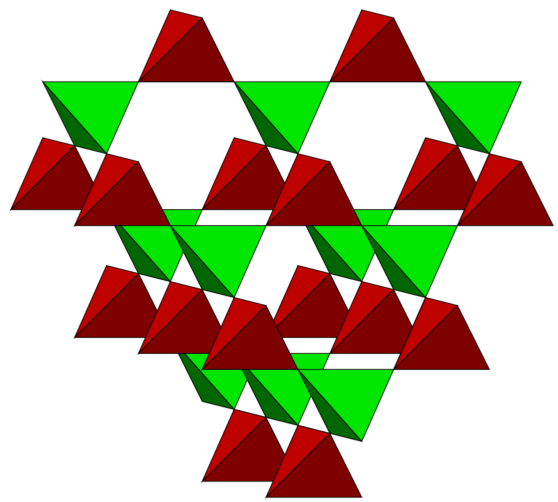
Quantum magnets with strong frustration



Oleg Tchernyshyov (JHU)

Thanks

- Colleagues:
  - A.G. Abanov (Stony Brook)
  - P. Fendley (UVA)
  - C.L. Henley (Cornell)
  - R. Moessner (ENS)
  - S.L. Sondhi (Princeton)
  - O.A. Starykh (Hofstra $\mapsto$ Utah)
  - Hong Yao (JHU $\mapsto$ Stanford)
- Funding:
  - NSF
  - Research Corporation

Outline

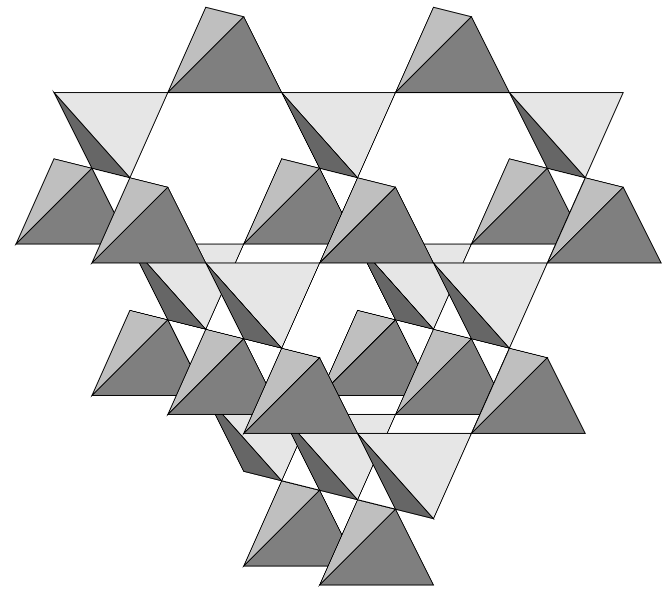
- Which magnets:

  pha.jhu.edu/$\sim$olegt/pyrochlore.html

- Large-S approach:
  - O.T., J.Phys.:Condens.Matter 16, S709 (2004).
  - O.T., Moessner, Starykh, A.G. Abanov, PRB 68, 144422 (2003).
  - O.T., H. Yao and R. Moessner, PRB 69 (June 1, 2004).
- Large-N approach:
  - O.T., R. Moessner and S.L. Sondhi, in preparation.
- Summary

Which magnets?

- Heisenberg SU(2) spins
- $H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$
- network of tetrahedra
- 3D pyrochlore lattice



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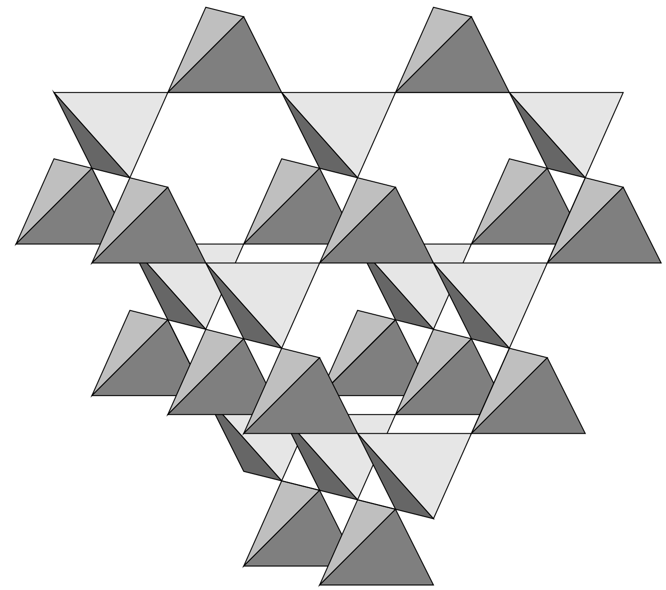

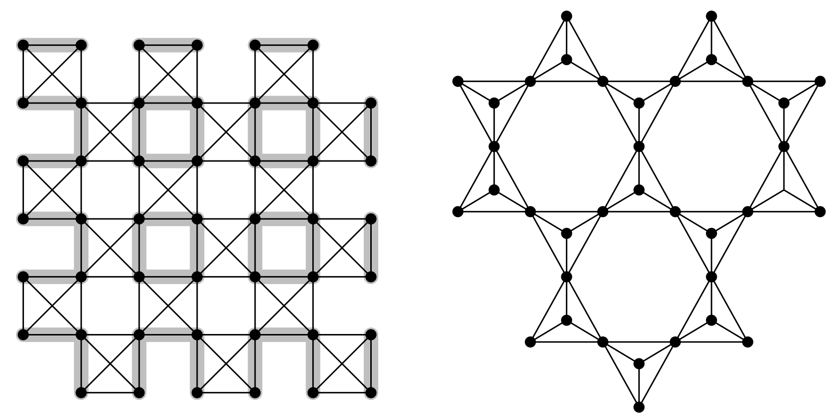

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- Heisenberg SU(2) spins
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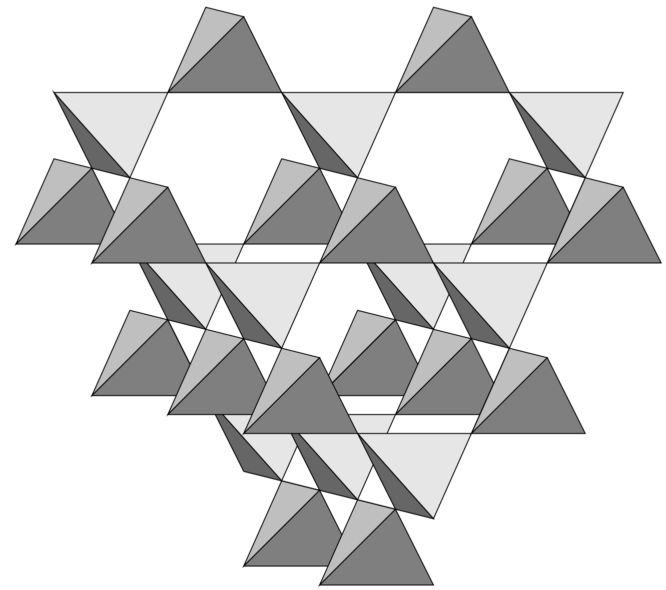
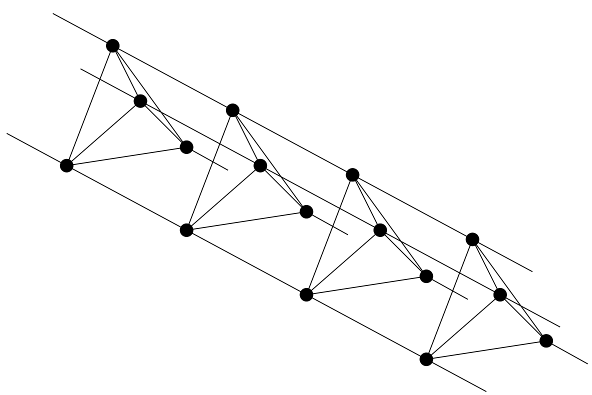
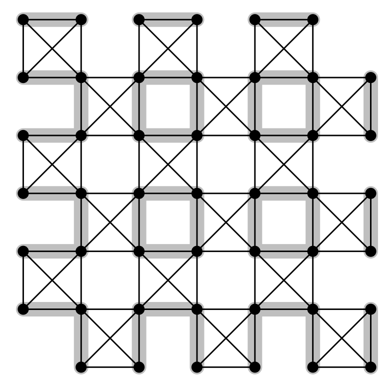
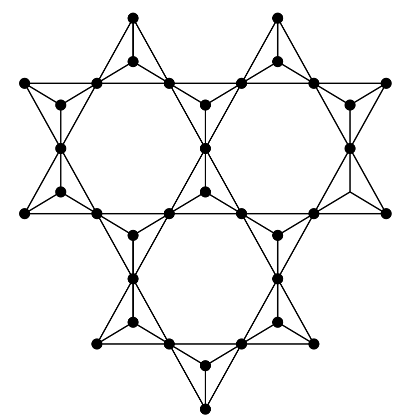
- 3D pyrochlore lattice
- + analogs in 2D and 1D



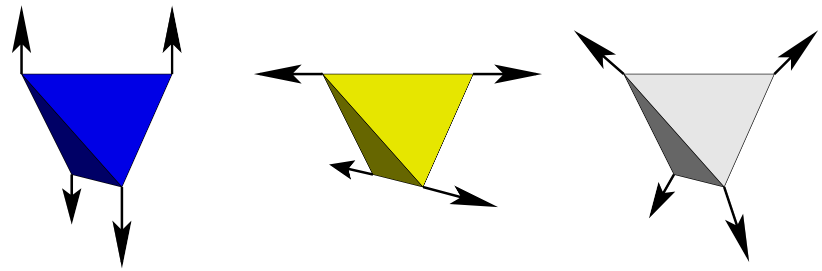


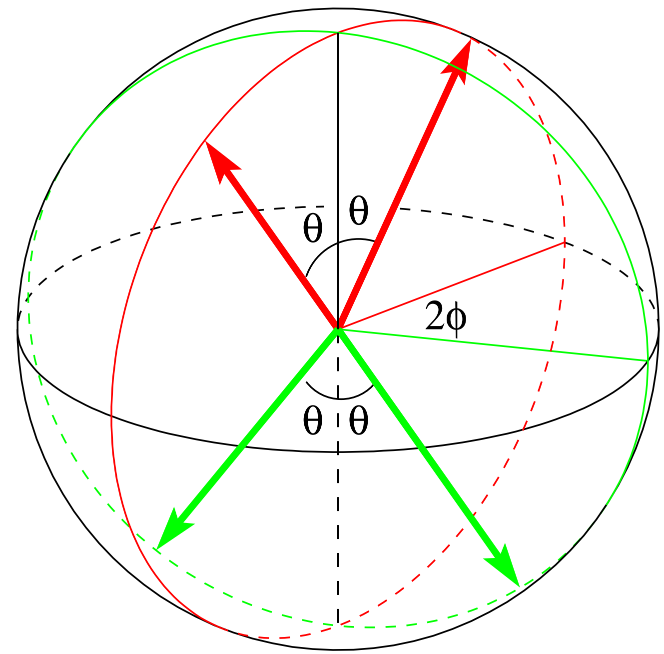




Heisenberg spins on a tetrahedron

- Degenerate ground state.
- $\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 = 0$.
- Classical ground states: distinct *relative* orientations form a manifold S_2/D_2.
- Quantum ground states: $2S + 1$ singlets labeled by total spins of bond 12 or 34: $S_{12} = S_{34} = 0, 1, 2 \ldots 2S$.
- Very strong frustration.



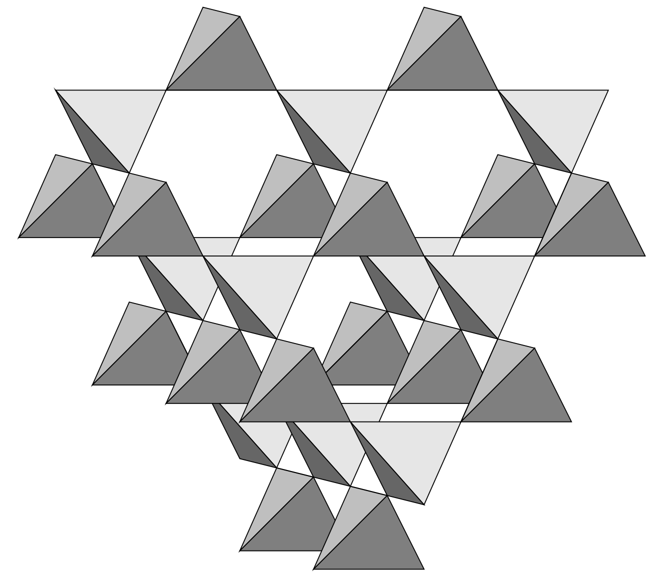


O.T., R. Moessner and S.L. Sondhi, PRB 66, 064403 (2002).

Pyrochlore lattice: classical spins

- Down to $T = 10^{-4} JS^2$:
  - No magnetic order
  - No spin-Peierls order
  - No thermodynamic singularities

Moessner and Chalker, 1998.



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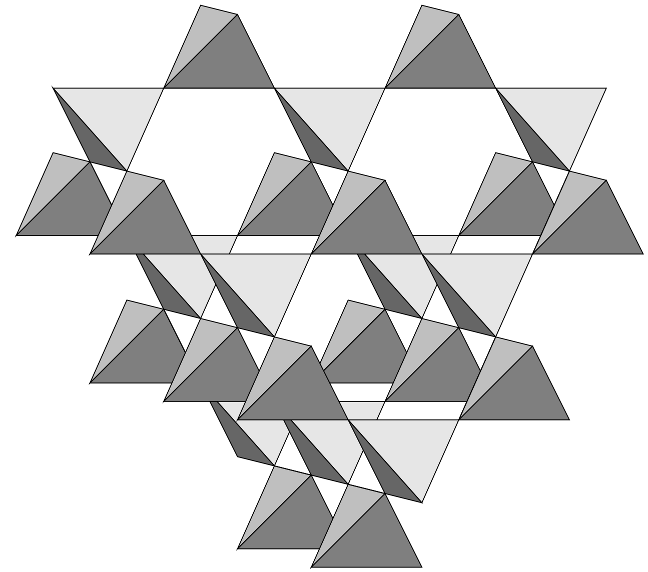

- Reminiscent of $ZnCr_2O_4$ ($S = 3/2$) at $T > 13$ K.

S.-H. Lee *et al.*, Nature 418, 856 (2002).

Quantum effects as a perturbation: $S \gg 1$

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  - Frustration is defined in the classical limit $S \to \infty$.
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- Challenges:
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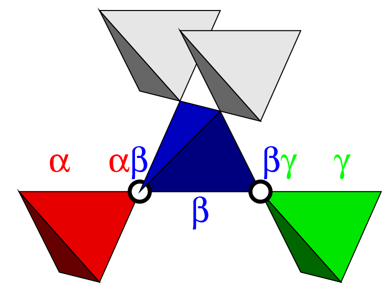
- Solutions:
  - Effective interactions for zero-point motion.
  - Gauge-like Z_2 symmetry at $\mathcal{O}(1/S)$ kills Neel order.

C.L. Henley (unpublished).

Zeroth order in $1/S$

Geometry:

- Tetrahedra α, β, γ,...
  form a diamond lattice.
- Spins live on links $\alpha\beta$, $\beta\gamma$,...
  of the diamond lattice.



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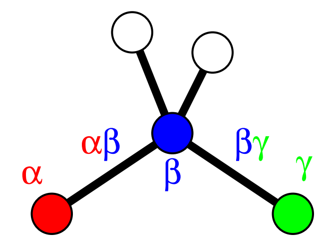

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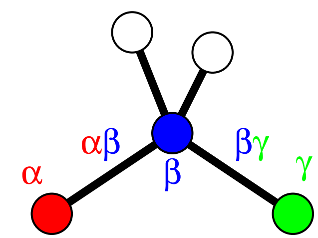

Classical energy $\mathcal{O}(S^2)$:

- $E_0 = J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j = (J/2)\sum_\alpha |\mathbf{L}_\alpha|^2 -$ const, where $\{\mathbf{S}_i\}$ is a classical spin configuration.
- Minimized by configs in which $\mathbf{L}_\alpha \equiv \sum_\beta \mathbf{S}_{\alpha\beta} = 0$.

Leading-order correction $\mathcal{O}(1/S)$

- Zero-point magnon energy:
  - Classical ground states are not eigenstates of H.
  - Virtual excitations are pairs of magnons.
  - Energy of zero-point quantum motion is $\mathcal{O}(1/S)$:
    - $E_1 =$ const $+ \sum_a \hbar|\omega_a|/2$.
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- Collinear states are the best bet:
  - Spin waves are *transverse* excitations.
  - More ways to make waves in *collinear* states.
  - More virtual excitations $\Rightarrow$ lower energy.

Collinear states: Ising gauge symmetry

- All spins point along, say, $\pm\hat{\mathbf{z}}$.
- New Ising variables $\sigma_{\alpha\beta} = \pm 1$: $\mathbf{S}_{\alpha\beta}/S = \sigma_{\alpha\beta}\hat{\mathbf{z}}$.

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- Use eqns of motion to obtain $\{\omega_a\}$:
  $\hbar\,\mathrm{d}\mathbf{L}_\alpha/\mathrm{d}t = J\,\mathbf{S}_{\alpha\beta} \times \mathbf{L}_\beta$. (Moessner and Chalker)
- Transverse fluctuations $\lambda = L_x + iL_y$:
  $$\hbar\omega\,\lambda_\alpha = JS\,\sigma_{\alpha\beta}\,\lambda_\beta.$$

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- "Gauge" symmetry: $\lambda_\alpha \mapsto \Lambda_\alpha\lambda_\alpha$, $\sigma_{\alpha\beta} \mapsto \Lambda_\alpha\sigma_{\alpha\beta}\Lambda_\beta^{-1}$.
- $\Lambda_\alpha = \pm 1$: keep/flip spins on tetrahedron α.
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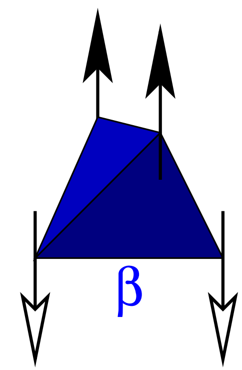
- Gauge-equivalent states have identical spectra. (Henley)
- Substantial degeneracy kills Néel order!

Caveat

- Not exactly a gauge symmetry: Constraint $\sum_\beta \sigma_{\alpha\beta} = 0$ on every tetrahedron α.



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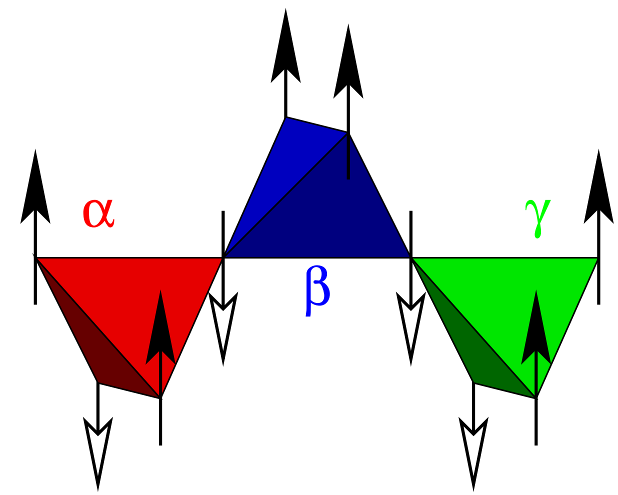

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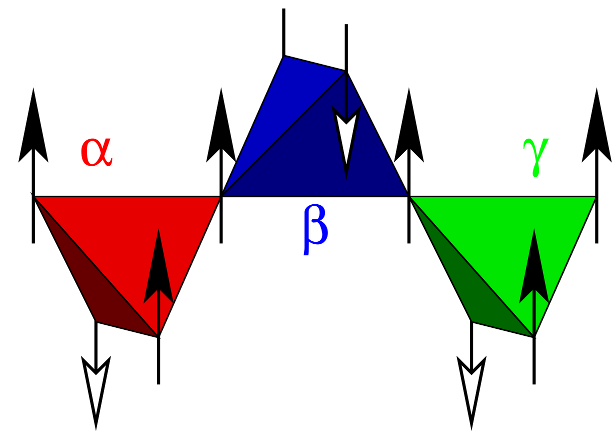

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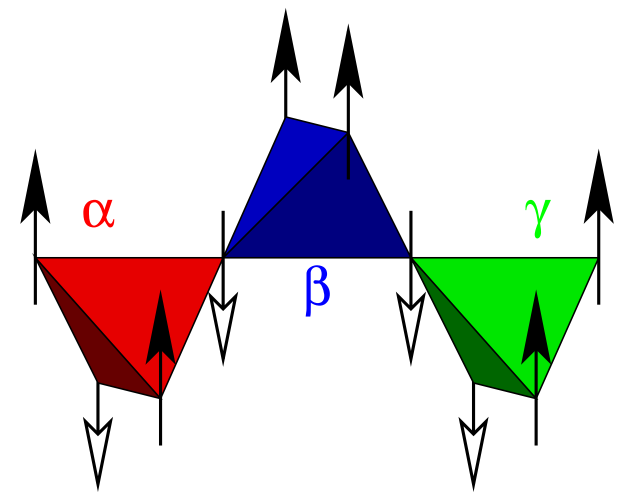
- Some gauge transformations violate it.
- $N_{\text{vacua}} \neq 2^{N_{\text{tetrahedra}}}$.
- Nonetheless, N_{vacua} is large enough to kill Néel order.



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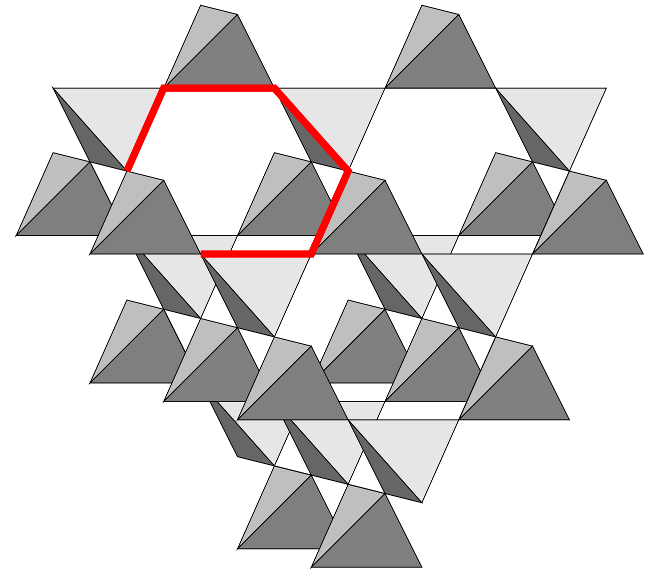
Effective interaction

- H_{eff} must be gauge-invariant.
- Physical variables are Z_2 fluxes
  - $\phi(\hexagon) = \bar{\sigma}_{12}\sigma_{23}\ldots\bar{\sigma}_{56}\sigma_{61} = \pm 1$.
  - where $\bar{\sigma} = -\sigma$.
- Cluster expansion for Z_2 fluxes:



$$\frac{E_1}{N} = \frac{1}{N}\sum_{\gamma} a_1 \phi_\gamma + \frac{1}{2N^2}\sum_{\gamma,\gamma'} a_2(\gamma,\gamma')\,\phi_\gamma\,\phi_{\gamma'} + \ldots$$

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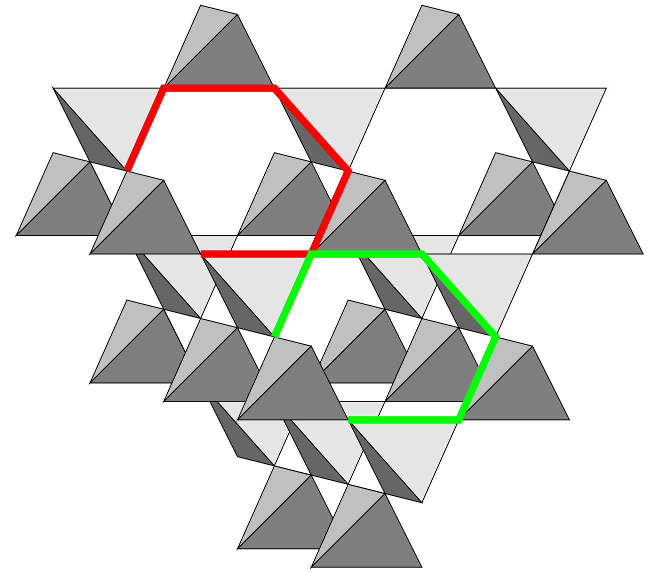

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- Does not converge well (spin waves are gapless).

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- $T = \mathcal{O}(JS)$: Gibbs ensemble of discrete classical states.
  - Roughly collinear: $\mathbf{S}_i \cdot \mathbf{S}_j \approx \pm S^2$.
  - No Néel order: $\langle \mathbf{S}_i \rangle = 0$ (thanks to Z_2 “gauge”).
  - Possibly valence-bond order: $\langle \mathbf{S}_i \cdot \mathbf{S}_j - \mathbf{S}_k \cdot \mathbf{S}_l \rangle \neq 0$.

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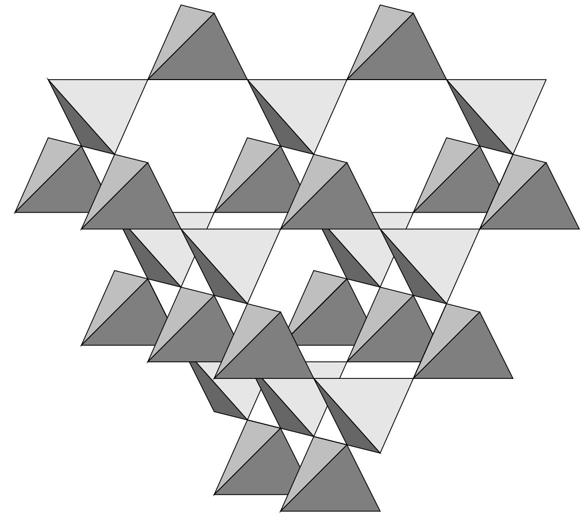
- $T = \mathcal{O}(J)$: unique collinear state (Henley):
  - Néel order: $\langle \mathbf{S}_i \rangle \neq 0$.
  - Very large magnetic unit cell (64 spins in $ZnCr_2O_4$).

Large-S results

- 3D pyrochlore lattice:
  - work in progress



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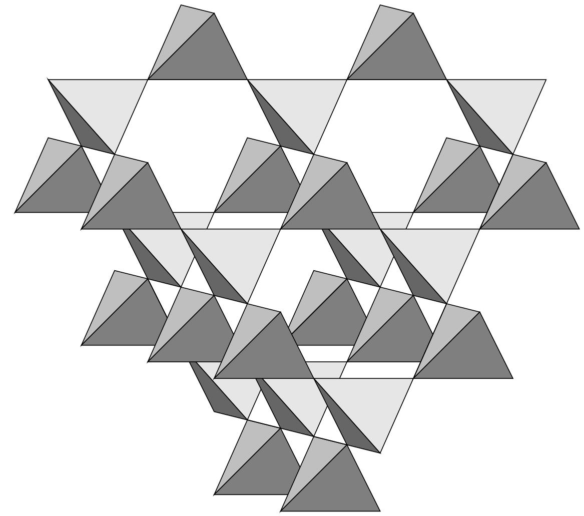
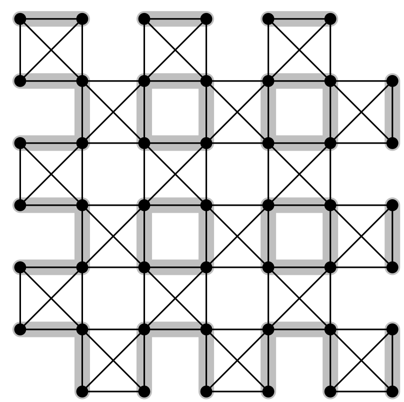
  - $Z_2 \times Z_2$ order parameter
  - similar to $S = 1/2$





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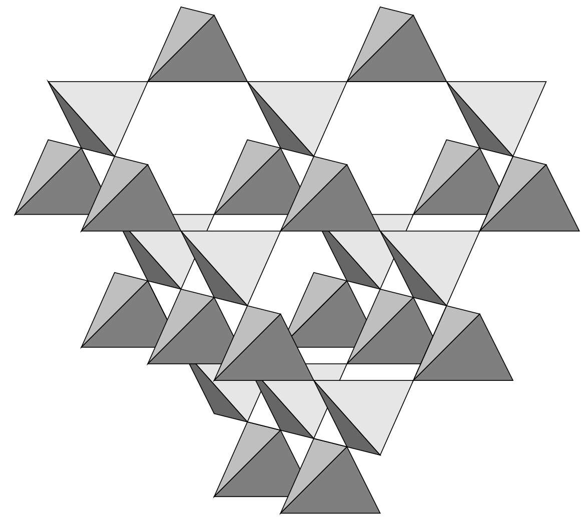
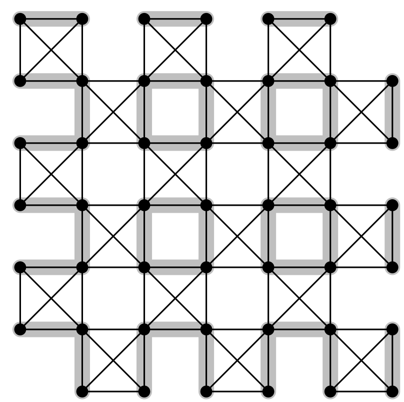
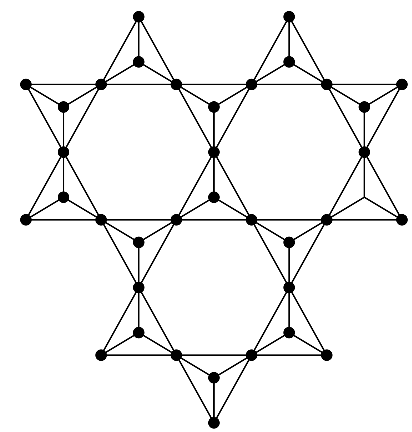
  - $q = 4$ Potts.

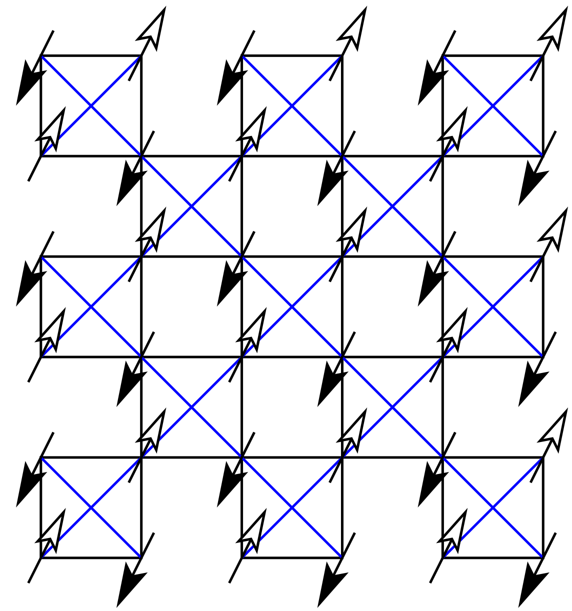






Checkerboard AF at large S

- 2^L classical vacua selected:
  - $\phi(\Box) = \bar{\sigma}_1 \sigma_2 \bar{\sigma}_3 \sigma_4 = +1$.
  - bonds across $\Box$ equally happy



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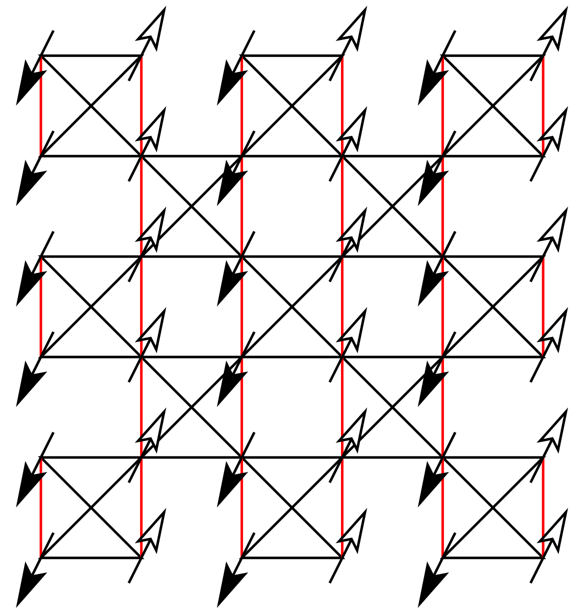

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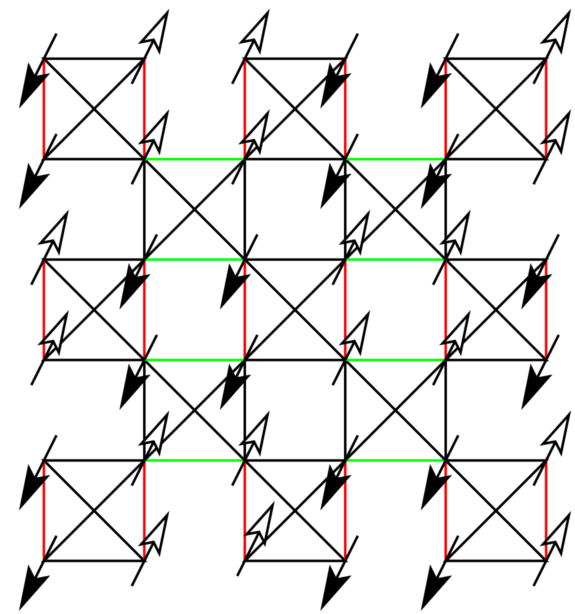

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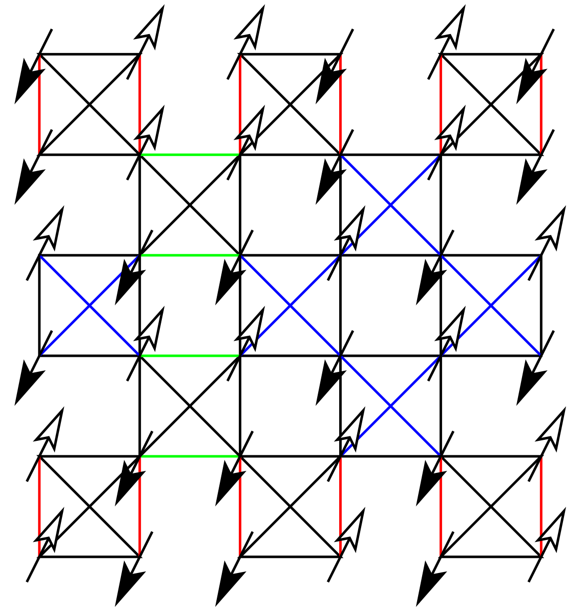

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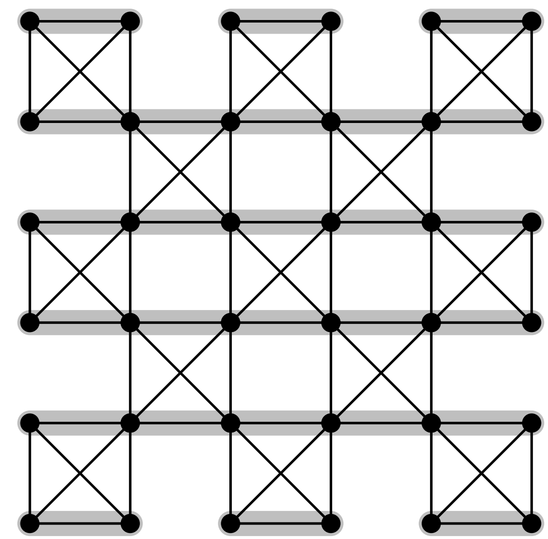

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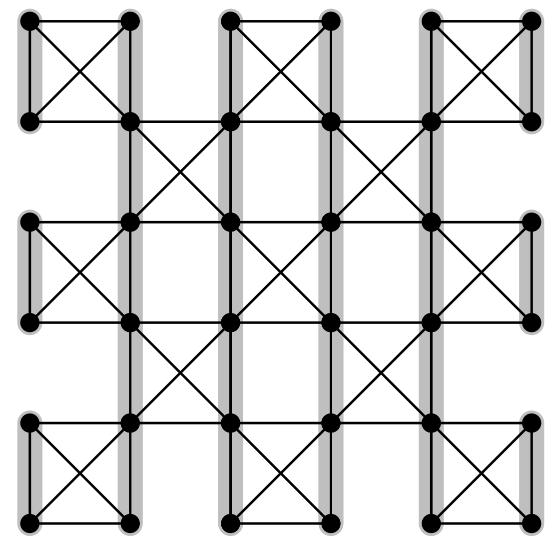

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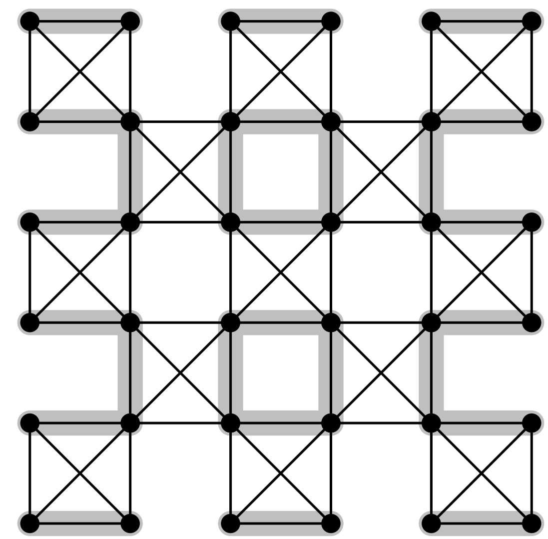

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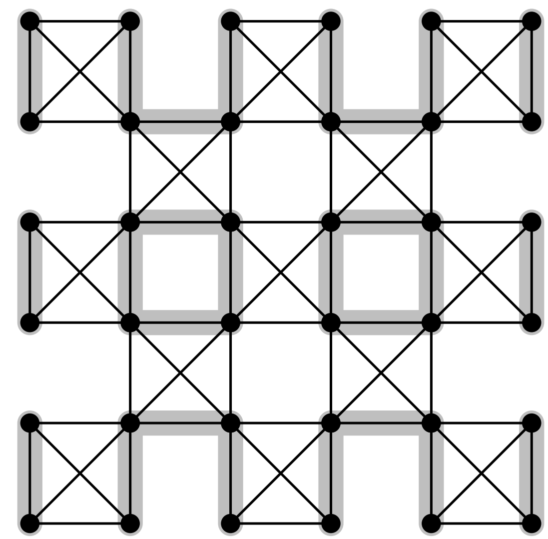
  - Location of happy bonds on 2 sublattices of $\boxtimes$:
    - H $\times$ H, V $\times$ V,
    - H $\times$ V, V $\times$ H.

  $S = 1/2$: Lhuillier *et al.* (2001).



- $Z_2 \times Z_2$ valence-bond order.
  - Thermal phase transition paramagnet $\mapsto$ valence-bond crystal: C. Xu and J.E. Moore, cond-mat/0405271.

(111) slice of the pyrochlore lattice

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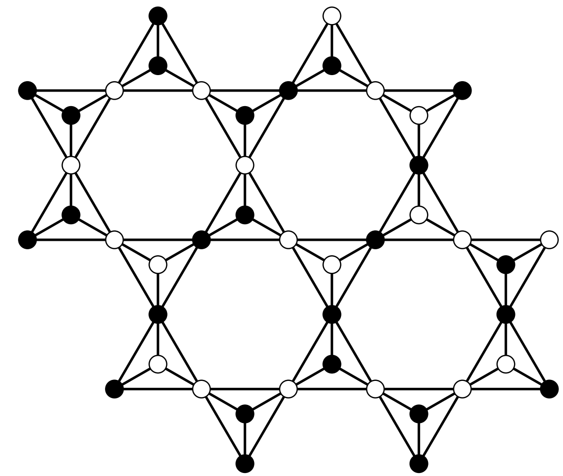

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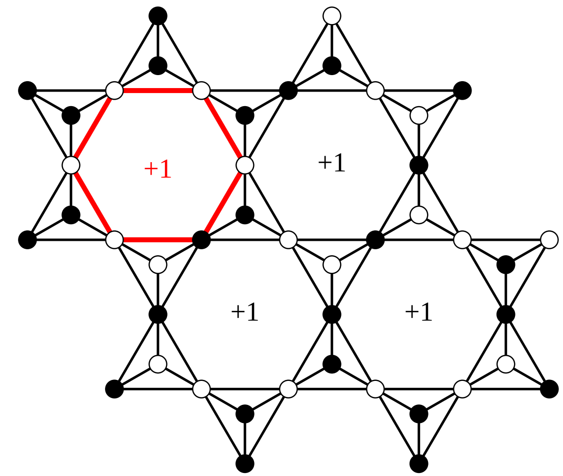

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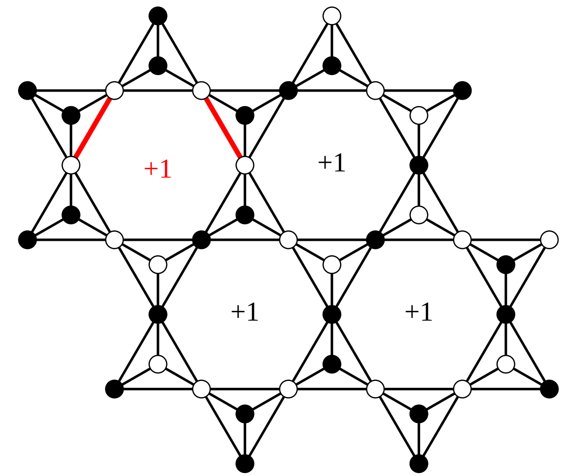

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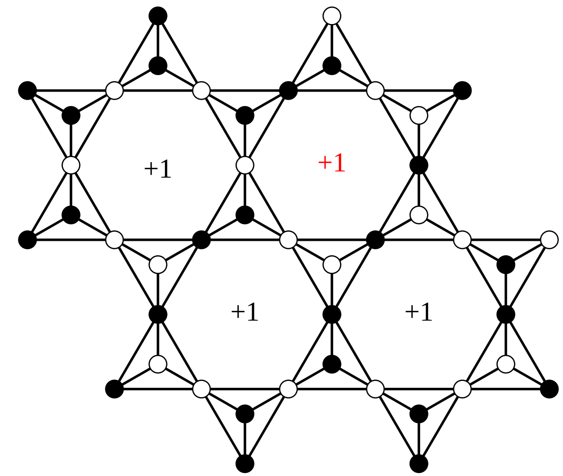

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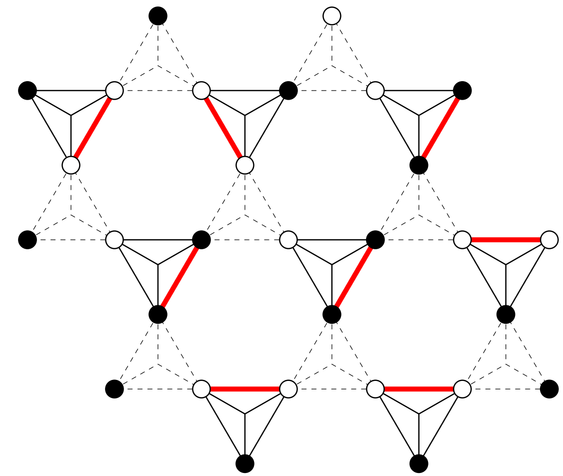

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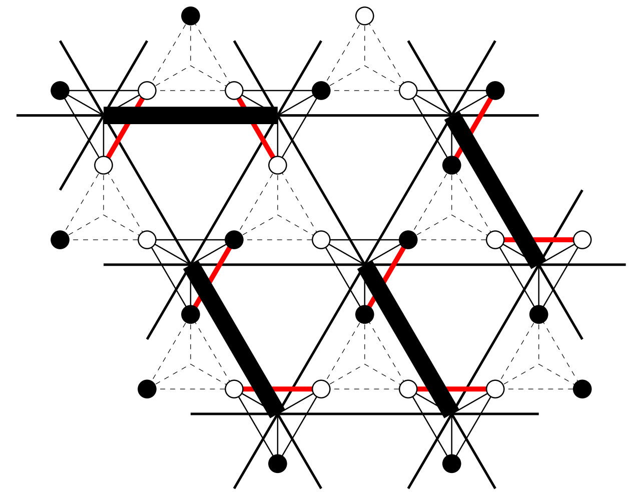

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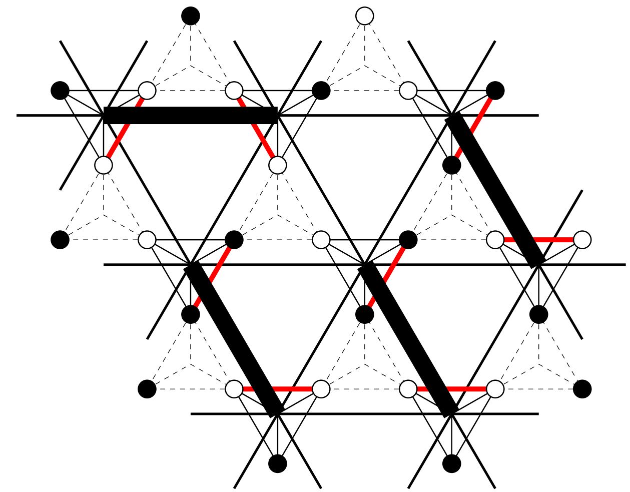

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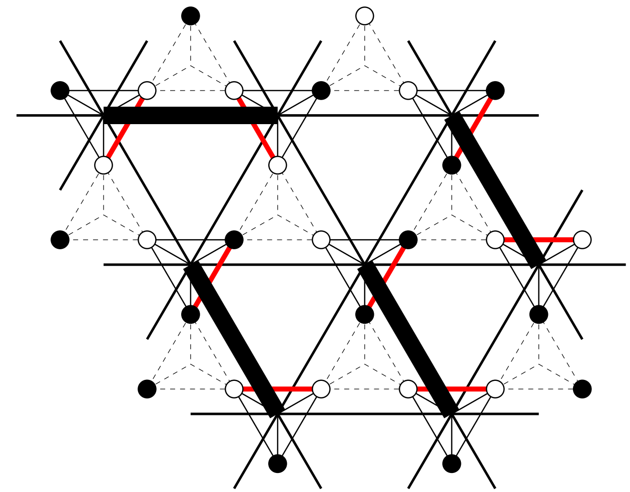

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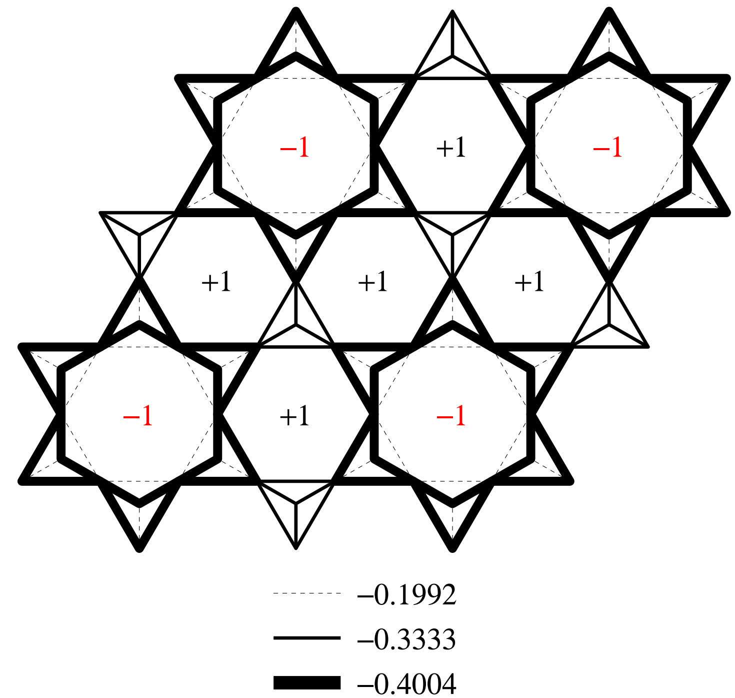
- Numerical minimization:



Actual ground states

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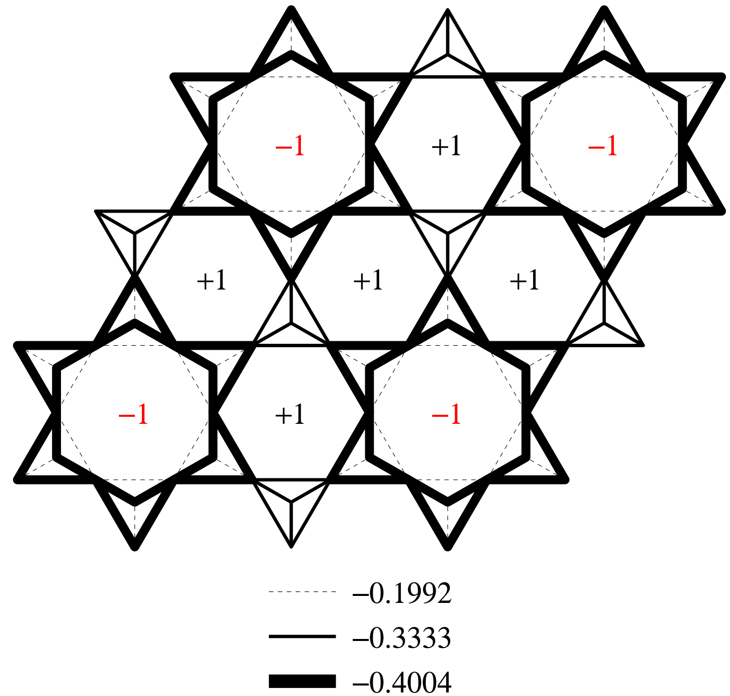

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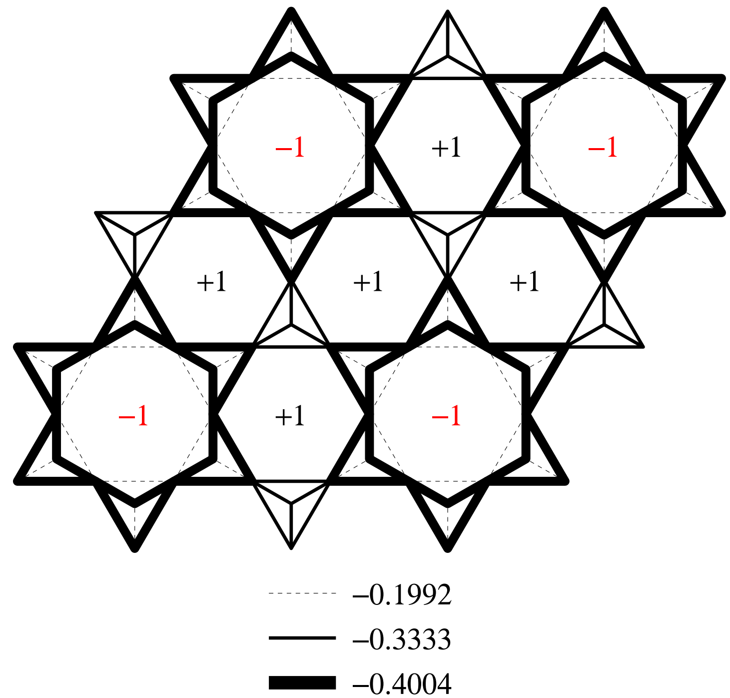

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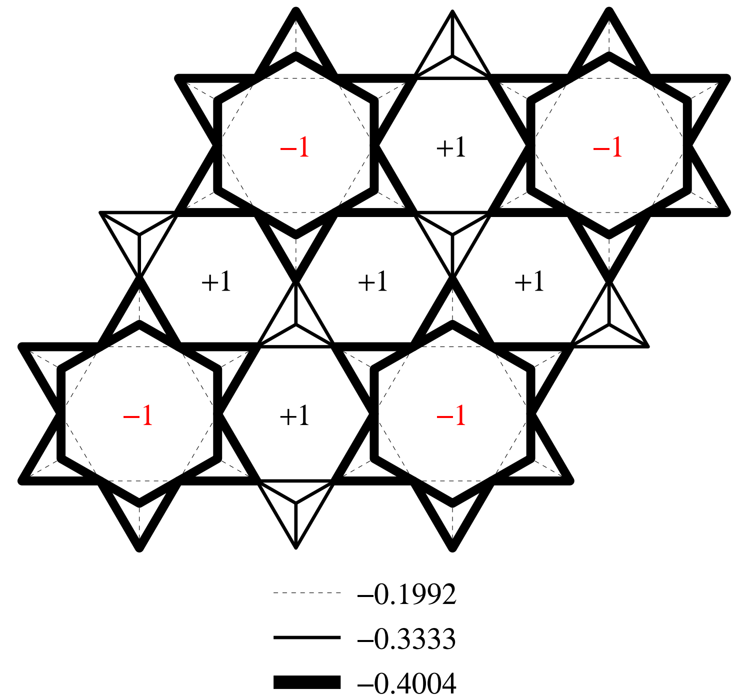

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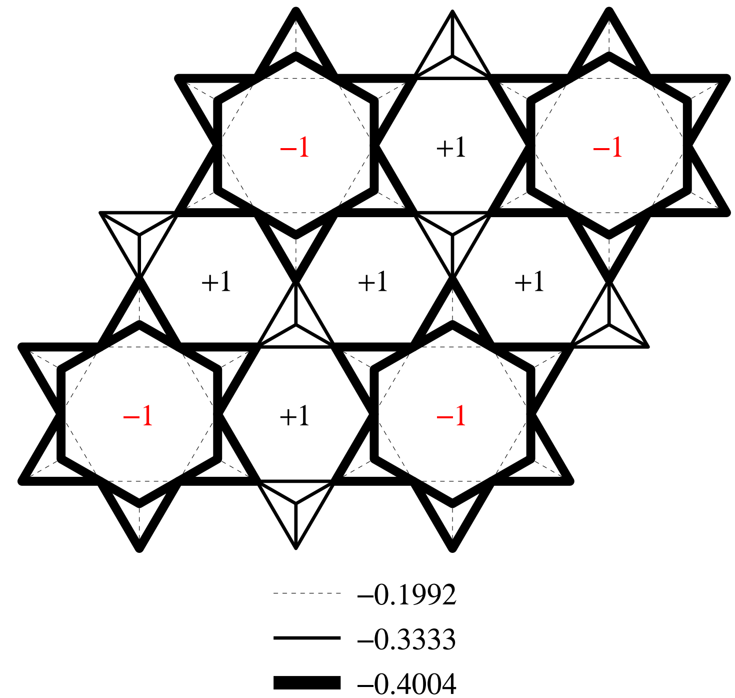

- Broken symmetries:
  - Spin SU(2) is intact: $\langle \mathbf{S}_i \rangle = 0$.
  - Valence-bond order: non-uniform $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$.

$S = 1/2$: A.B. Harris, Berlinsky and Bruder (1991).

Alternative approach: Schwinger bosons

- Represent spins in terms of bosons carrying $S = 1/2$:
  - $\mathbf{S} = \frac{1}{2} b^\dagger_\alpha \boldsymbol{\sigma}_{\alpha\beta} b_\beta, \qquad S = \frac{1}{2} b^\dagger_\alpha b_\alpha, \qquad \alpha = \uparrow, \downarrow.$
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- Method particuarly suitable for finding spin liquids:
  - Featureless quantum ground state.
  - Deconfined $S = 1/2$ excitations.
  - Topological order.
  - Square lattice with frustration, triangular, kagome.

N. Read and S. Sachdev, late 1980s.

Schwinger bosons in a pyrochlore

- Ground state breaks:
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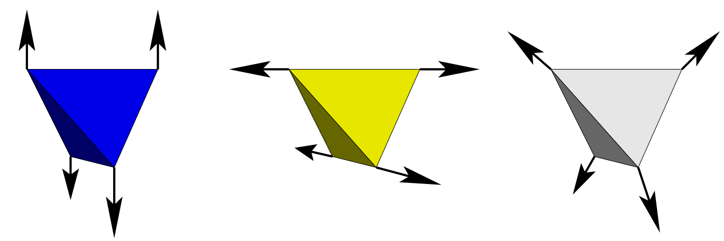
Schwinger bosons in a pyrochlore



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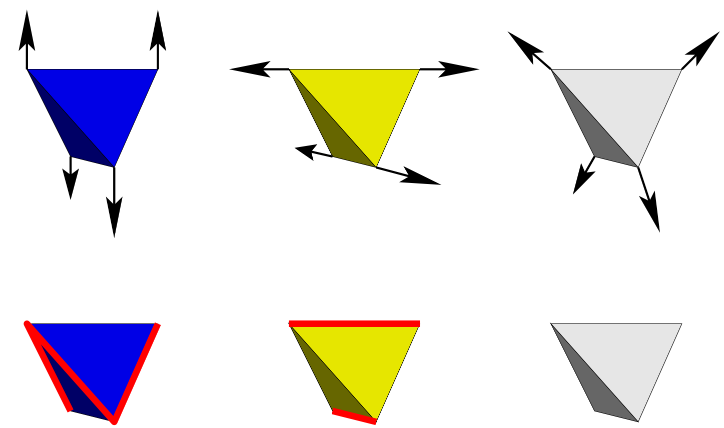

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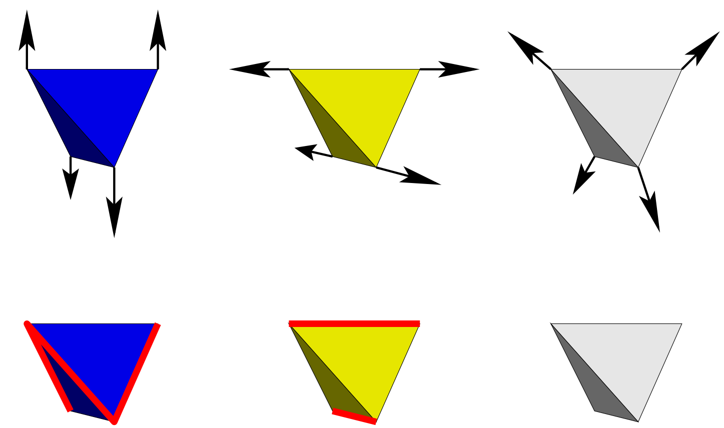

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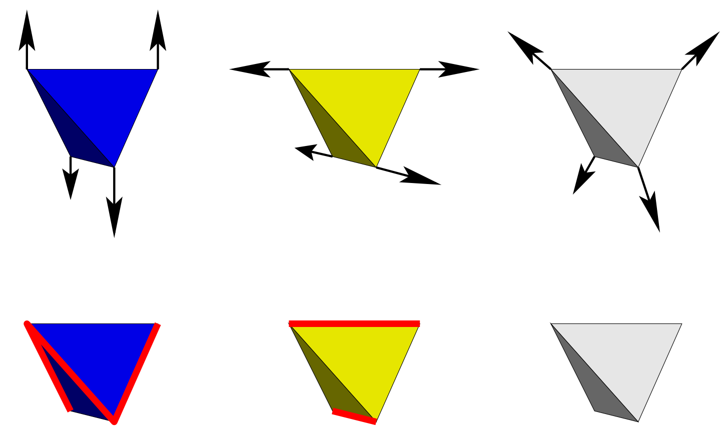

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