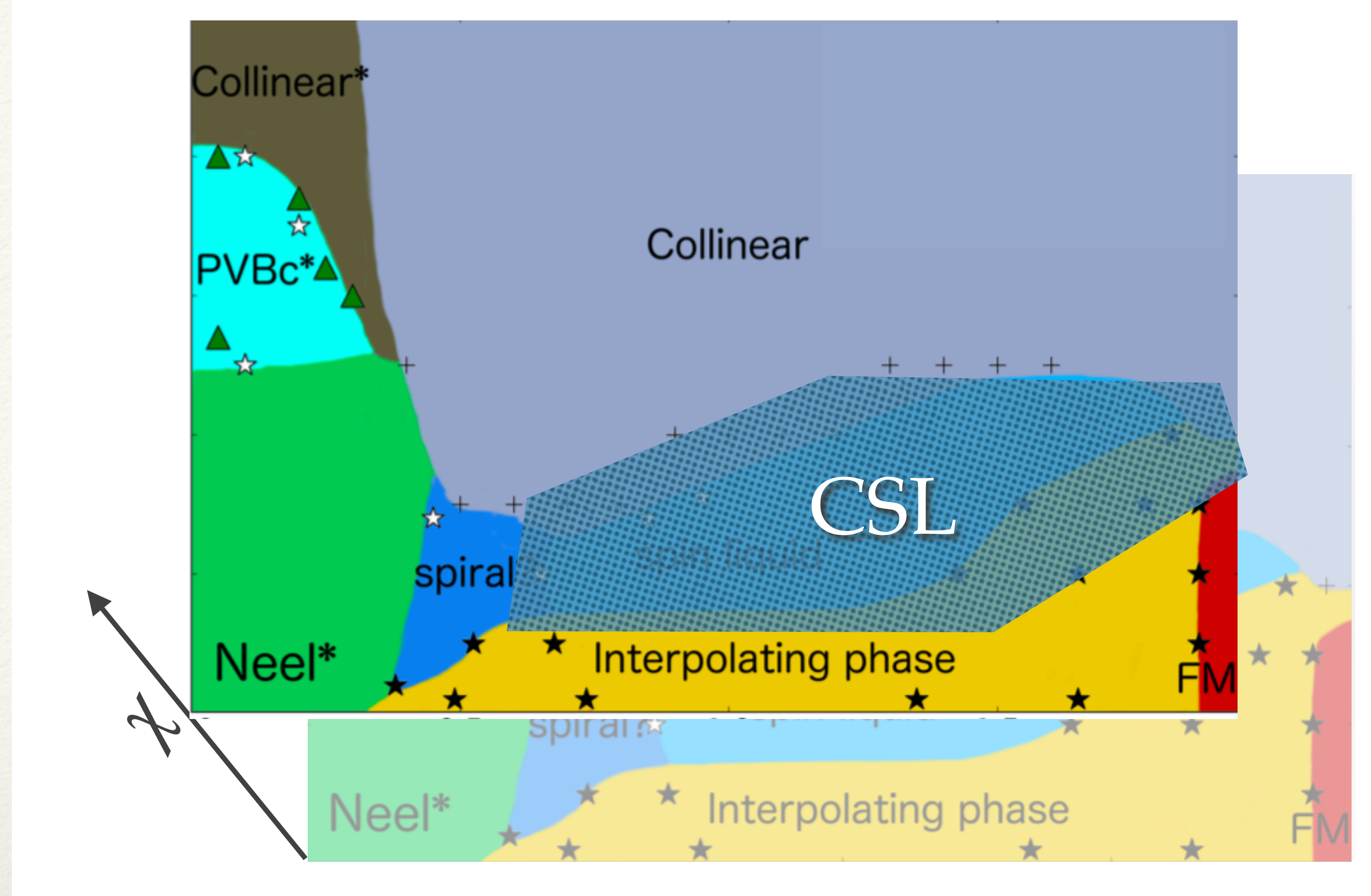
Q: What type of spin liquid(s)?

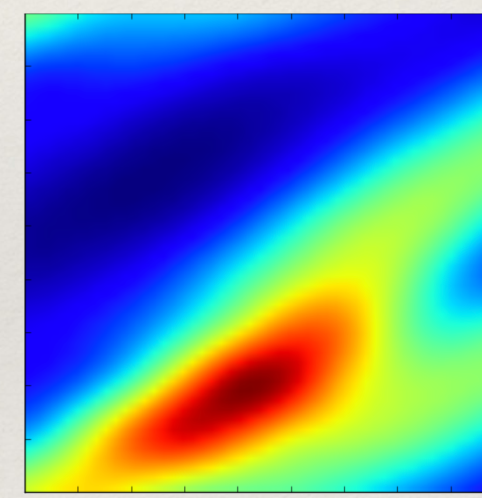
Create 2 anyons

Braid them

$S_{ab} =$ 





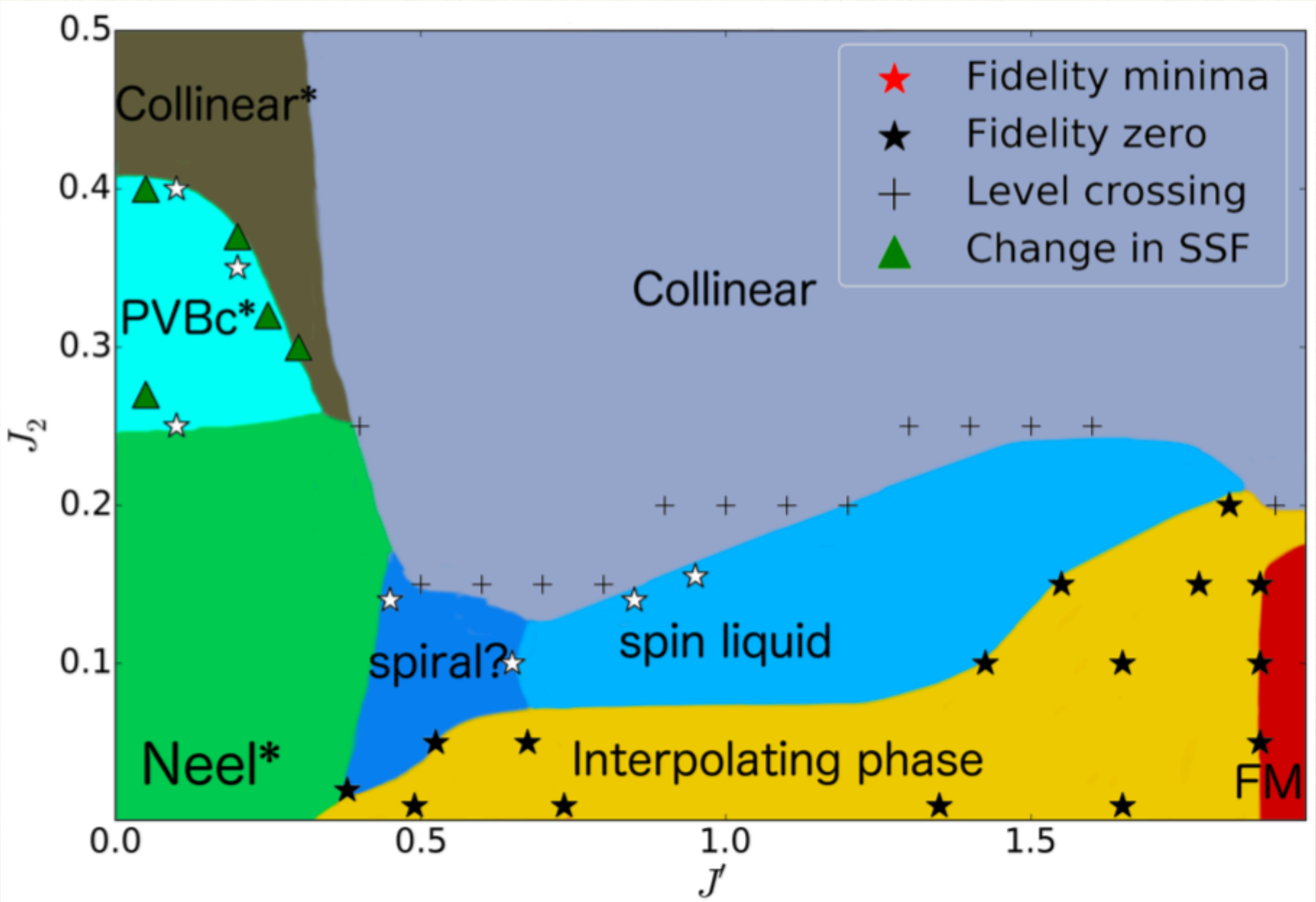


Modular matrix gives topological quantum field theory.

$$S_{24} = \begin{pmatrix} 0.74 & 0.74 \\ 0.67 & -0.67 \end{pmatrix} \qquad S_{36} = \begin{pmatrix} 0.77 & 0.6 \\ 0.6 & -0.83 \end{pmatrix} \qquad S_{CSL} = \begin{pmatrix} 0.707 & 0.707 \\ 0.707 & -0.707 \end{pmatrix} \tag{4.2}$$

Q: What type of spin liquid(s)?

There are many spin-liquids.
But they all have no-order.
What makes them different?



$$H = \sum_{\langle i,j \rangle} S_i^a \cdot S_j^a$$

$$S_i^a = \frac{1}{2} f_i^\dagger \sigma_a f_i$$

$$H = \sum_{\langle i,j \rangle} \frac{1}{2} f_i^\dagger \sigma_a f_i f_j^\dagger \sigma_b f_j$$

(constrain g.s. to one electron per site)

mean field

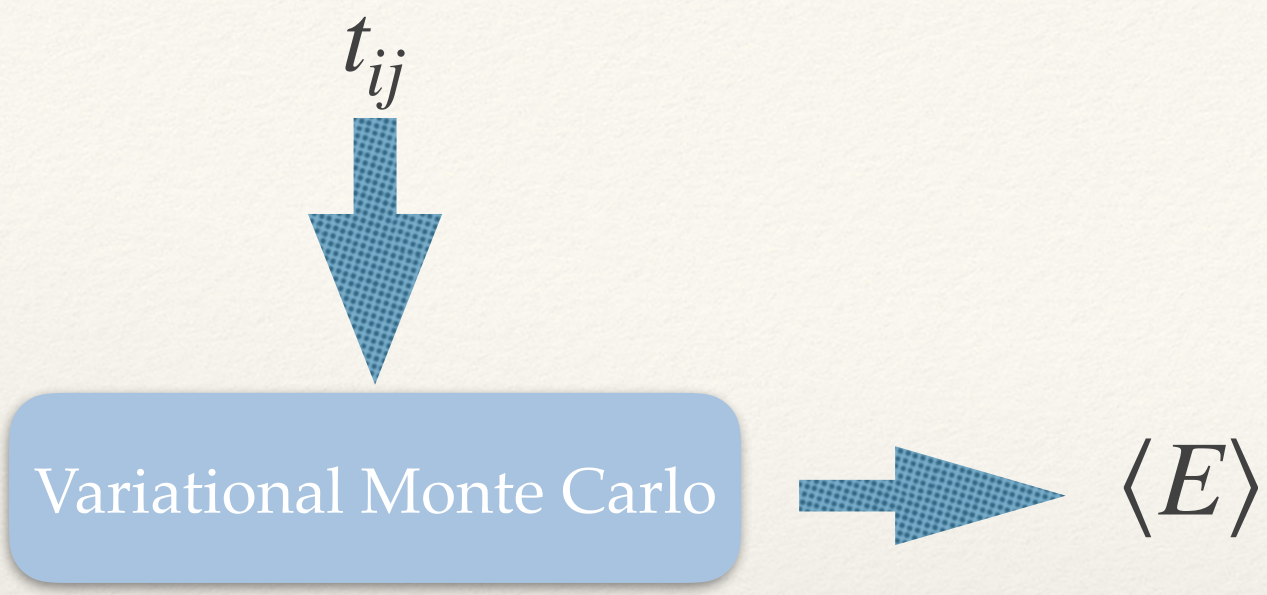
$$H = \sum_{ij} t_{ij} f_i^\dagger f_j$$

(constrain g.s. to one electron per site)

The t_{ij} determine the type of spin-liquid.

How should we determine the t_{ij} ?

How should we determine the t_{ij} ?



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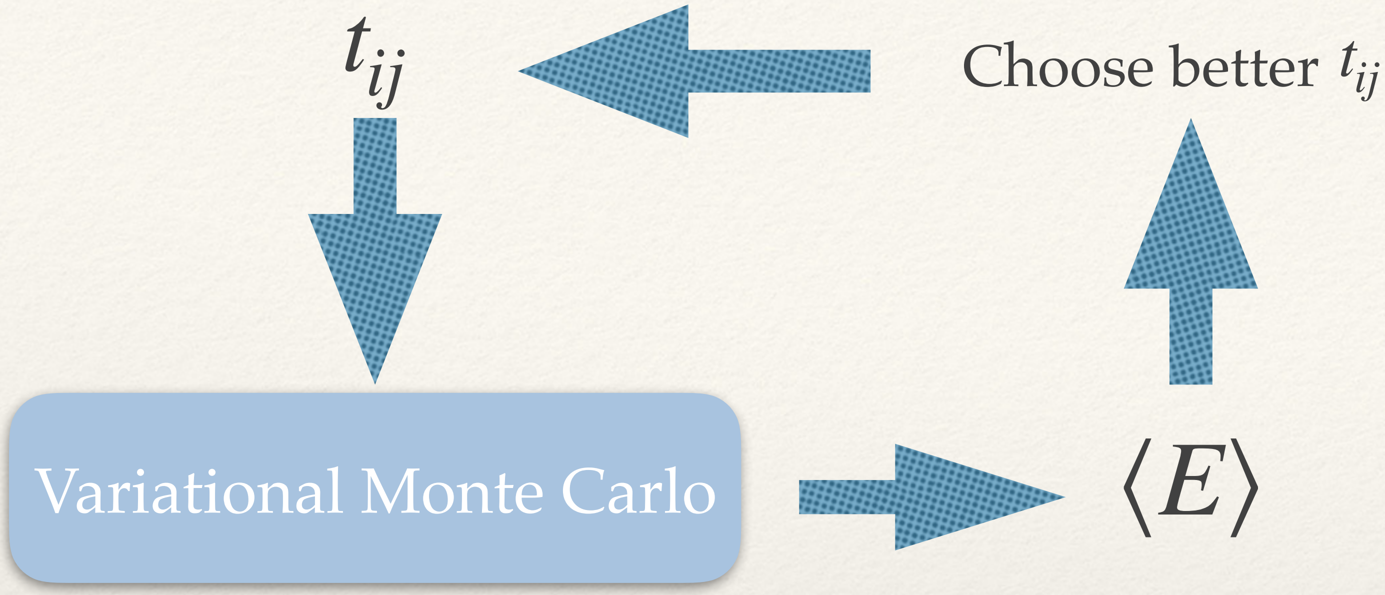
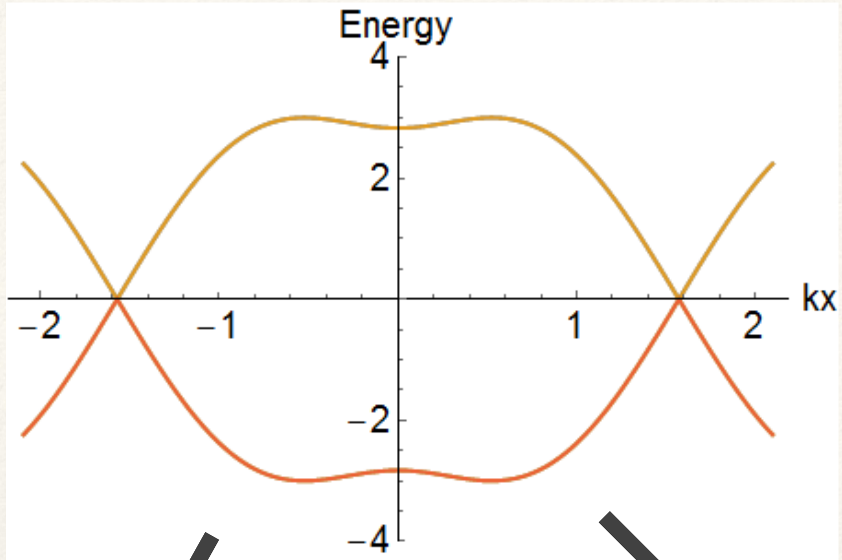


What is the band structure that wins?

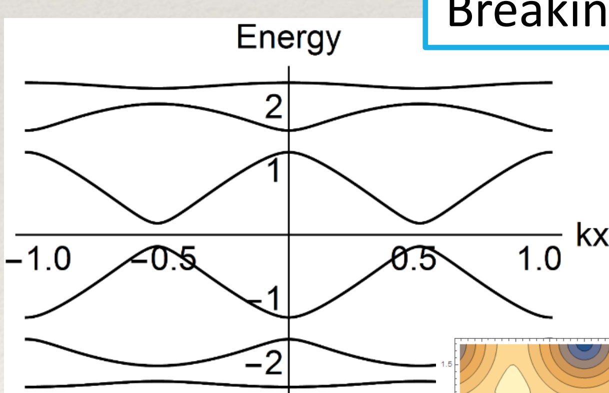


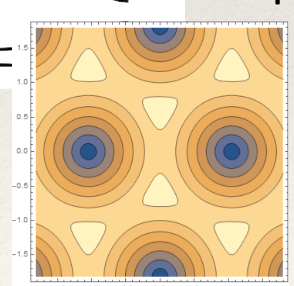
Single spinon dispersion
Nearest neighbor hopping only
No on-site potentials
Dirac cones at Γ point (6-fold symmetry)
Expected to be unstable to gapped Z_2 spin liquid

All competitive for triangle

PSG \`A′ and \`B′ competitive for stuffed honeycomb.

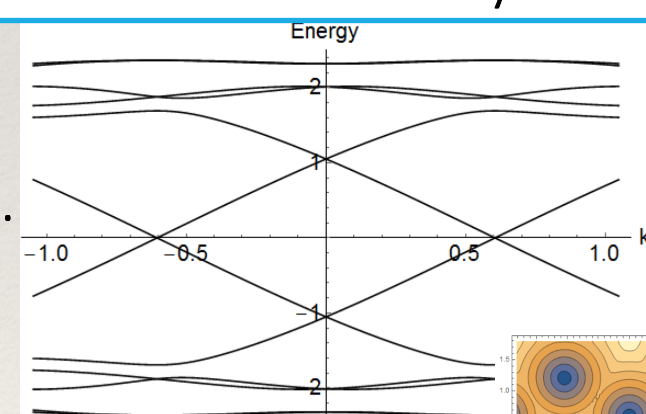
Breaking triangular lattice symmetry down to stuffed honeycomb symmetry

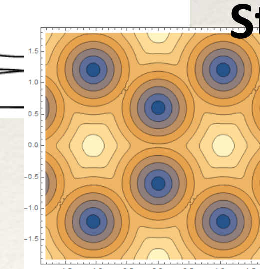




PSG "A"

2^{nd} neighbor hopping ok
Onsite potentials ok
Dirac cones at Γ, 6-fold sym.
Gapped Z_2 spin liquid





PSG "B"

2^{nd} neighbor hopping ok
Onsite potentials ok
Dirac cones at K, K', 3-fold sym.
A Z_2 Dirac spin liquid
Stable to perturbations

Conclusion

History (Summarized)

Lodestone (ferromagnet)

Anti-ferromagnet

Ferri-magnet

Paramagnet

Spin-liquid

Chiral Spin Liquid

The stuffed honeycomb's phase diagram simultaneously encompass years of magnetism history.