Solving the sign problem for a class of frustrated antiferromagnets

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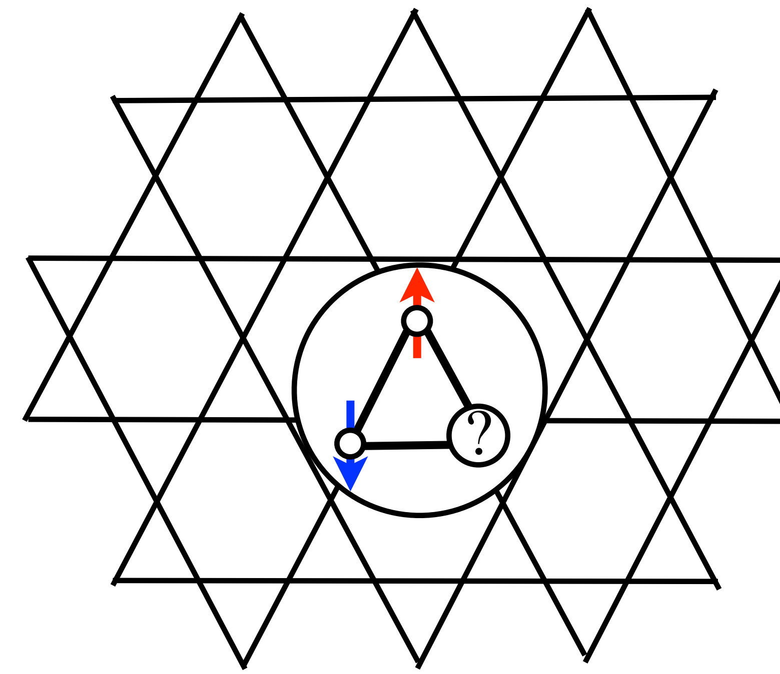
UNIVERSITÉ TOULOUSE III PAUL SABATIER

Université de Toulouse

Workshop SIGN2017
Seattle, March 2017

Motivations : frustrated magnets

- Frustration destabilises « simple » orders such as antiferromagnetism



kagome antiferromagnet

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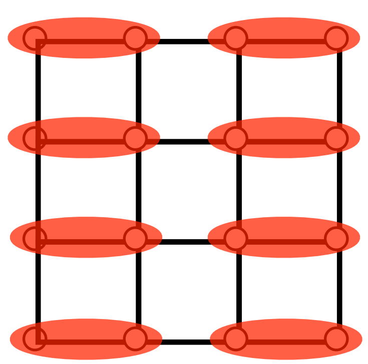
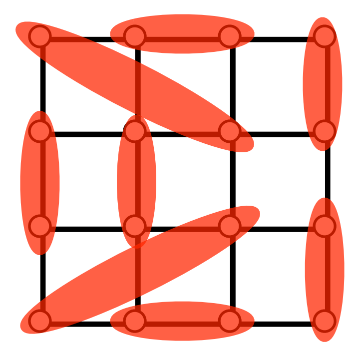
- Condensed matter theory motivations :

  Understand (ground-state) properties in presence of frustration and strong quantum fluctuations

  New resulting non-magnetic states of matter

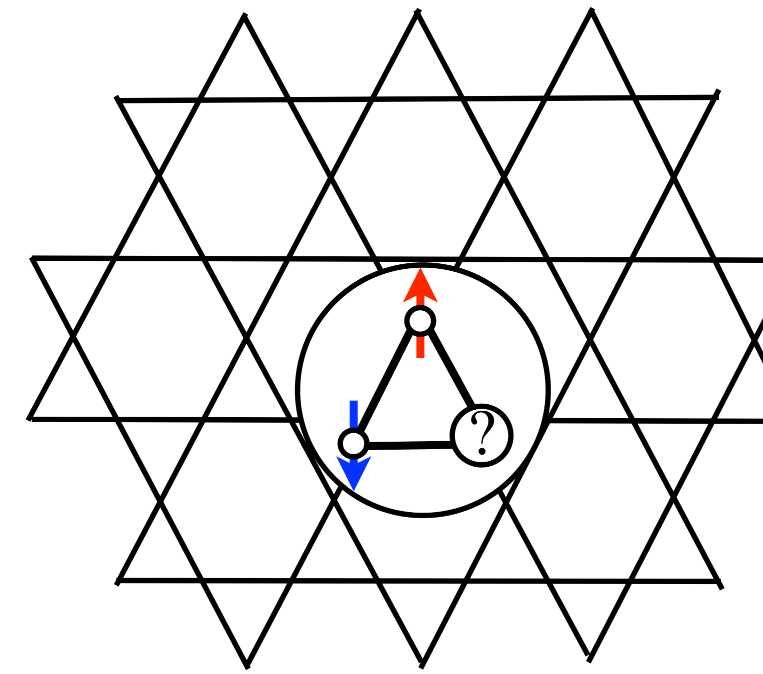


Valence bond crystals



Spin liquids

 $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$



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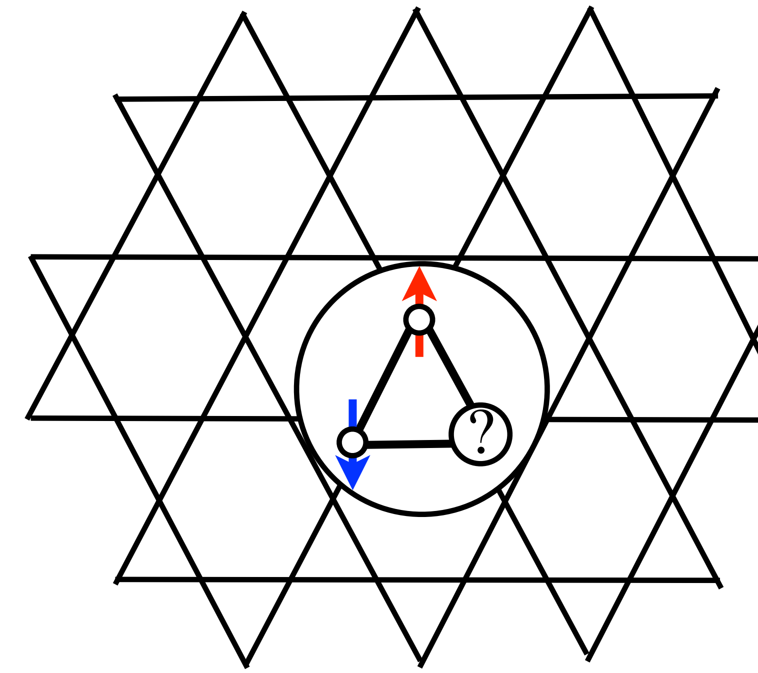
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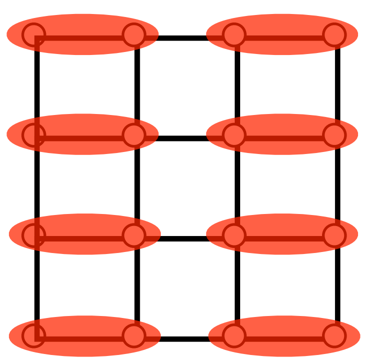
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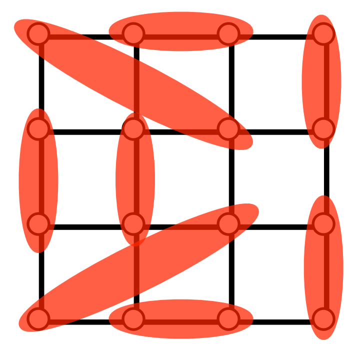
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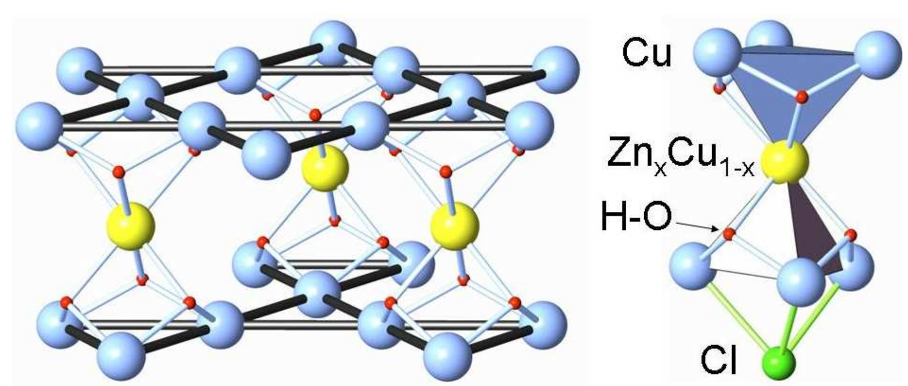
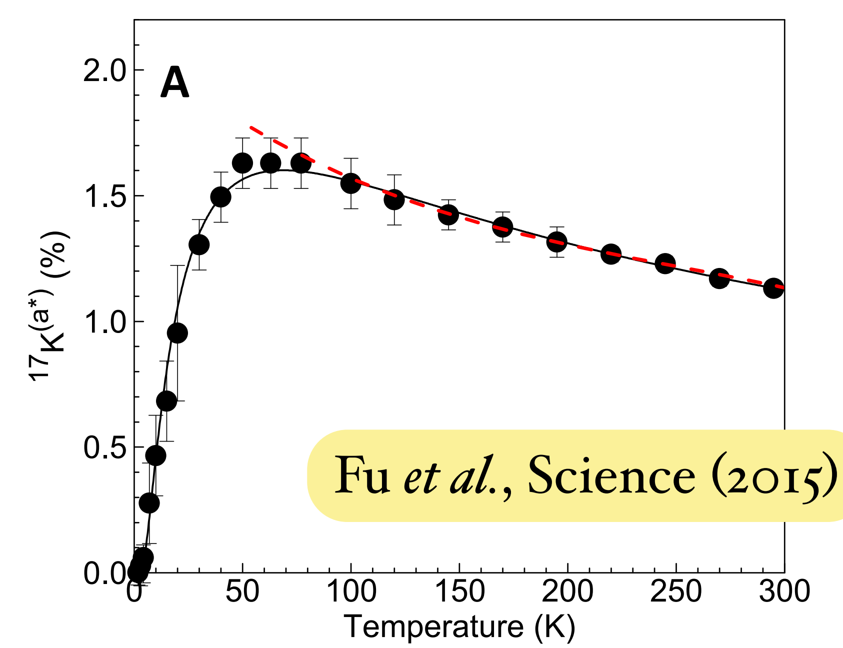
- Condensed matter experimental motivations:


Herbertsmithite



$ZnCu_3(OH)_6Cl_2$



• Experiments often start with thermodynamics : finite-temperature methods more than welcome

QMC, frustration & sign problem

Quantum Monte Carlo & spin systems

- Typical model in mind : spin 1/2 Heisenberg or XXZ model

$$H_{\mathrm{XXZ}} = \sum_{b=\langle i,j \rangle} \underbrace{J_\perp/2(S_i^+ S_j^- + S_i^- S_j^+)}_{H_b^\pm} + \underbrace{J_z S_i^z S_j^z}_{H_b^z}$$

- Heisenberg model (SU(2) symmetry) : $J_\perp = J_z$
- Antiferromagnetism : $J_\perp, J_z > 0$

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Sandvik

$$Z = \sum_i \langle i|\exp(-\beta H)|i\rangle = \sum_i \sum_n \frac{\beta^n}{n!}\langle i|(-H)^n|i\rangle \qquad H = \sum_b H_b$$

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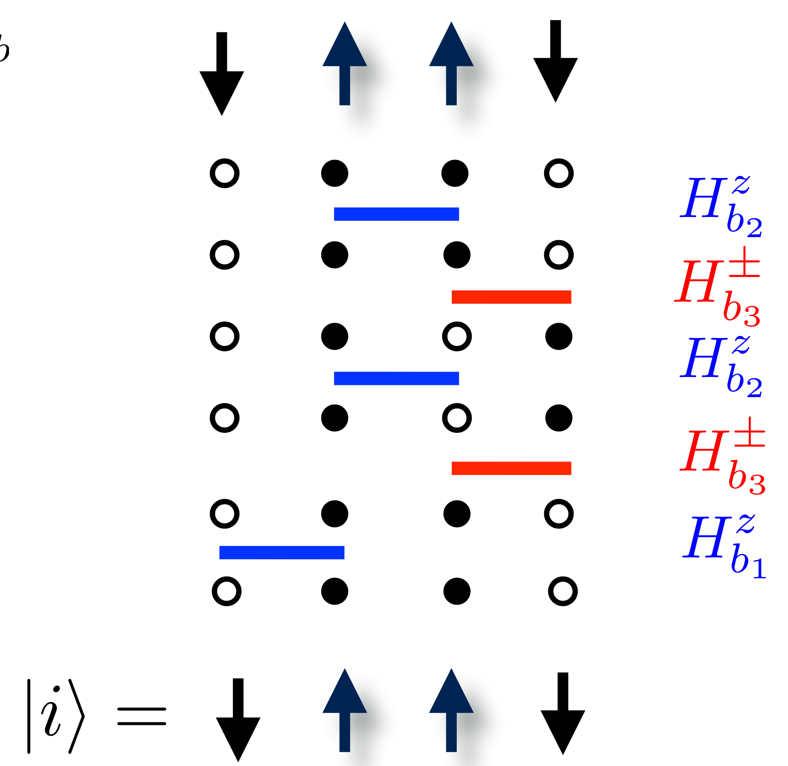

ex : 4 spins 1/2, n=5

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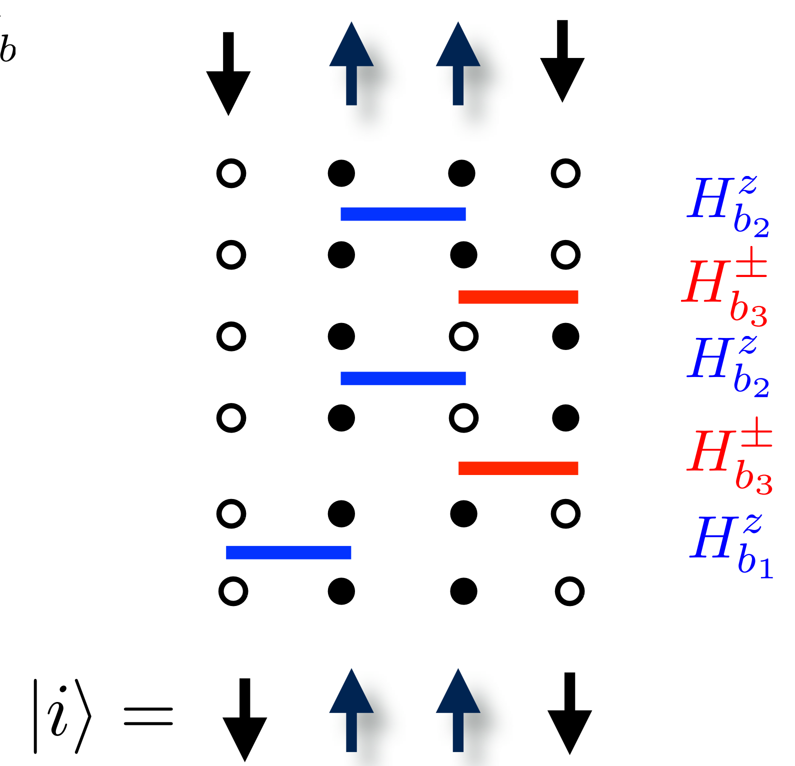

ex : 4 spins 1/2, n=5

- Often use the S^z basis $\{|i\rangle\} = \{S^z\} = \{|\uparrow\downarrow\downarrow\uparrow\dots\rangle, \dots\}$

$H_b^\pm$: off diagonal, carry sign problem

Sign problem in the S^z basis

- Inspect sign of off-diagonal matrix elements (frustration in the diagonal is OK)
  - Heisenberg ferromagnet : $H_b^{\pm} = -\frac{1}{2}(S^+S^- + S^-S^+)$ $\langle \uparrow\downarrow | H_b^{\pm} | \downarrow\uparrow \rangle < 0$ ✓ Sufficient condition

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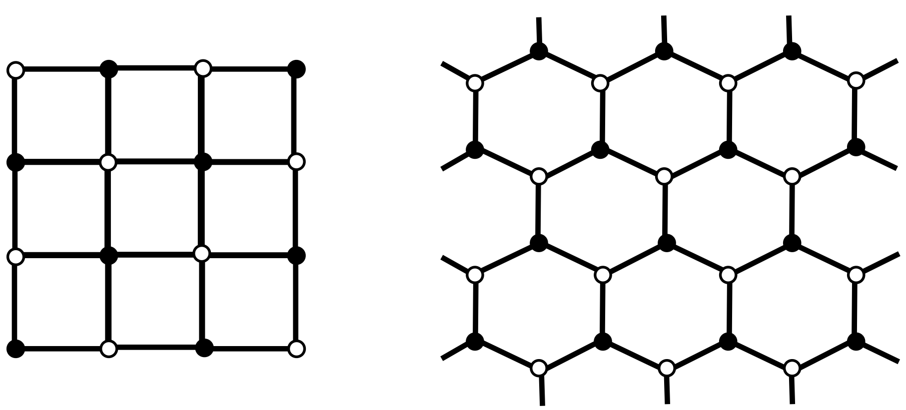
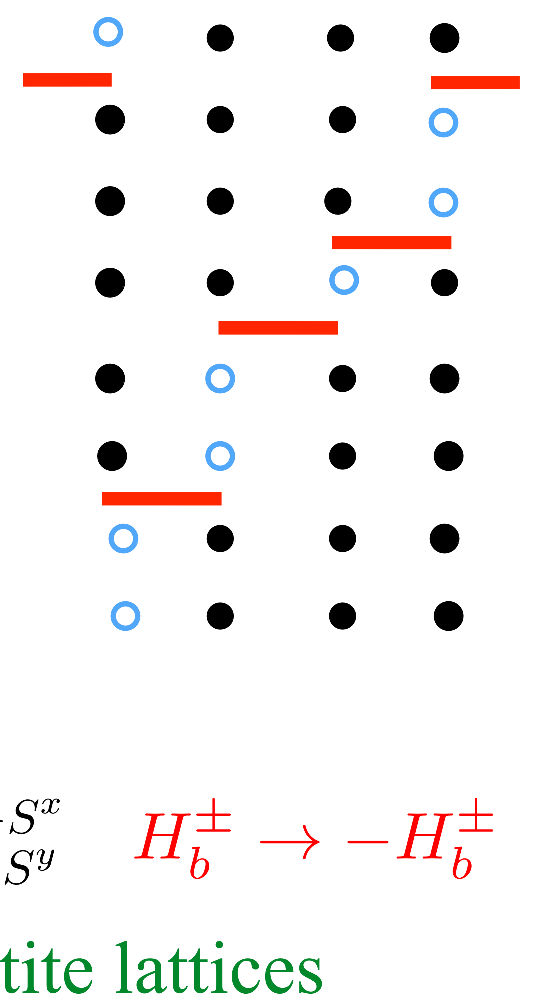
Bipartite lattice: even loops





$H_b^{\pm}$ always come in even numbers

Alternatively, unitary transform on one sublattice: $\begin{array}{l} S^x \to -S^x \\ S^y \to -S^y \end{array}$ $\quad H_b^{\pm} \to -H_b^{\pm}$

QMC possible for AF on bipartite lattices

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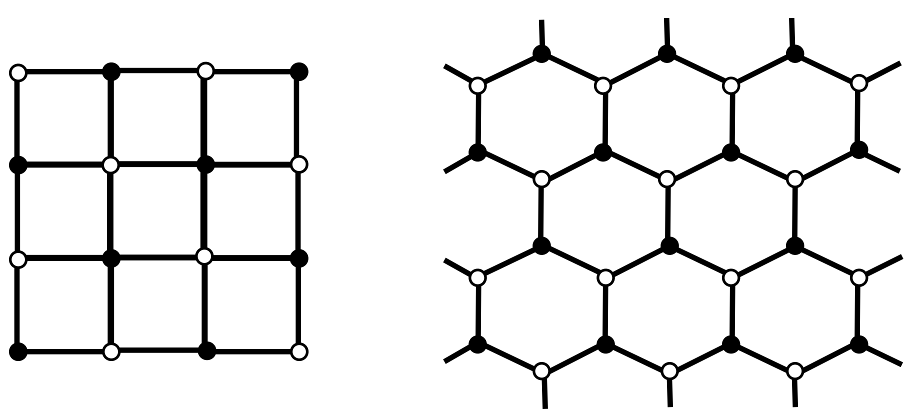

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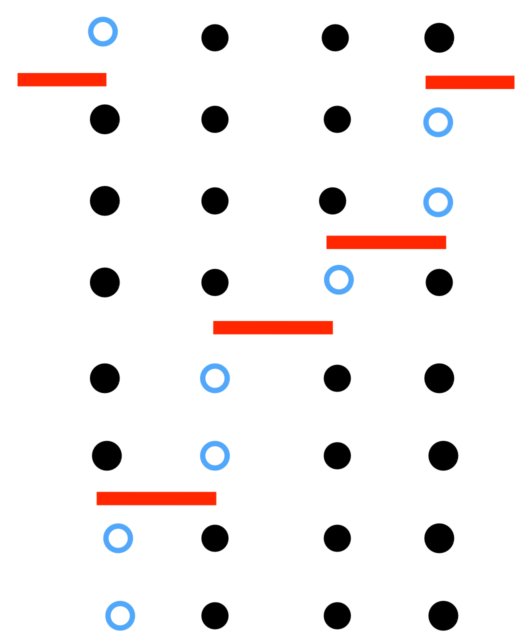

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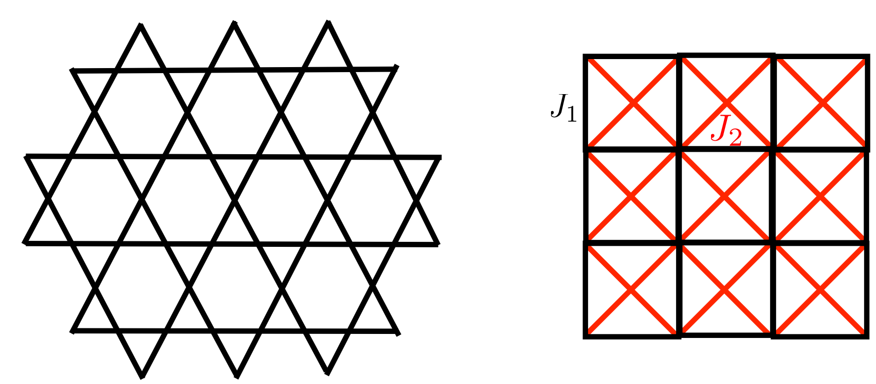
Frustrated lattice: odd loops



Sign problem for AF on frustrated lattices

Sign problem is basis dependent

- This talk : find frustrated models for which a specific change of $\{|i\rangle\}$ solves the sign problem

(a posteriori) Strategy

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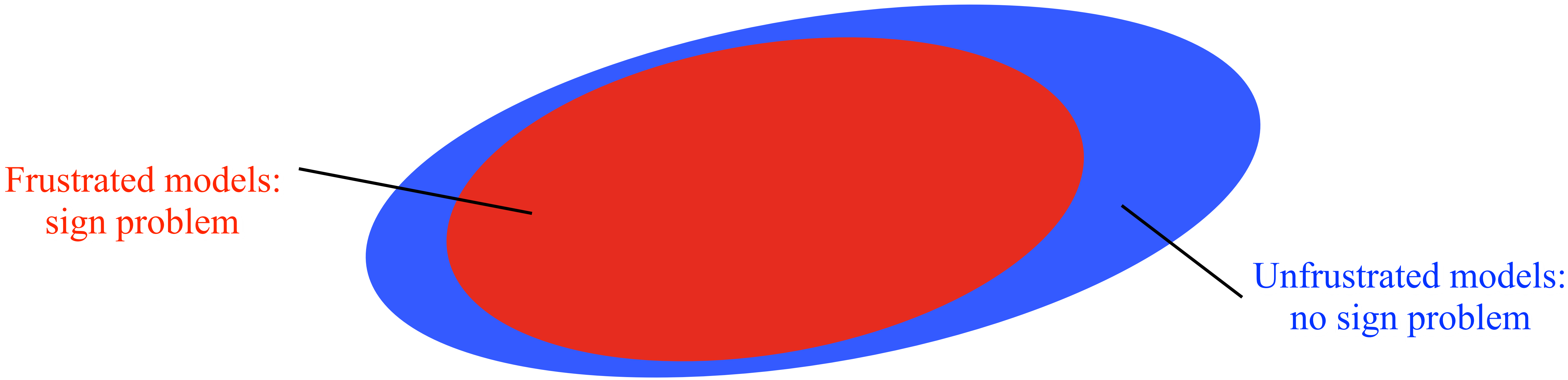

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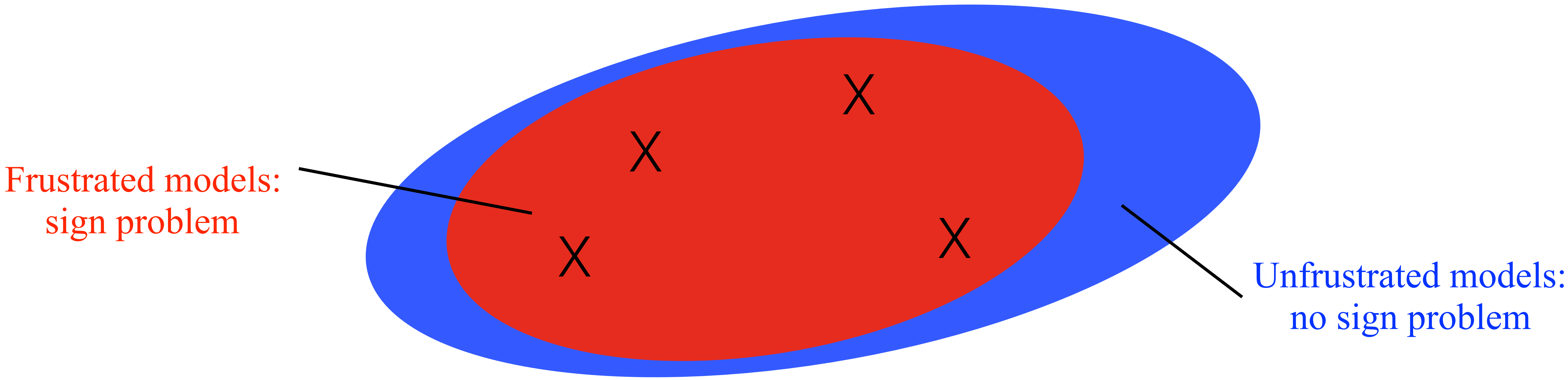
1. Exhibit particular frustrated models with specific symmetry conditions

Here namely : an extensive number of local conserved quantities



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2. Go to the « natural basis » for this symmetry. It solves the sign problem. The model keeps non-trivial.

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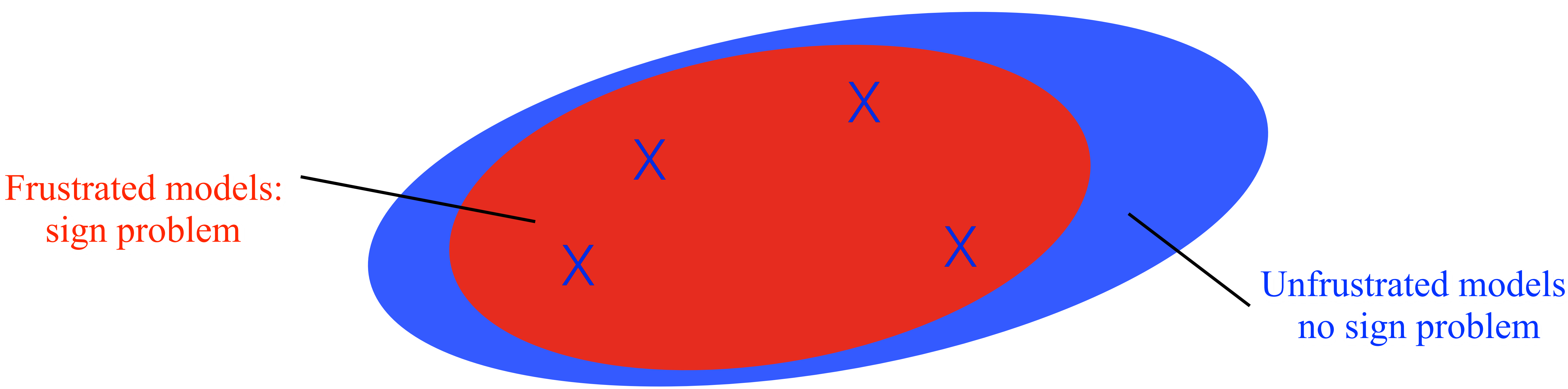

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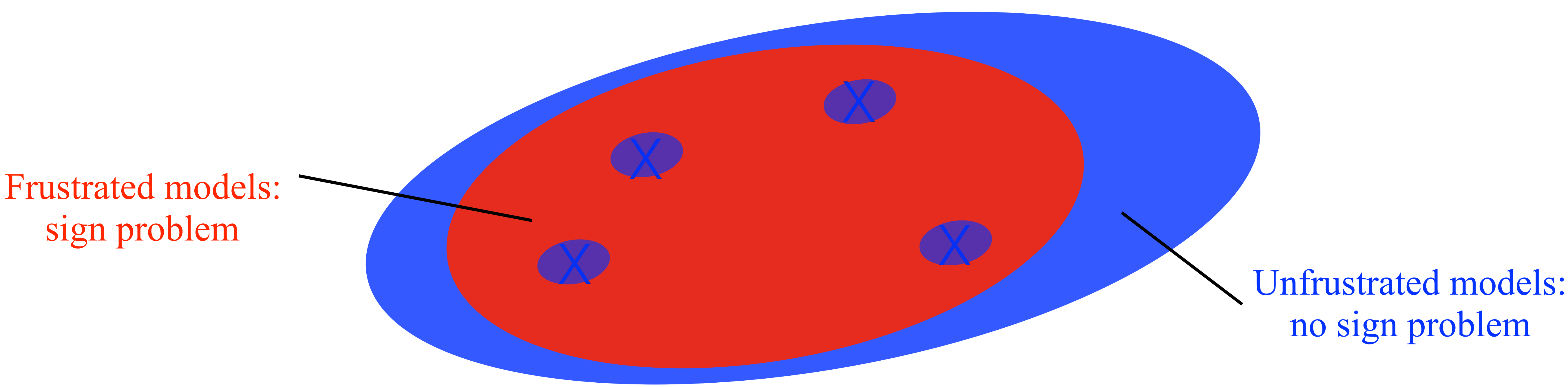
3. Keep this basis. Perturb the symmetric Hamiltonian such that the symmetry is longer present, but the sign problem is still gone

Choose the perturbation according to their off-diagonal contribution in this basis



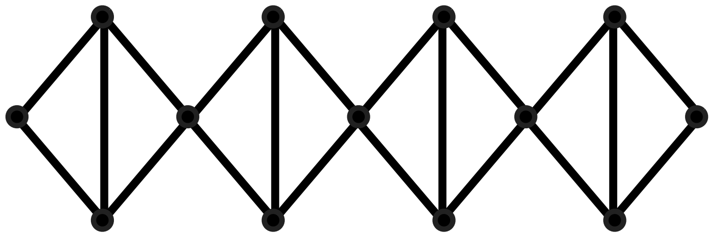
Start with a simple example

PRL **117**, 197203 (2016)

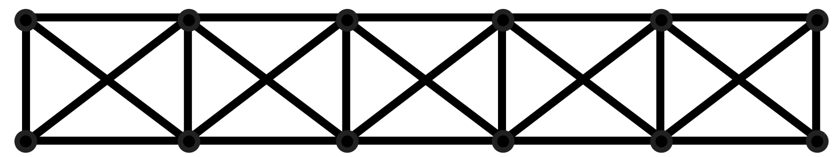
See also Stefan's talk and Honecker *et al.*, PRB (2016)

Solving the sign problem for a class of frustrated AF

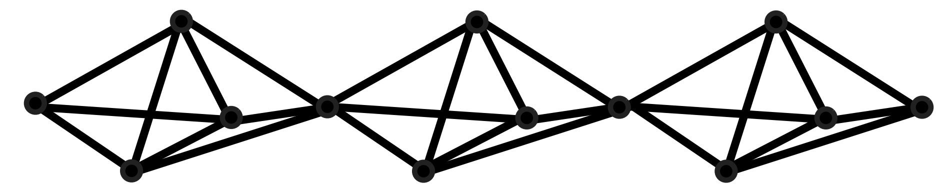
- Sign problem can be solved for the Heisenberg antiferromagnet on these lattices (and others …)



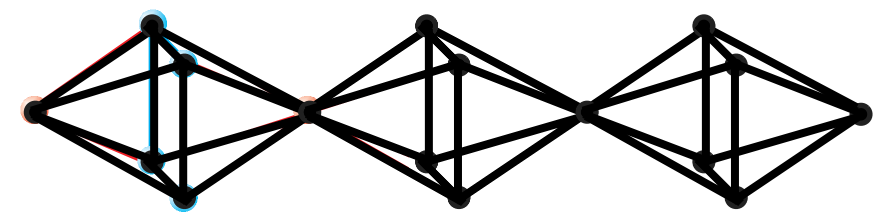
Diamond chain



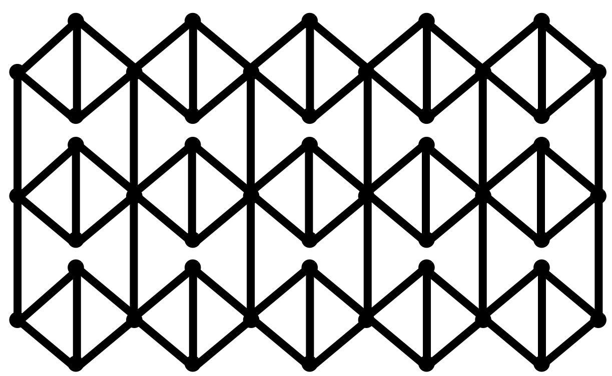
Fully frustrated spin ladder



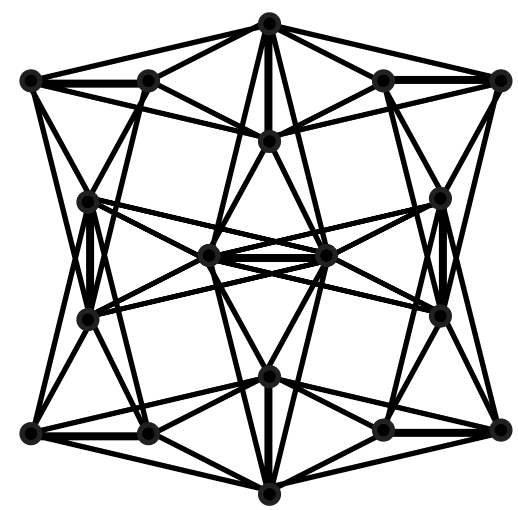
1d pyrochlore



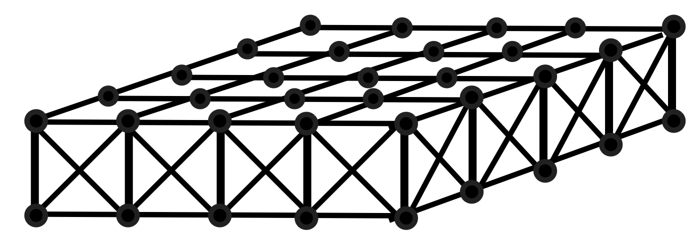
Spin octahedral chain



Coupled diamonds



Extended Shastry-Sutherland



Fully-frustrated bilayer

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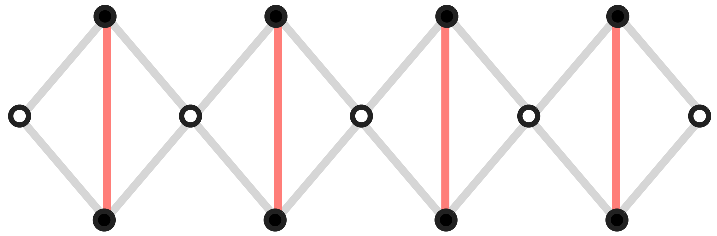

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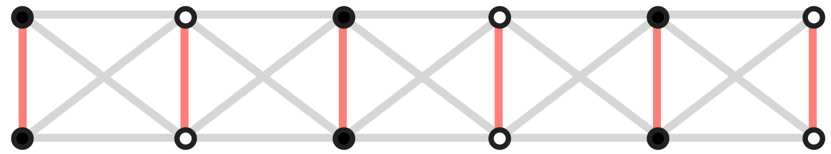

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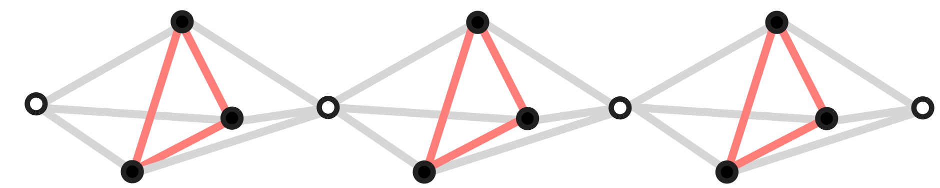

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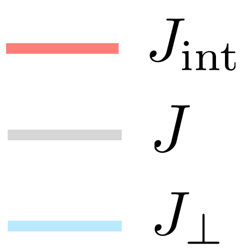

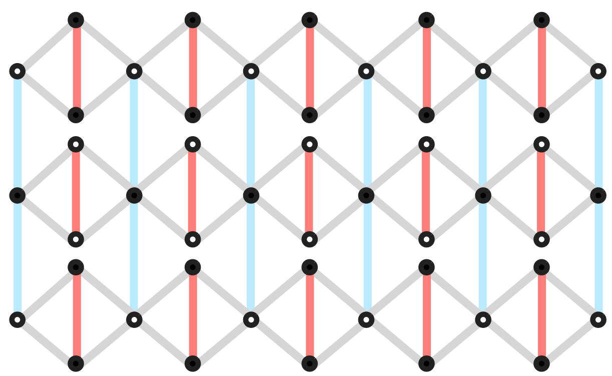

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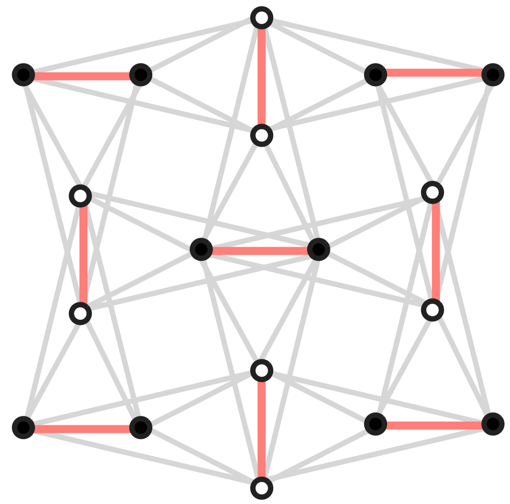

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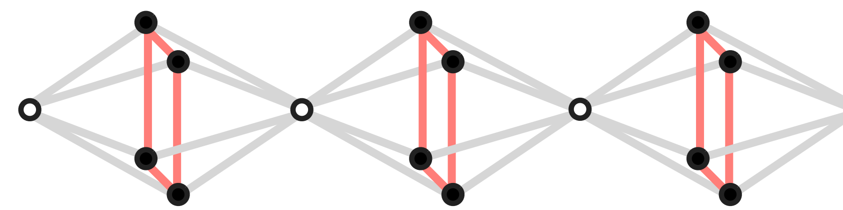
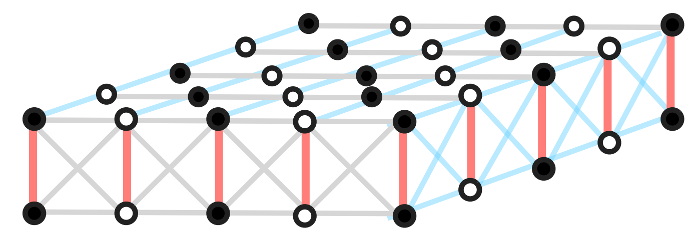
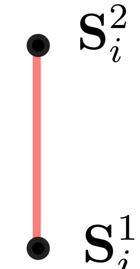


Spin octahedral chain



Fully-frustrated bilayer

- **Key idea :** form the total spin on a red cluster $\mathbf{T}_i = \mathbf{S}_i^1 + \mathbf{S}_i^2$



- Work in the singlet / triplet basis of $\mathbf{T}_i$

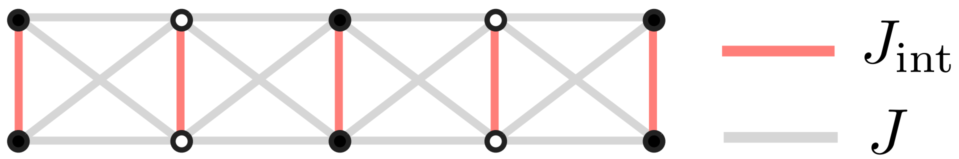
$$T = 0 \qquad |{\color{red}\bullet}\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$|\bullet\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$T = 1$$

$$|\blacktriangle\rangle = |\uparrow\uparrow\rangle \quad |\blacktriangledown\rangle = |\downarrow\downarrow\rangle$$

Showing the sign-freeness



- AF Heisenberg model for the fully-frustrated ladder

$$H = J_{\text{int}} \sum_i (\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}) + J \sum_i (\mathbf{S}_{i,1} + \mathbf{S}_{i,2}).(\mathbf{S}_{i+1,1} + \mathbf{S}_{i+1,2})$$

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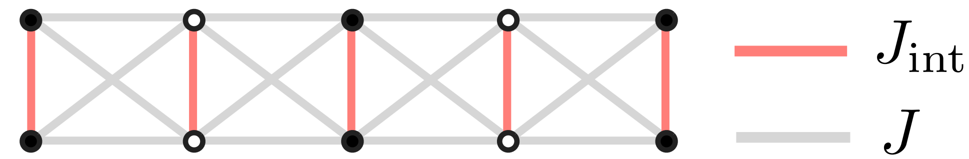

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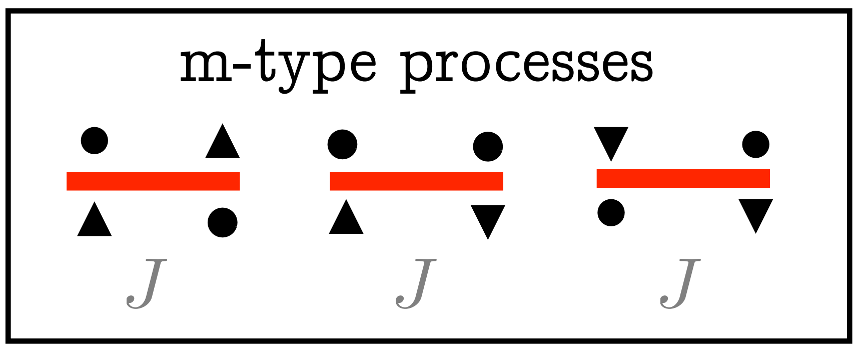
- Inspect off-diagonal matrix elements in the new basis

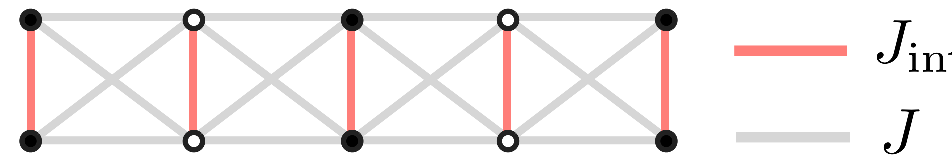
$$\langle \blacktriangle \bullet |H| \bullet \blacktriangle \rangle = \langle \blacktriangledown \bullet |H| \bullet \blacktriangledown \rangle = \langle \blacktriangle \blacktriangledown |H| \bullet \bullet \rangle = J > 0$$

Sign problem?



Conservation of m=T^z
quantum number

Showing the sign-freeness



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$$H = {\color{red}J_{\mathrm{int}}} \sum_i (\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}) + {\color{gray}J} \sum_i (\mathbf{S}_{i,1} + \mathbf{S}_{i,2}).(\mathbf{S}_{i+1,1} + \mathbf{S}_{i+1,2})$$

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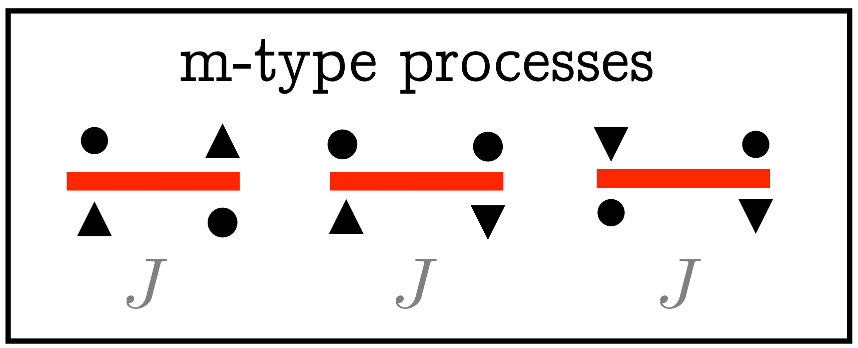
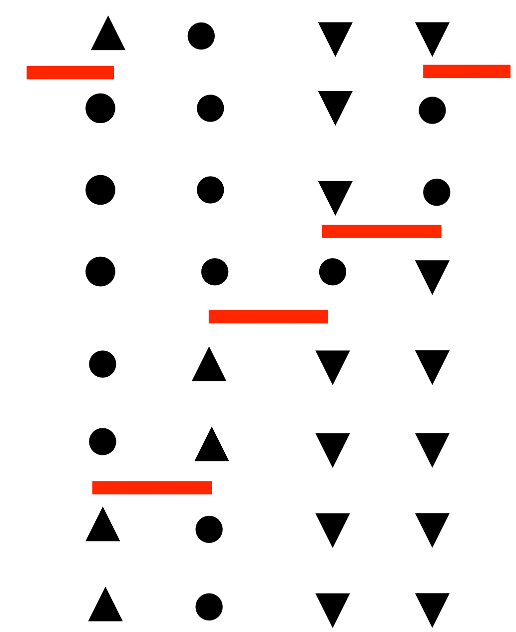
$$\langle \blacktriangle \bullet | H | \bullet \blacktriangle \rangle = \langle \blacktriangledown \bullet | H | \bullet \blacktriangledown \rangle = \langle \blacktriangle \blacktriangledown | H | \bullet \bullet \rangle = {\color{gray}J} > 0$$

Sign problem?



Conservation of m=T^z quantum number

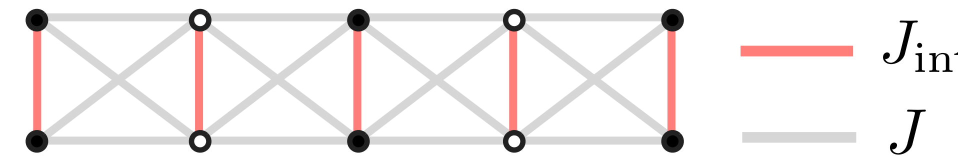


- On a bipartite lattice (even loops): always even number of J terms

No sign problem in the new basis!

Showing the sign-freeness

- AF Heisenberg model for the fully-frustrated ladder



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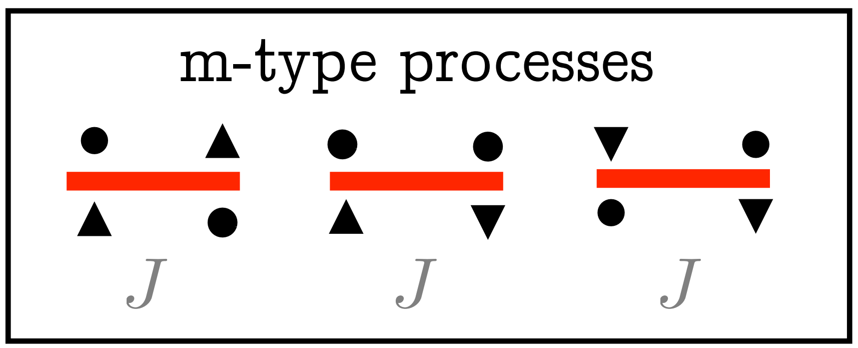

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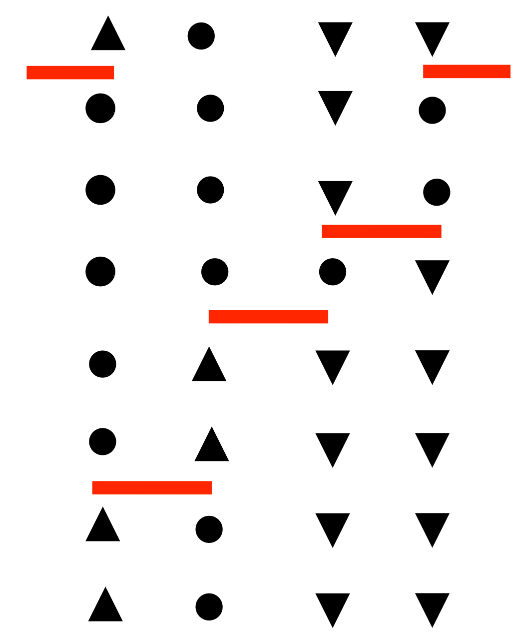


- On a bipartite lattice (even loops): always even number of J terms

No sign problem in the new basis!

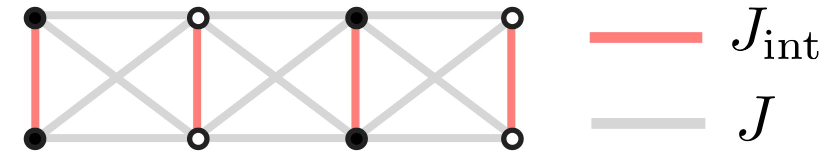
- Now (almost) standard QMC methods can be applied

Worm algorithm for m-type particles

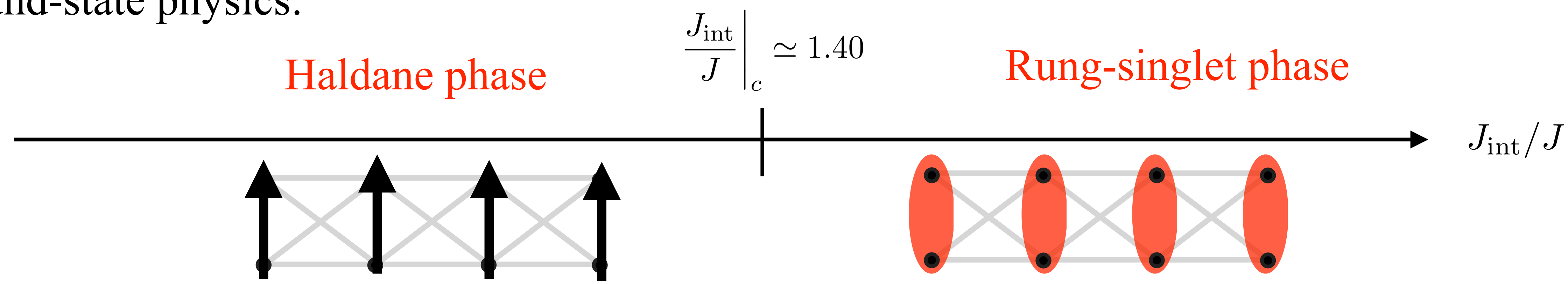
Local update that swaps T=0 and T=1

Parallel tempering for low temperatures

Thermodynamics of FF ladder



- Ground-state physics:



- Thermodynamics : magnetic susceptibility

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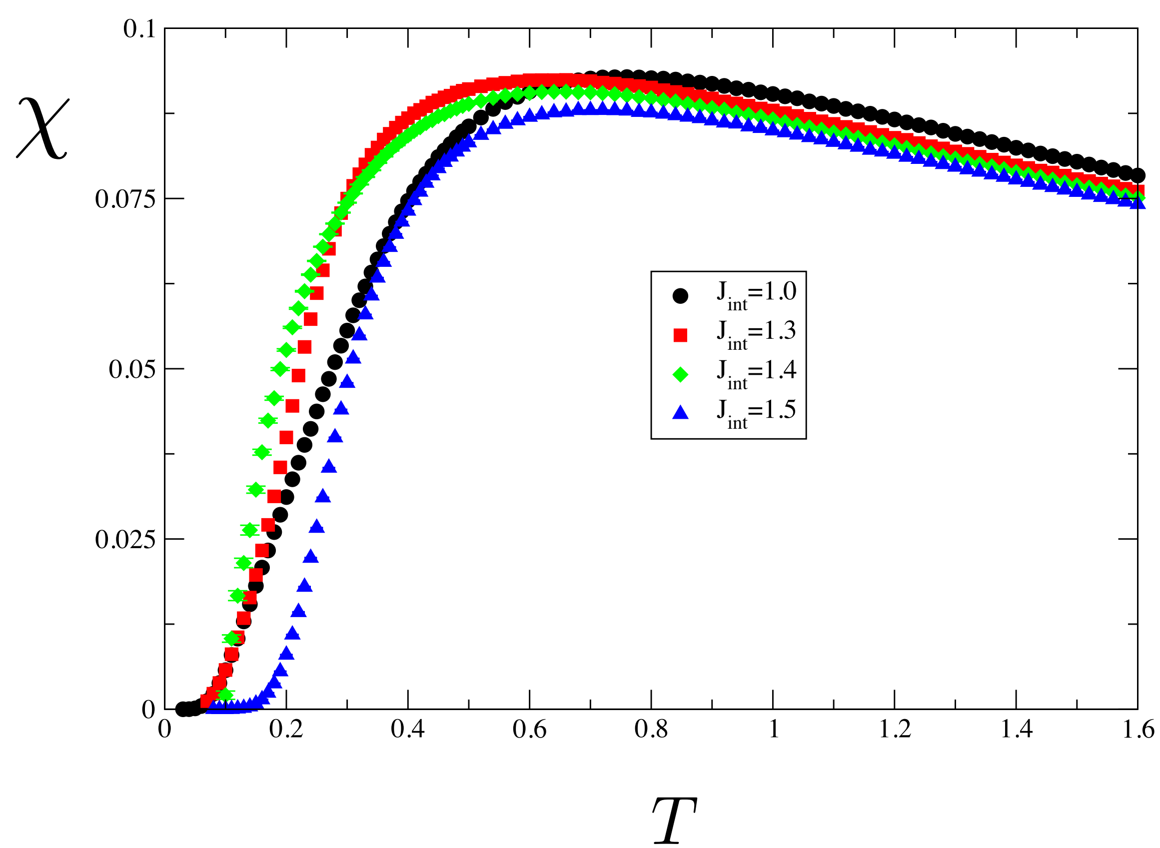

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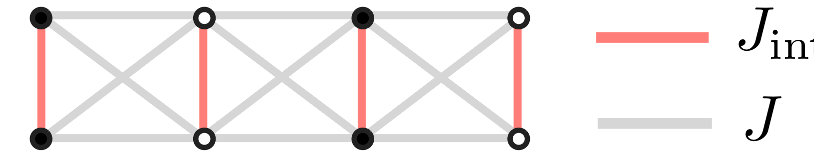

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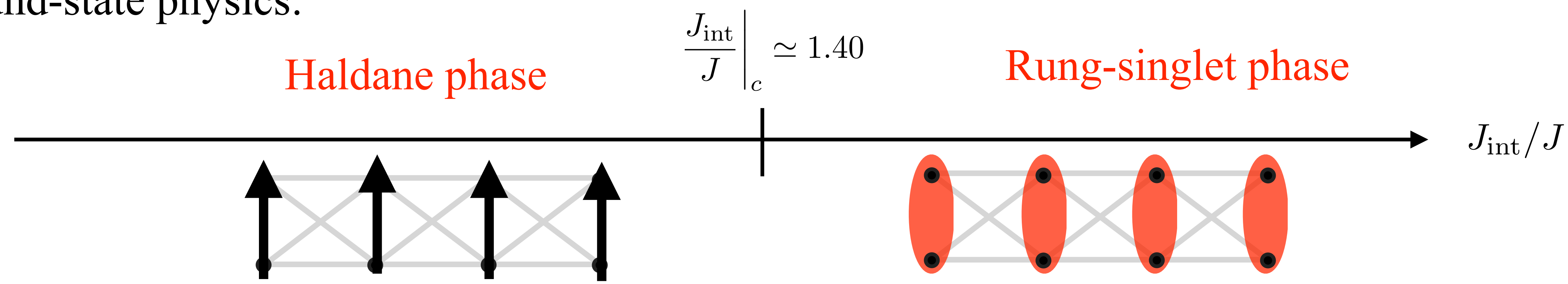

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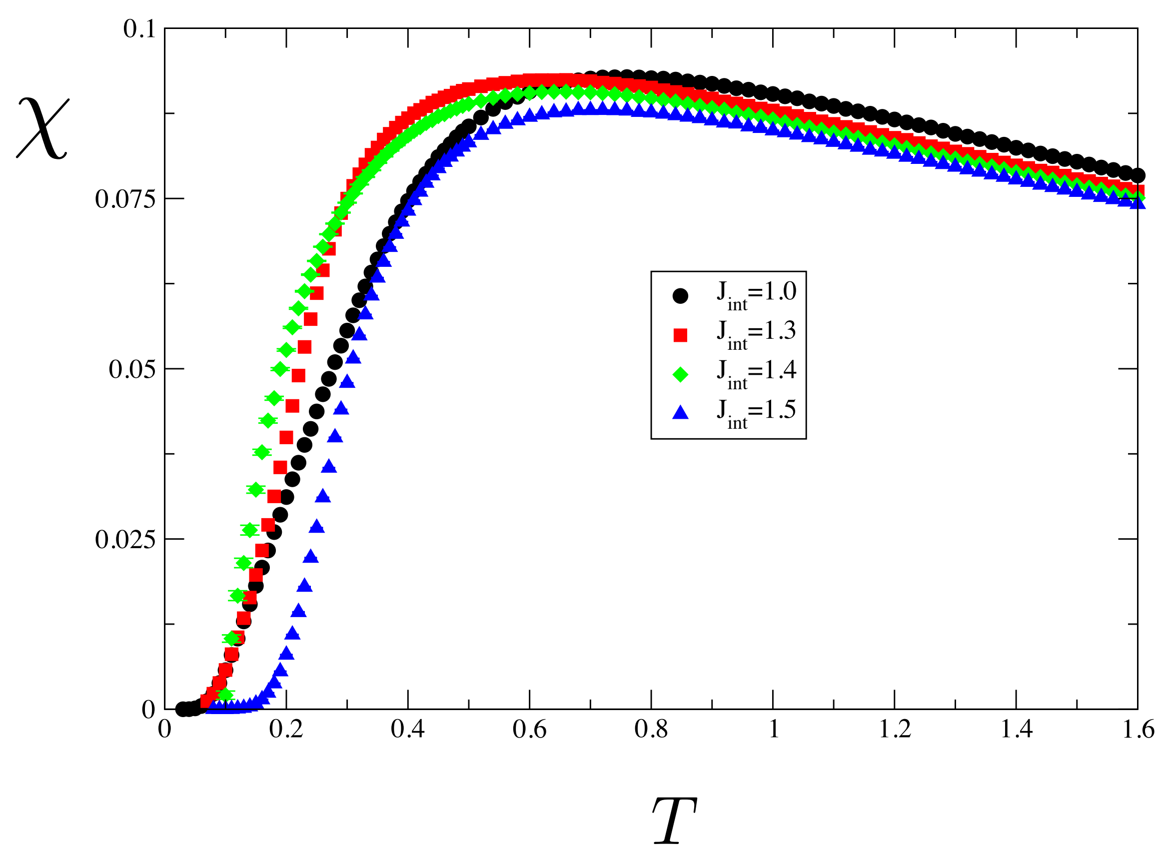
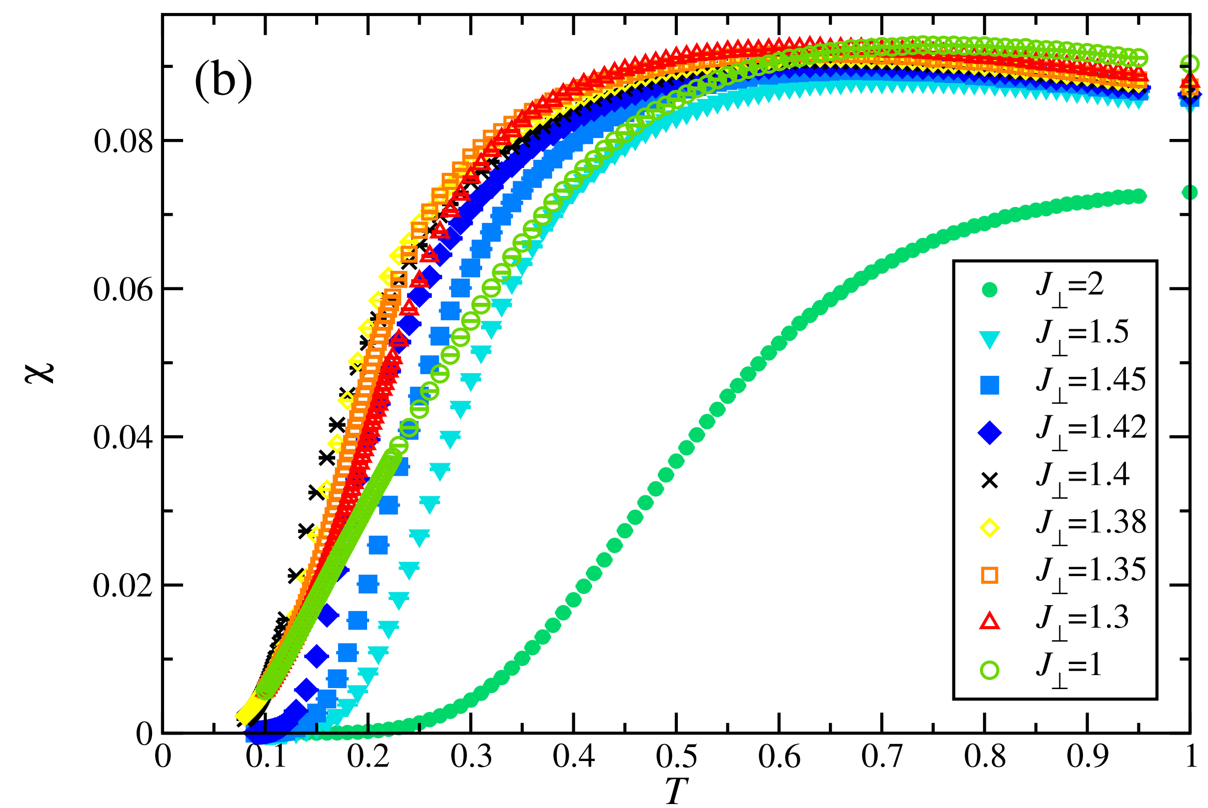
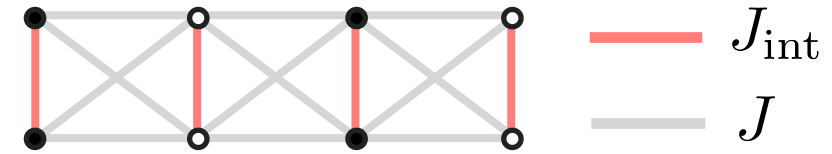
Honecker *et al.*, PRB (2016)

PRL **117**, 197203 (2016)





Thermodynamics of FF ladder



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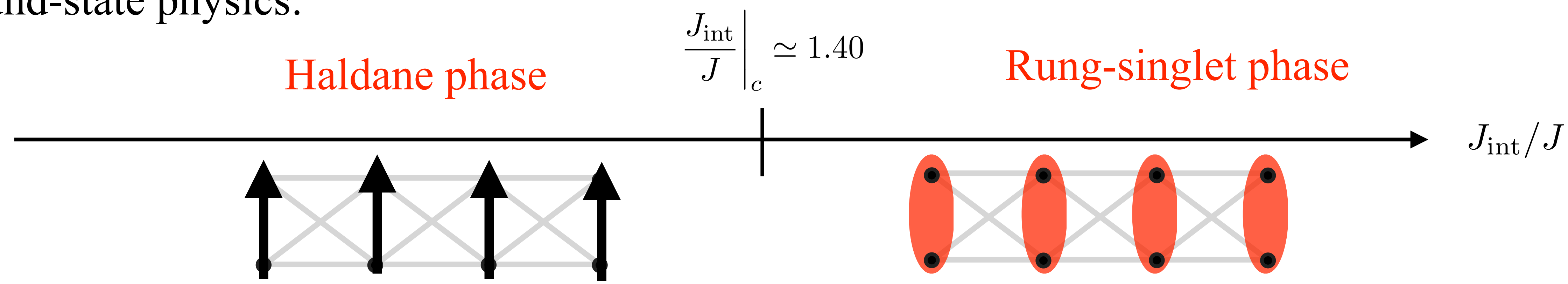
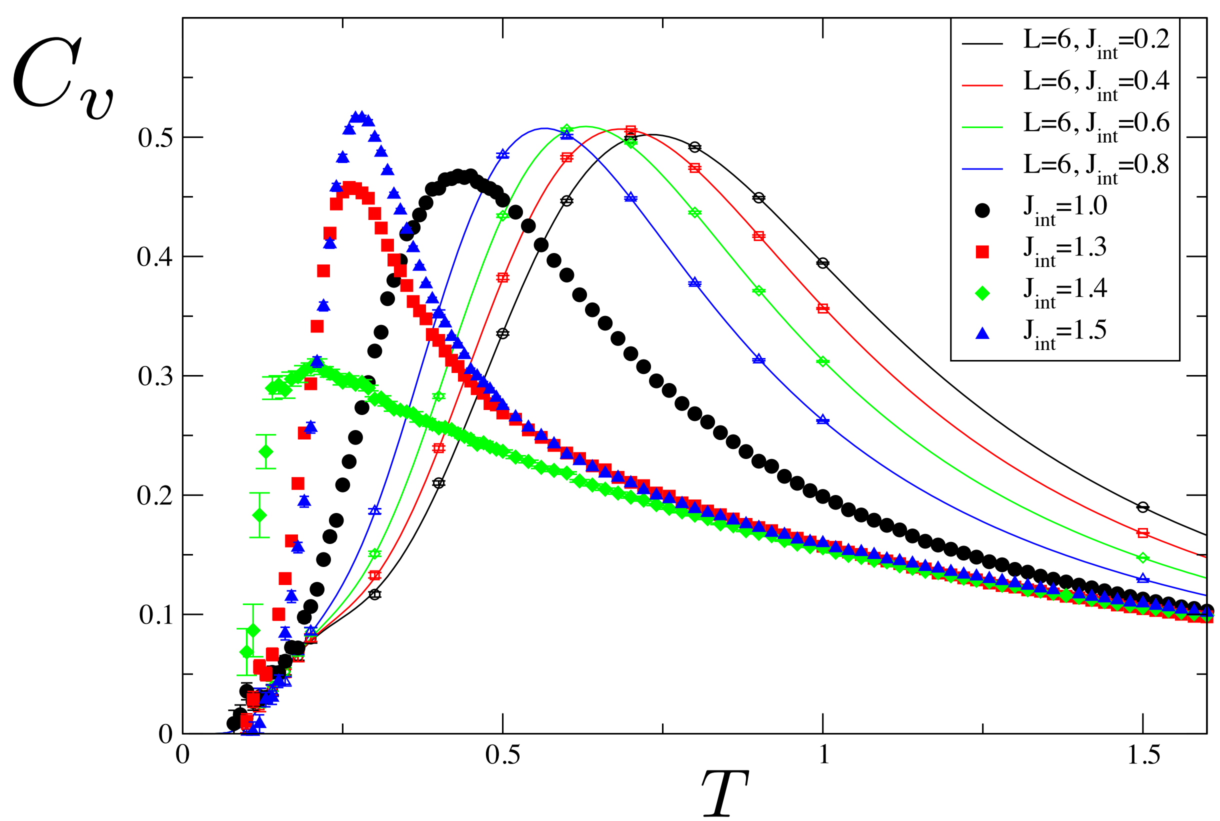
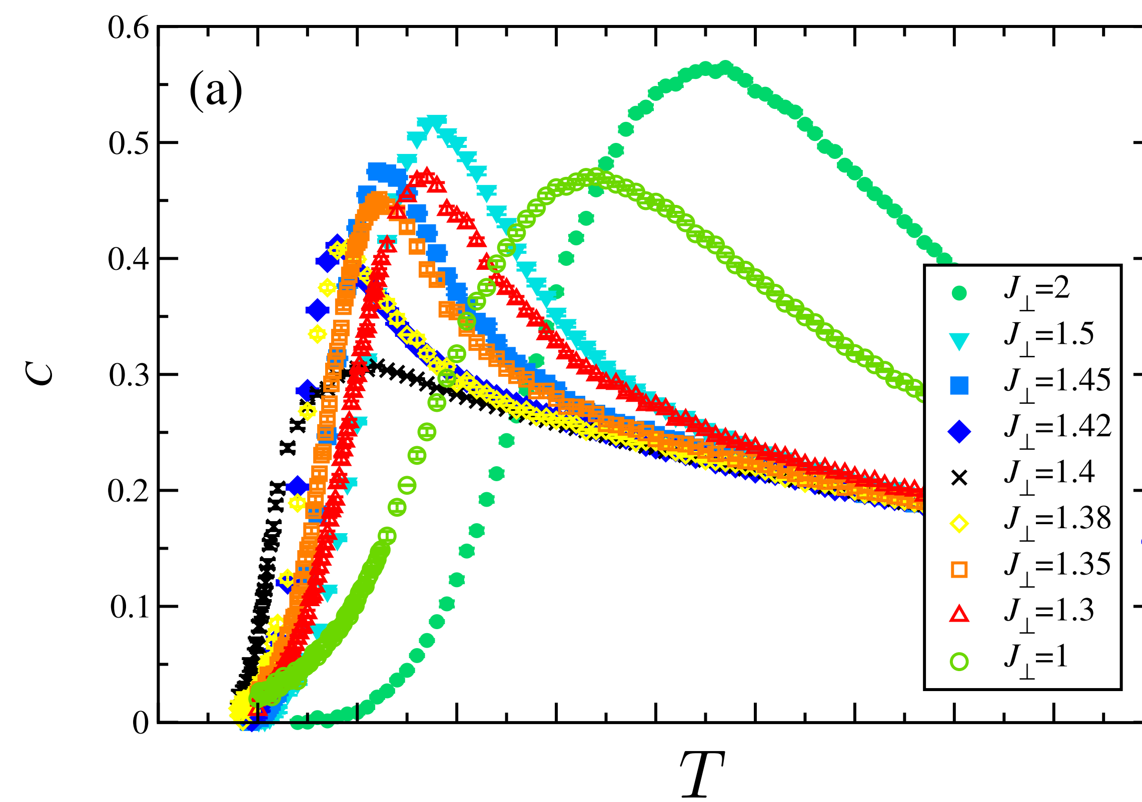


- Thermodynamics : specific heat

PRL **117**, 197203 (2016)

Honecker *et al.*, PRB (2016)





- Sharp narrowing peak approaching and sudden drop at the quantum phase transition

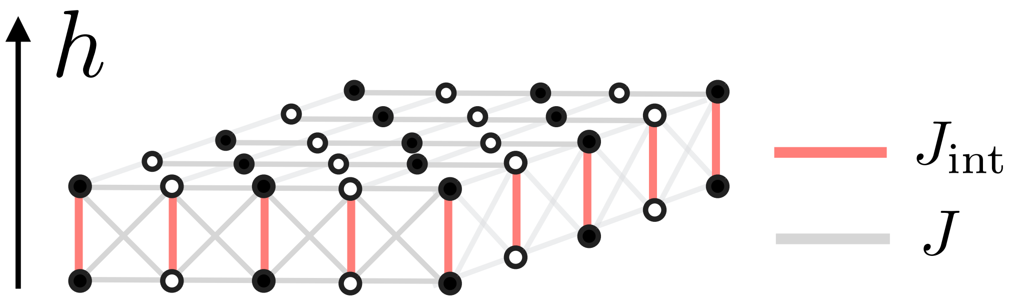
- Can be understood from accumulation of n-triplon states above the gap

Honecker *et al.*, PRB (2016)

Field-induced transition in the FF bilayer

- The method also works in a field (z direction) : study of magnetization curves, plateaus …

- Fully-frustrated bilayer in a field



- At large J_{int}, rung-singlets dominate but large enough field brings back the polarized triplets

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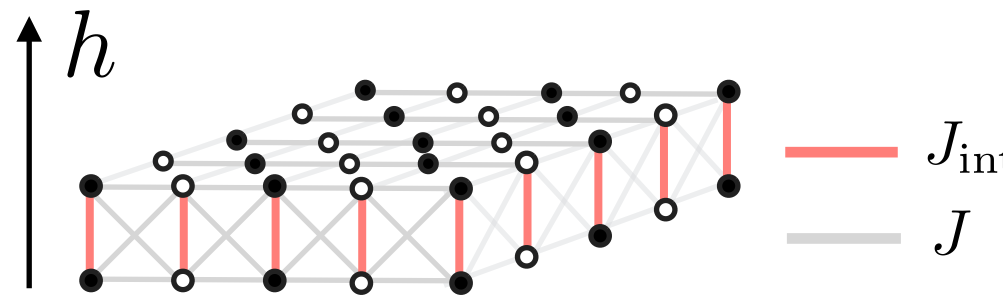
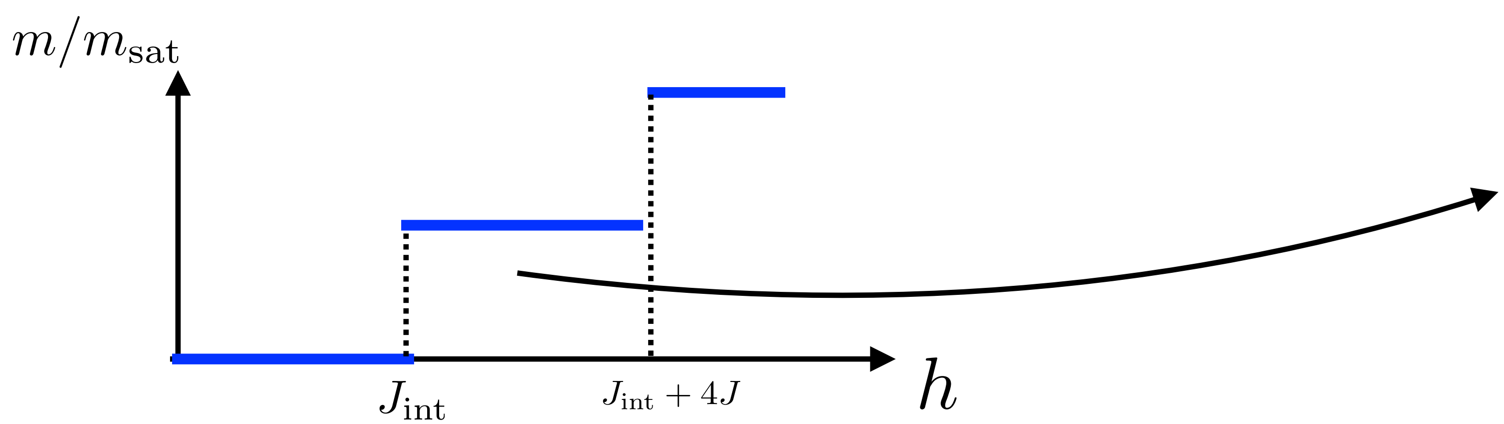
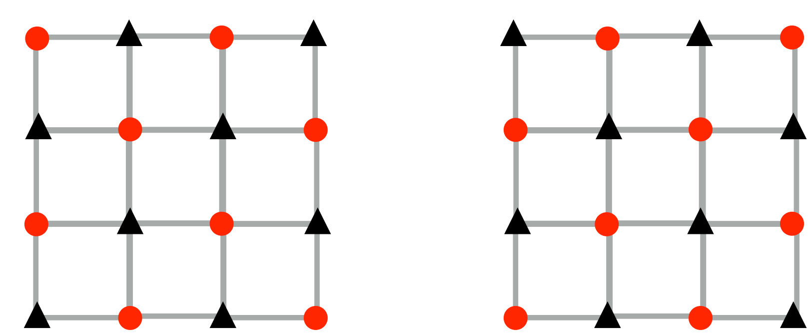


- At large J_{int}, rung-singlets dominate but large enough field brings back the polarized triplets
- T=0 : Magnetization plateau for intermediate fields

Derzhko, Richter …

$$|\bullet\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \qquad |\blacktriangle\rangle = |\uparrow\uparrow\rangle$$





view from top

Field-induced transition in the FF bilayer

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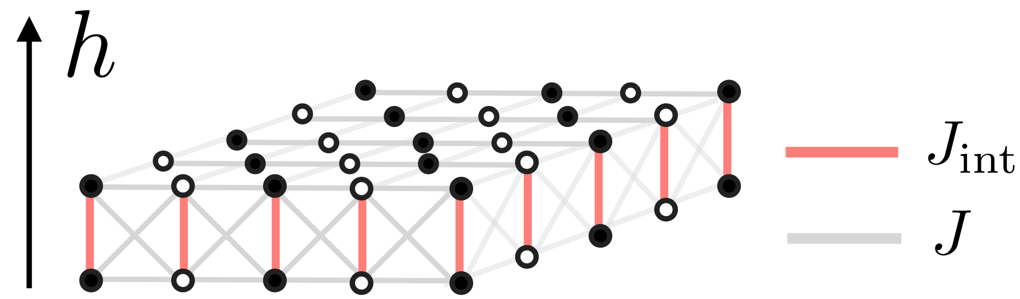
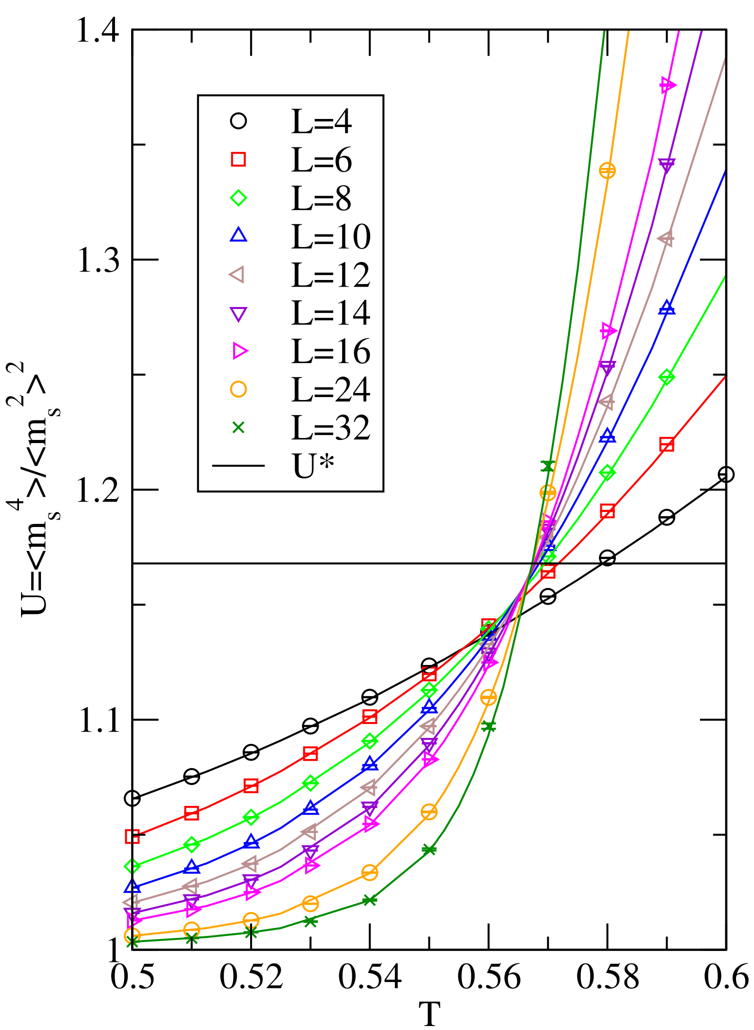
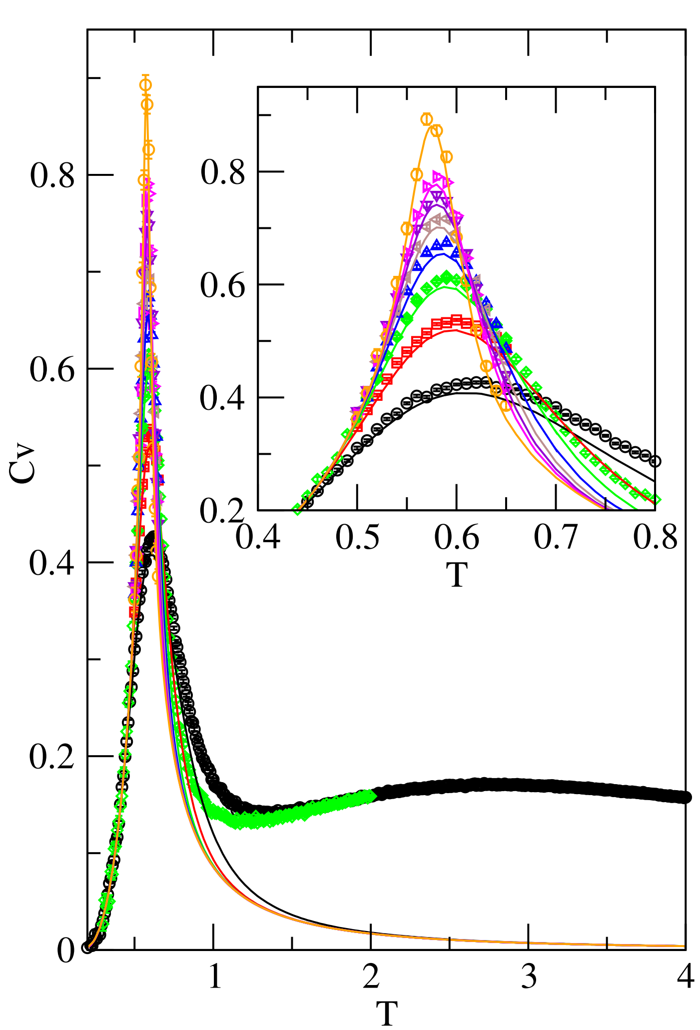
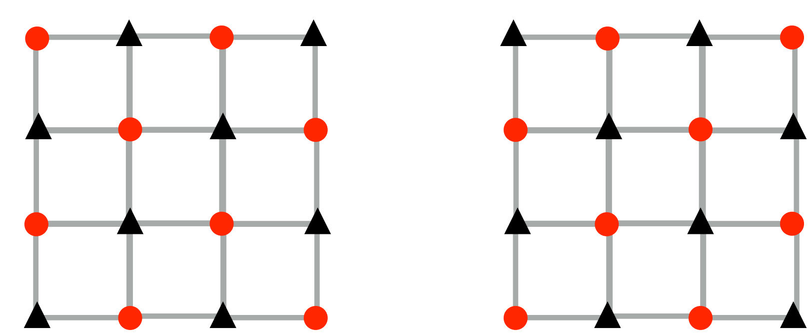


- At large J_{int}, rung-singlets dominate but large enough field brings back the polarized triplets
- QMC : finite-temperature transition where sublattice symmetry is spontaneously broken





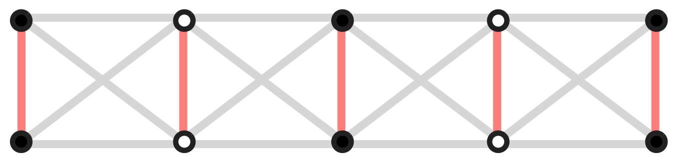


2d Ising universality class

Generalization out of the fully frustrated case

PRL **117**, 197203 (2016)

Extending the sign-freeness

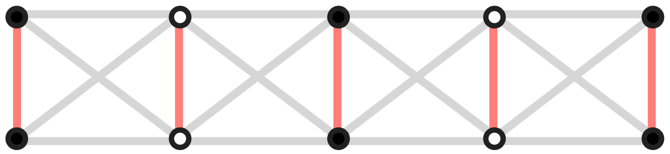


- All seems to work because $\mathbf{T}_i$ are locally conserved quantum numbers :

$$[H, \mathbf{T}_i^2] = 0$$

$$H = J_{\text{int}} \sum_i (\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}) + J \sum_i (\mathbf{S}_{i,1} + \mathbf{S}_{i,2}).(\mathbf{S}_{i+1,1} + \mathbf{S}_{i+1,2}) = J \sum_i \mathbf{T}_i.\mathbf{T}_{i+1} + \frac{J_{\text{int}}}{2} \sum_i \mathbf{T}_i^2 + \text{Ct}$$

Extending the sign-freeness



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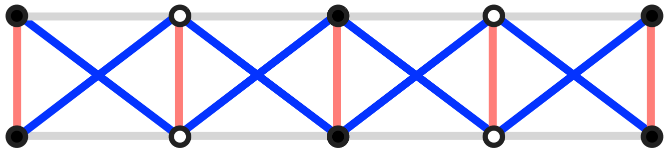
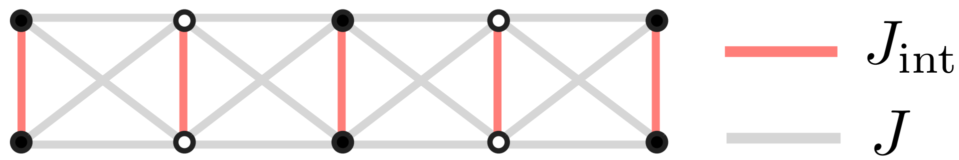
- NO ! To see this, generalize the FF ladder to XXZ different couplings



$$\begin{aligned} H = {} & J_{\rm int} \sum_i \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} \\ & + \sum_i J_{=}^z (S^z_{i,1} S^z_{i+1,1} + S^z_{i,2} S^z_{i+1,2}) + J_{=}^{\perp} (S^+_{i,1} S^-_{i+1,1} + S^+_{i,2} S^-_{i+1,2} + h.c.) \\ & + \sum_i J_{\times}^z (S^z_{i,1} S^z_{i+1,2} + S^z_{i,1} S^z_{i+1,2}) + J_{\times}^{\perp} (S^+_{i,1} S^-_{i+1,2} + S^+_{i,1} S^-_{i+1,2} + h.c.) \end{aligned}$$

Extending the sign-freeness



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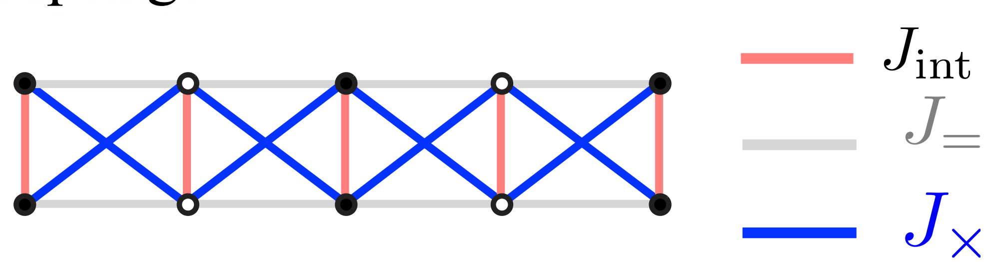


$$H = J_{\text{int}} \sum_i \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2}$$
$$+ \sum_i J_{=}^{z} (S_{i,1}^z S_{i+1,1}^z + S_{i,2}^z S_{i+1,2}^z) + J_{=}^{\perp} (S_{i,1}^+ S_{i+1,1}^- + S_{i,2}^+ S_{i+1,2}^- + h.c.)$$
$$+ \sum_i J_{\times}^{z} (S_{i,1}^z S_{i+1,2}^z + S_{i,1}^z S_{i+1,2}^z) + J_{\times}^{\perp} (S_{i,1}^+ S_{i+1,2}^- + S_{i,1}^+ S_{i+1,2}^- + h.c.)$$

- One shows: no sign problem if $J_{=}^{z} = J_{\times}^{z}$ or $J_{=}^{\perp} = J_{\times}^{\perp}$ or $J_{\text{int}} = 0$

New basis can solve the sign problem even when no local conserved numbers

Classification of matrix elements

- Off-diagonal matrix elements

$$\langle \blacktriangle \bullet | H | \bullet \blacktriangle \rangle = \langle \blacktriangledown \bullet | H | \bullet \blacktriangledown \rangle = \langle \blacktriangle \blacktriangledown | H | \bullet \bullet \rangle = \frac{J^{\perp}_{=} + J^{\perp}_{\times}}{2} \equiv J^{\perp}$$

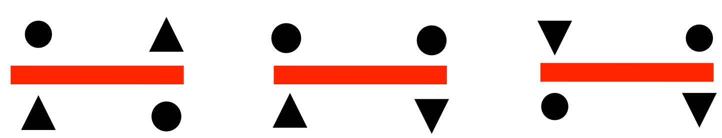
$$|\bullet\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$|\blacktriangle\rangle = |\uparrow\uparrow\rangle$$

$$|\bullet\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$|\blacktriangledown\rangle = |\downarrow\downarrow\rangle$$

m-type processes



$J^{\perp}$

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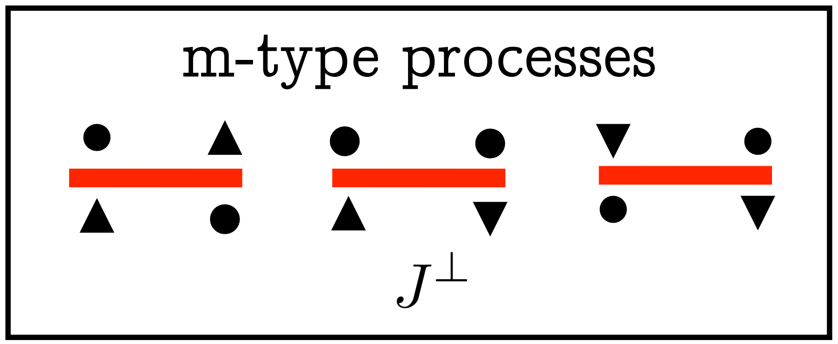
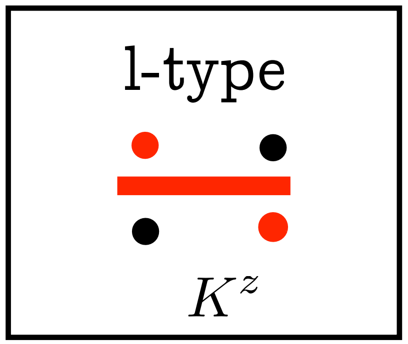
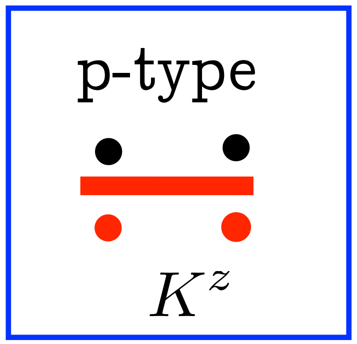
$$\langle \bullet \textcolor{red}{\bullet} |H| \textcolor{red}{\bullet} \bullet \rangle = \langle \bullet \bullet |H| \textcolor{red}{\bullet} \textcolor{red}{\bullet} \rangle = \frac{J^{z}_{=} - \textcolor{blue}{J^{z}_{\times}}}{2} \equiv K^{z}$$







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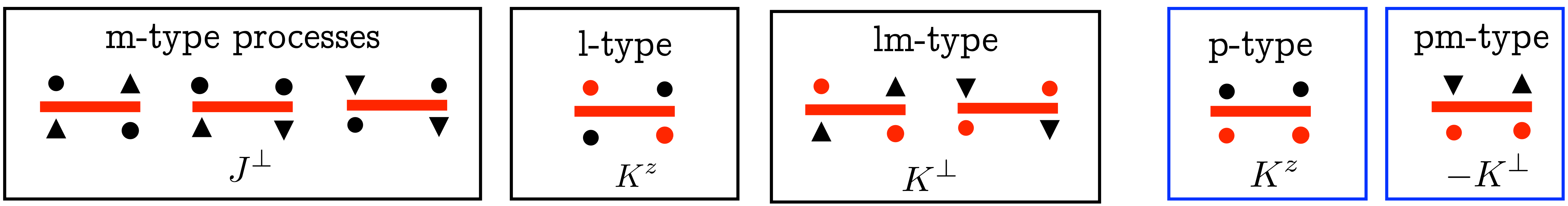

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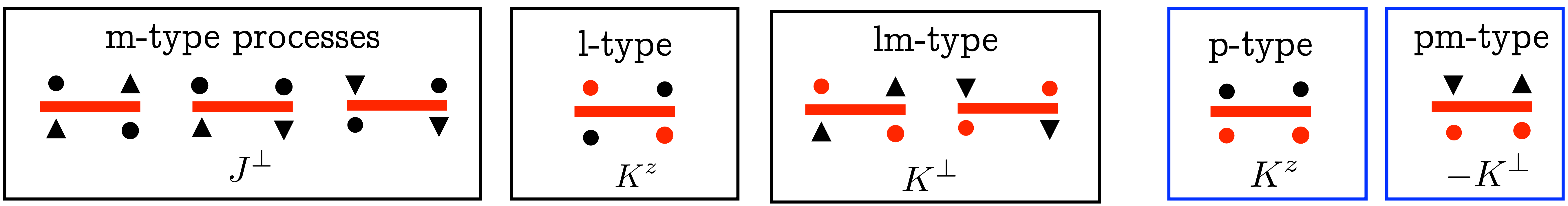
$$\langle \bullet{\color{red}\bullet}|H|{\color{red}\bullet}\bullet\rangle = \langle \bullet\bullet|H|{\color{red}\bullet}{\color{red}\bullet}\rangle = \frac{{\color{gray}J_{=}^{z}} - {\color{blue}J_{\times}^{z}}}{2} \equiv K^{z}$$



Hopings types

Pair-creation types

Classification of matrix elements

- Off-diagonal matrix elements

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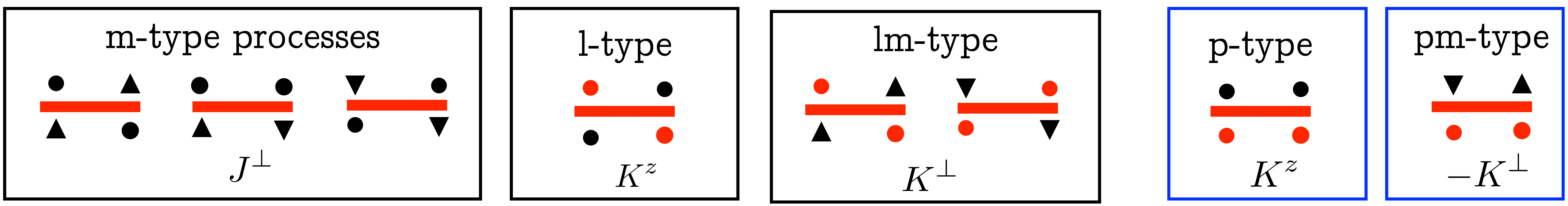


Hopings types

Pair-creation types

- Conservation rules + Bipartite lattice impose $J_{=}^{z} = J_{\times}^{z}$ or $J_{=}^{\perp} = J_{\times}^{\perp}$

  T^z, T quantum numbers

  Creations balance annihilations

  Even loops

  $(K^{z} = 0)$ $(K^{\perp} = 0)$

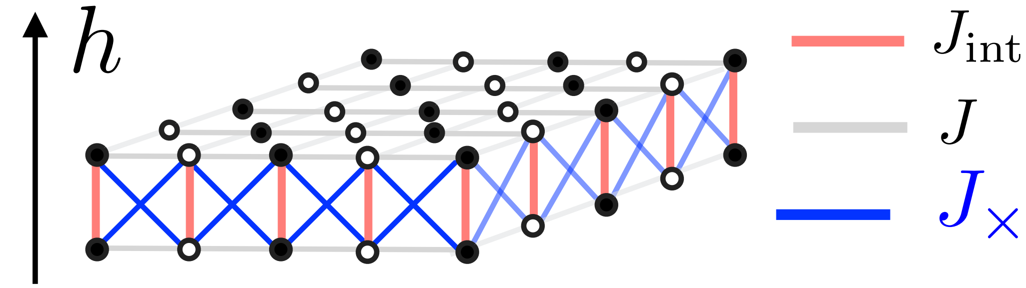
  or $J_{\text{int}} = 0$

- Equivalent local unitary transform exist …

PRL **117**, 197203 (2016)

Bilayer in a field away from fully-frustrated case

- The method also works in a field (z direction) : study of magnetization curves, plateaus …



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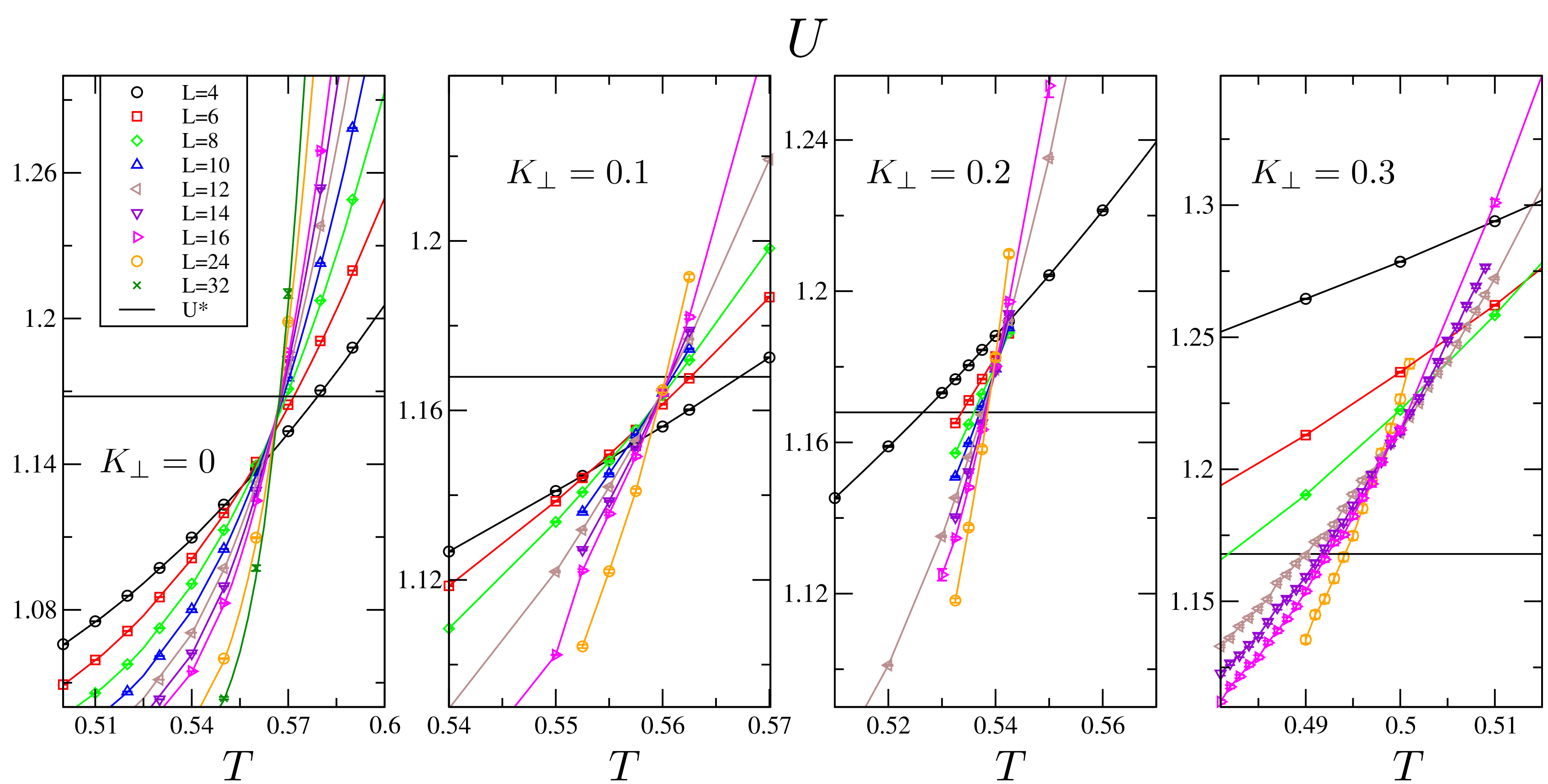
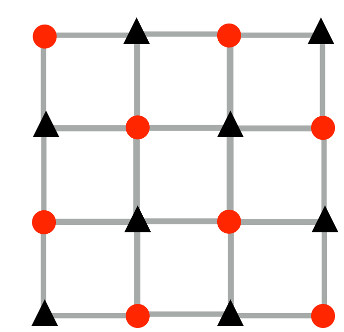
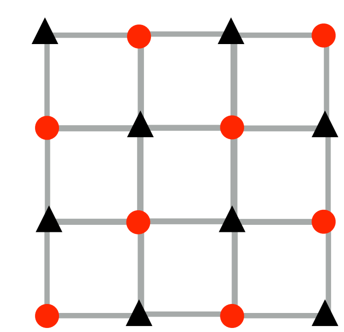


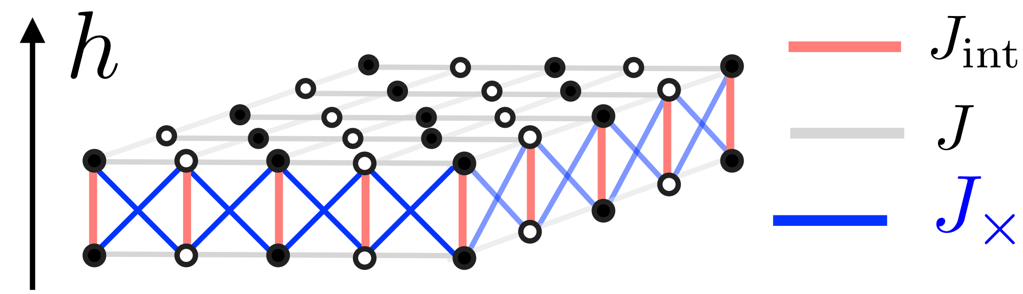




2d Ising universality class even in presence of $K^\perp$

Zero-temperature phase diagram

$$H_{\text{bilayer}} = D\sum_i \mathbf{S}_{i,1}\cdot\mathbf{S}_{i,2} - h\sum_{i,\alpha} S^z_{i,\alpha}$$
$$+\sum_{\langle i,j\rangle}\left[J^{\perp}_{\parallel}\mathbf{S}^{\perp}_{i,1}\cdot\mathbf{S}^{\perp}_{j,1} + J^{z}_{\parallel}S^z_{i,1}S^z_{j,1} + 1\leftrightarrow 2\right]$$
$$+\sum_{\langle i,j\rangle}\left[J^{\perp}_{\times}\mathbf{S}^{\perp}_{i,1}\cdot\mathbf{S}^{\perp}_{j,2} + J^{z}_{\times}S^z_{i,1}S^z_{j,2} + 1\leftrightarrow 2\right],$$



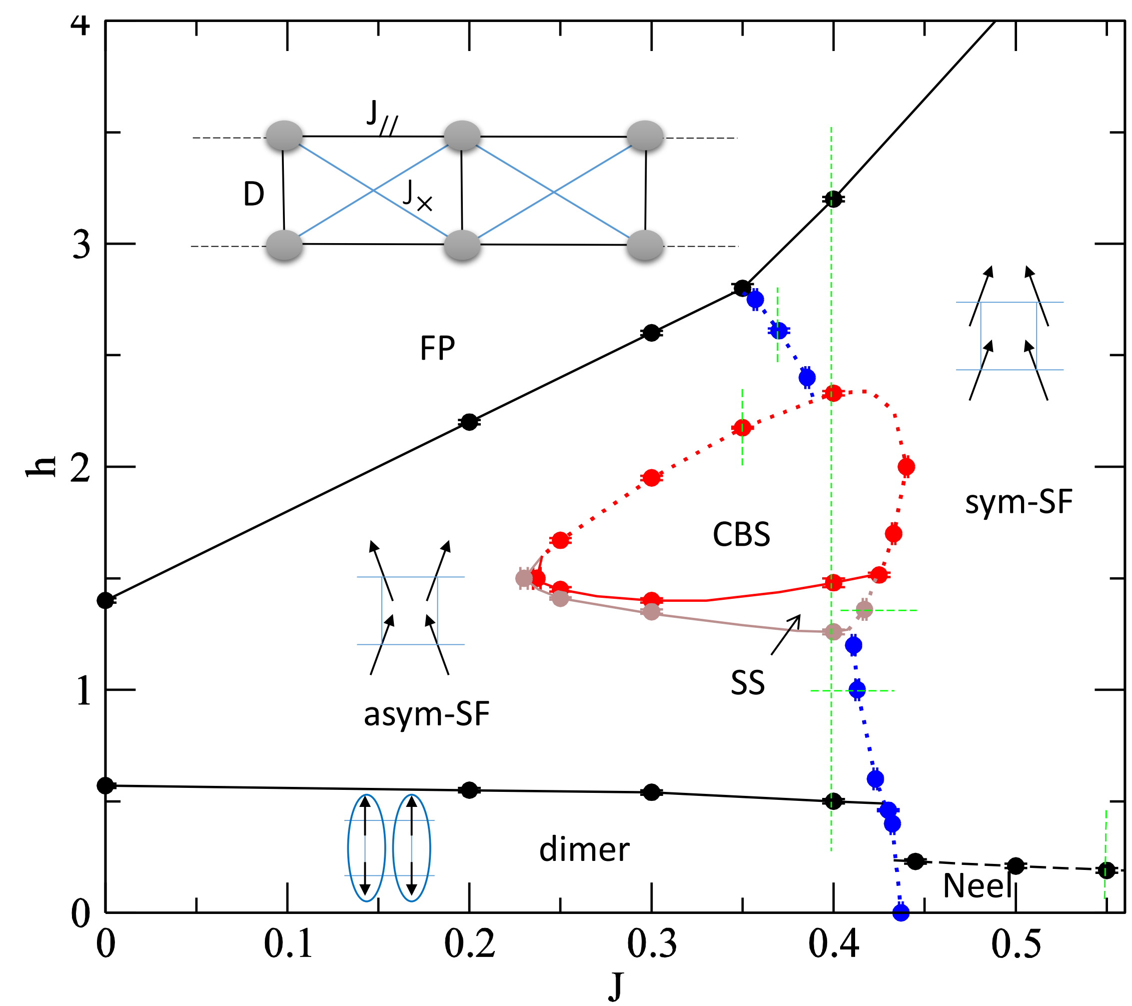


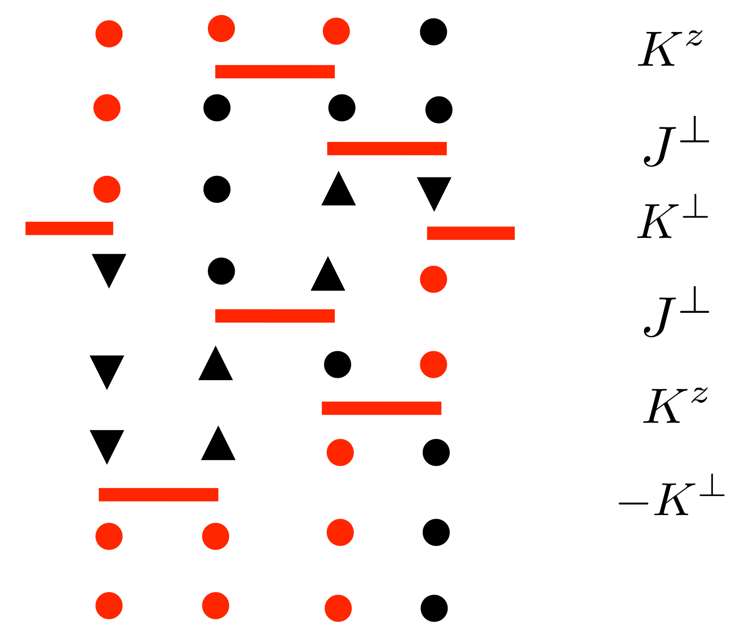
FIG. 1: (Color online) Ground-state phase diagram for the spin-1/2 bilayer spin model in Eq. (1) with the spin anisotropy $K = 0.1$, where $K = J^{\perp}_{\parallel} - J^{z}_{\parallel} = -(J^{\perp}_{\times} - J^{z}_{\times})$ and $J = J^{z}_{\parallel} = J^{z}_{\times}$. Here the interlayer coupling $D \equiv 1$. The dotted (solid)

Ng & Yang, PRB (2017)

When does the sign problem appear?

- Sign becomes negative for some configurations when both K^z and $K^\perp$ are present

- Example of a negative sign configuration



Stefan’s talk

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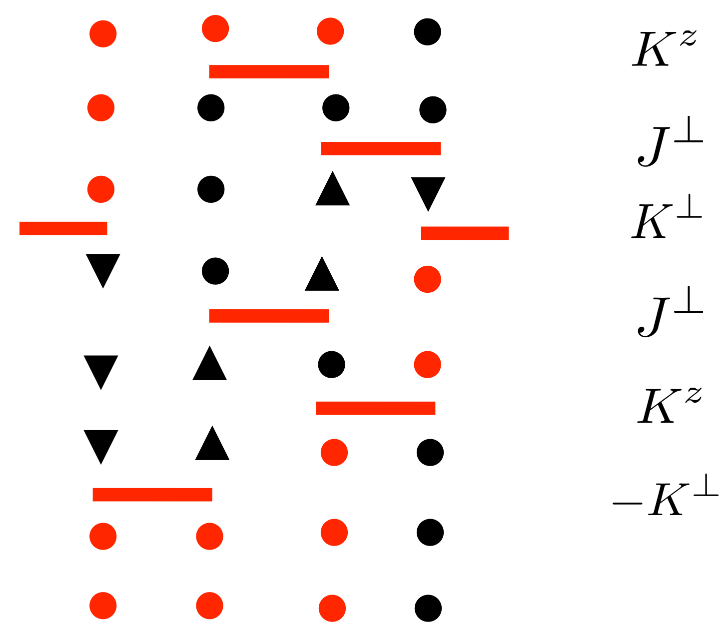
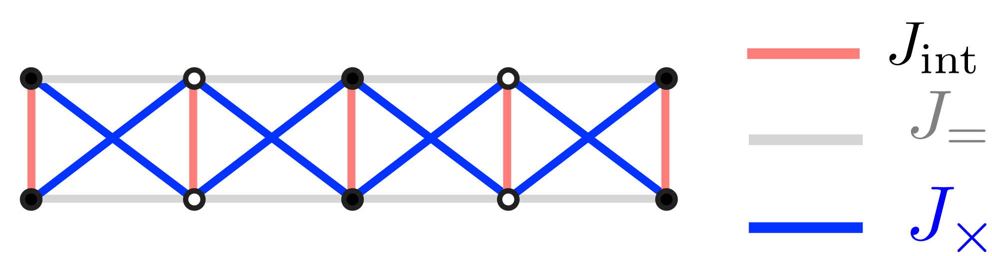


Only appears when closed loops !

- Consequences for 1d chains (regular ladders) :



  - Open boundary conditions : no sign problem
  - Periodic boundary conditions : small sign problem for large systems

Stefan's talk

Perspectives

- **Perspective 1:** How bad is the sign problem in the generic case with K^z and $K^{\perp}$?

Perspectives

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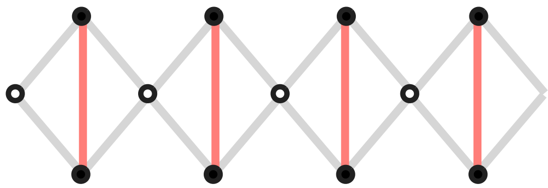
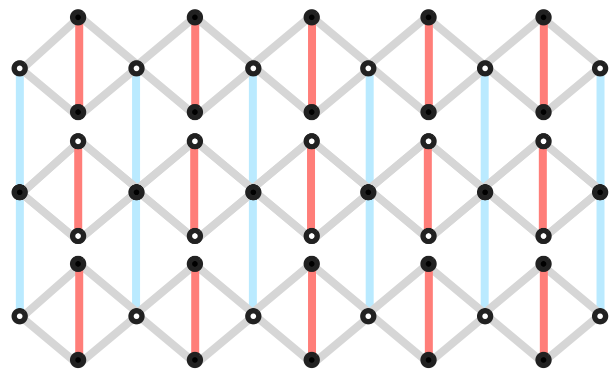
- **Perspective 2:** Many other lattices with interesting physics to be explored



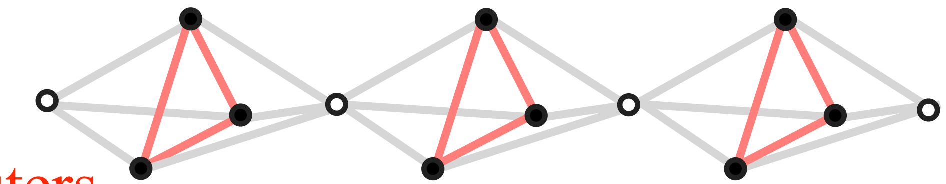
Diamond chain

Mixed-spin lattices



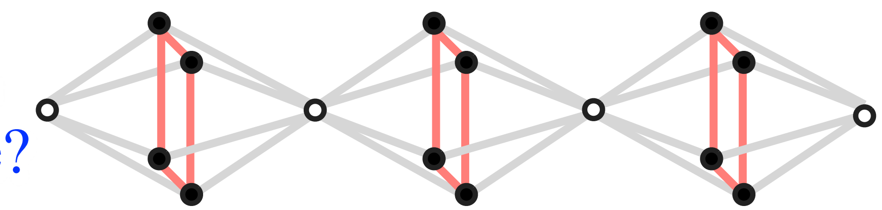
Coupled diamonds

3+ spins clusters



1d pyrochlore

Which terms are sign-problem free?



Spin octahedral chain

Perspectives

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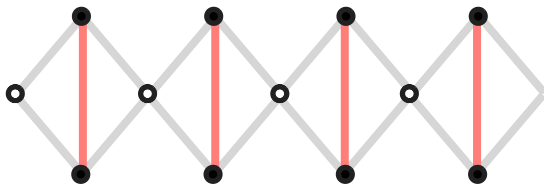
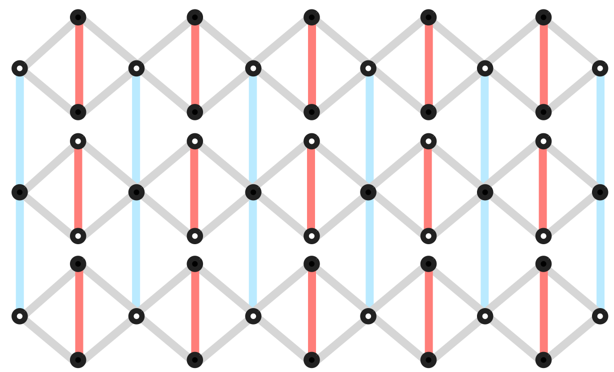


Diamond chain

Mixed-spin lattices



Coupled diamonds

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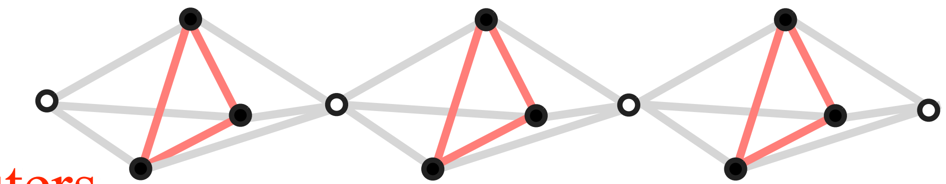

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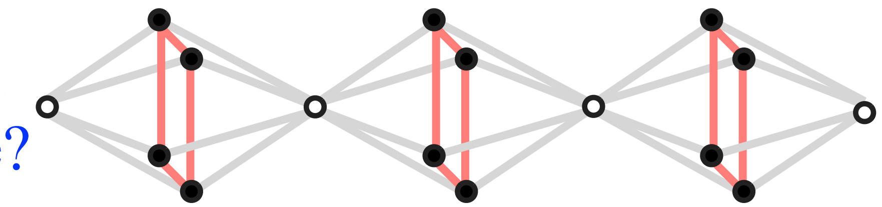

Spin octahedral chain

- **Perspective 3:** Other types of interactions beyond XXZ : Four-spin interactions, transverse fields…

Perspectives

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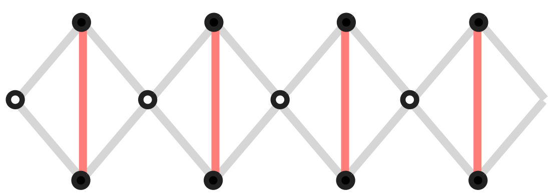
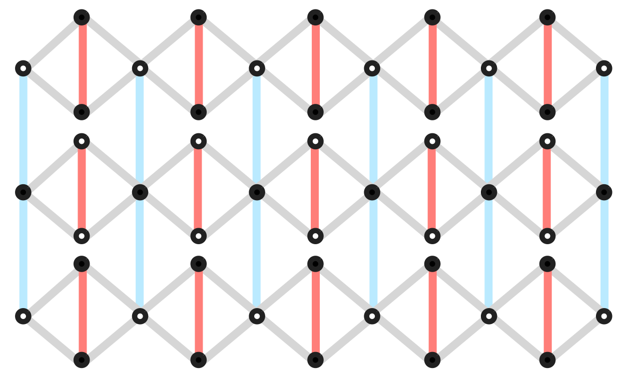
Mixed-spin lattices



Diamond chain



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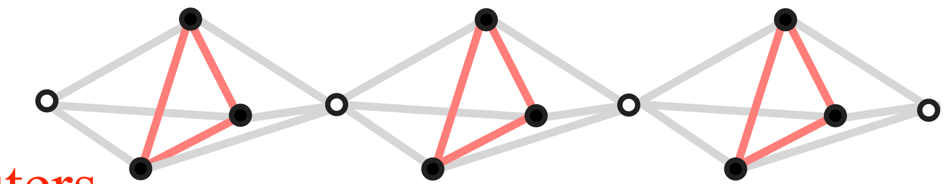

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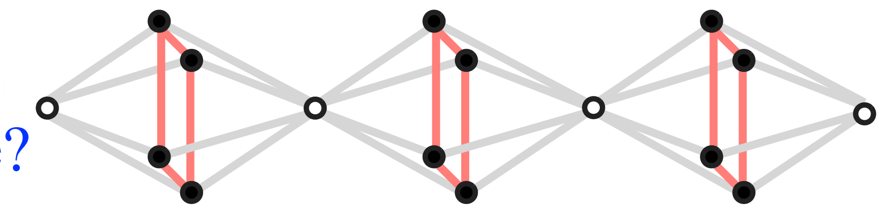


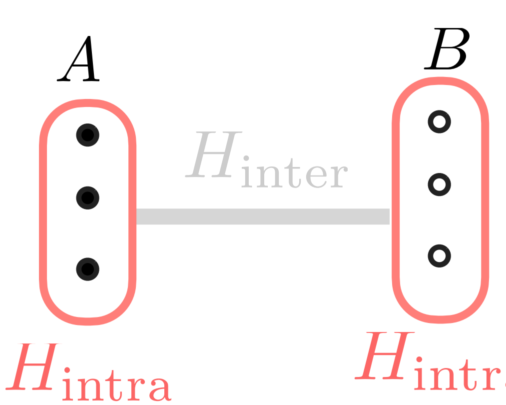
Spin octahedral chain

- **Perspective 3:** Other types of interactions beyond XXZ : Four-spin interactions, transverse fields…

- **Perspective 4:** Keep the « cluster » idea but change strategy

For a given frustrated model, search numerically for the « best » local unitary transform

$$H = H_{\mathrm{intra}} + H_{\mathrm{inter}}$$



$$H_{\mathrm{QMC}} = (U_A U_B)^{-1} H (U_A U_B)$$

with M. Mambrini

see also H. Shinaoka *et al.*, PRB (2016)

Perform small local rotations in the cluster basis, check *at the matrix element level / in a small run* if the sign problem is improved