Chiral spin states in the pyrochlore Heisenberg magnet : Fermionic mean-field theory & variational Monte-carlo calculations

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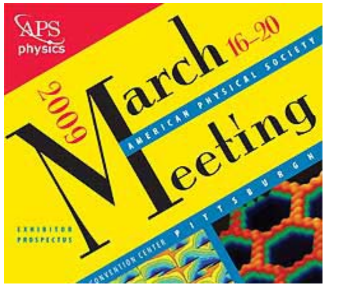
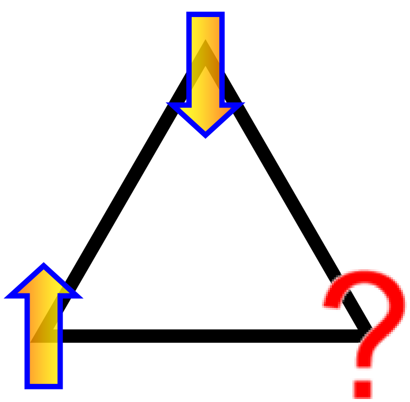


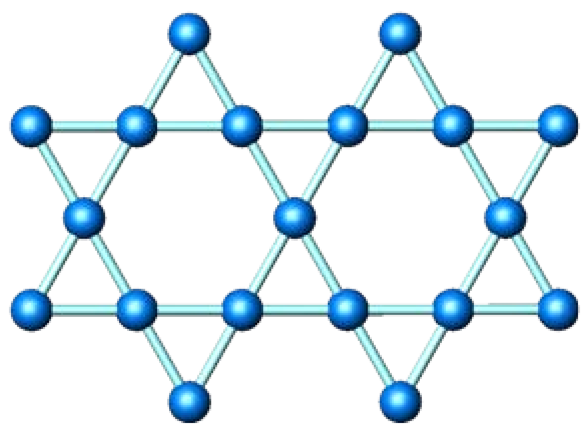
Introduction

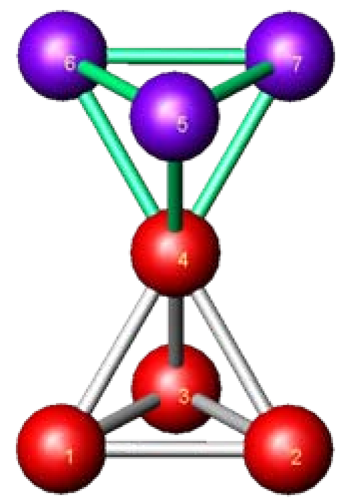
- We would like to better understand the quantum ground state of the spin-1/2 Heisenberg Hamiltonian on the pyrochlore lattice

- Frustrated Systems :
  - Systems in which all interactions cannot be simultaneously satisfied

➡ Can lead to exotic phases, excitations, ground states







Pyrochlore magnets

- (spin-ice) $Dy_2Ti_2O_7$, $Nd_2Mo_2O_7$
- (coop. para.) $Tb_2Ti_2O_7$
- (spin-Peierls) $ZnCr_2O_4$
- (Kondo lattice, AHE) $Nd_2Mo_2O_7$, $Pr_2Ir_2O_7$
- (Heavy fermion) LiV_2O_4
- Some are insulating, others metallic
  (We will focus on non-metallic pyrochlore magnet)
- Some spins Ising, others Heisenberg + anisotropy
- No known examples of insulating, S=1/2
  HAFM with pristine pyrochlore lattice

Classical magnet on pyrochlore lattice

- Classical Heisenberg AFM spins show
  No LRO, No ObyD, extensive GS degeneracy

Reimers PRB 45, 7287 (1992); Moessner, Chalker PRL 80, 2929 (1998)

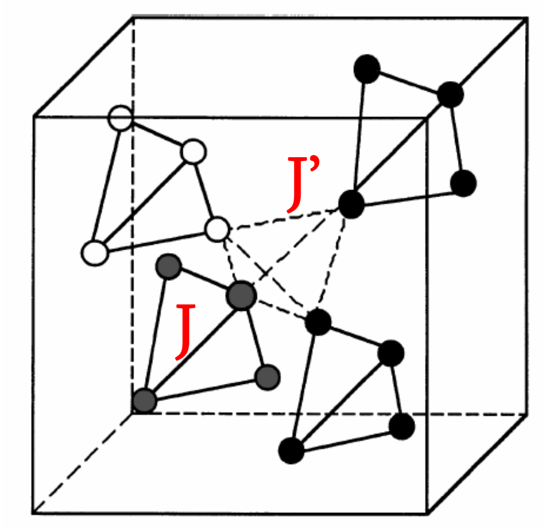
- Ising AFM spins show
  No LRO, No ObyD, extensive GS degeneracy,
  GS manifold shows dipolar spin-spin correlations

Anderson PR 102, 1008 (1956) ; Zinkin et al PRB 56, 11786 (1997);
Hermele et al. PRB 69, 064404 (2004); Isakov et al PRL 93, 167204 (2004);
Henley PRB 71, 014424 (2005)

Quantum S=1/2 magnet on pyrochlore

- Begin with one-tetrahedron solution of HAFM
- Inter-tetrahedra coupling is treated perturbatively (J'/J)

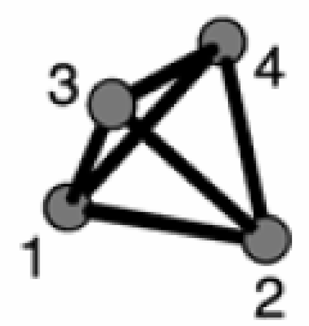
Harris, Berlinsky, Bruder, JAP 69, 5200 (1991)
Canals, Lacroix, PRL 80, 2933 (1998)
Tsunetsugu, JPSJ 70, 640 (2000); PRB 65, 024415 (2001)



Single tetrahedron

- Three dimer solutions of S=1/2 HAFM
  [12][34] , [13][24], [14][23],
  only two are independent

$$[ij] = (\uparrow_i \downarrow_j - \downarrow_i \uparrow_j)$$



- Two chiral solutions

$$\chi|\pm\rangle = \pm|\pm\rangle$$

$$\chi = \chi_{123} + \chi_{243} + \chi_{341} + \chi_{142}$$

$$\chi_{ijk} = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$$

Scalar spin chirality

A non-magnetic state with nonzero averages of scalar spin chirality was proposed by Wen, Wilczek, Zee in connection with high-Tc cuprates (sCSL)

$$\chi_{ijk} = \langle \mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k \rangle$$

sCSL breaks T (Time reversal symmetry) while
vCSL breaks I (Inversion symmetry)

Both spin chiralities arise due to some sort of frustration, including one of geometric nature (triangular, kagome, pyrochlore, etc)

Lattice of Tetrahedra

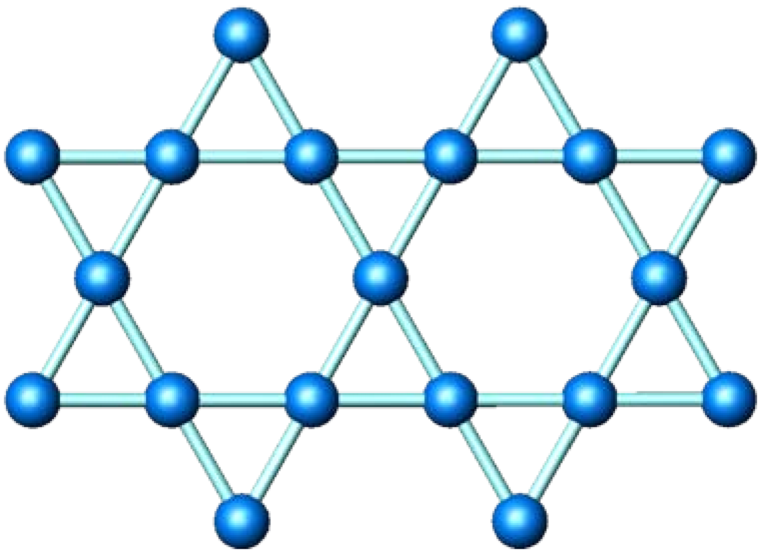
- When continued to pyrochlore lattice, the quantum GS may be

  (i) dimer solid with broken translational symmetry
  (ii) chiral spin liquid with broken time symmetry
  (iii) mixture of the two

- Previous theories based on J'/J expansion found enhanced dimer correlations, no sign of T-breaking

- We find T-breaking chiral spin liquid

VMC work on Kagome



$$H = \sum_{\langle ij \rangle} S_i \cdot S_j$$

$$S_i = \frac{1}{2} f^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} f_{i\beta}$$

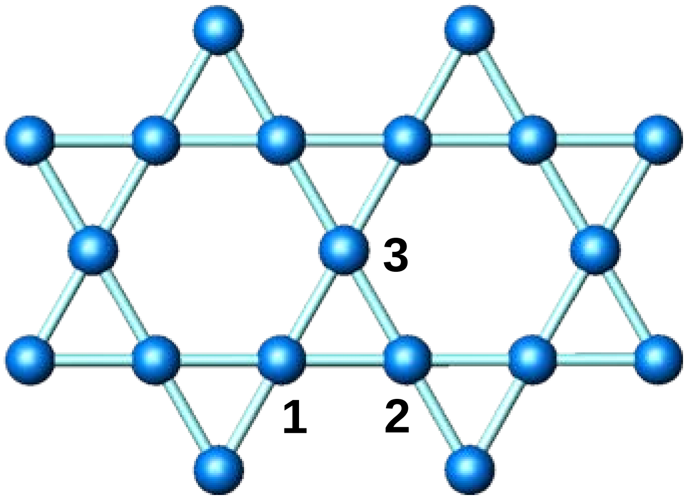
Solve Heisenberg model on the kagome lattice by

(1) Re-writing spin as a fermion bilinears
(2) Solve the mean-field theory with $\chi_{ij} = \langle \sum_\sigma f^{\dagger}_{j\sigma} f_{i\sigma} \rangle$
(3) Refine the state with Gutzwiller projection of doubly occupied sites

Ran et al. PRL 98, 117205 (2008); Hermele et al. arXiv:0803.1150v2

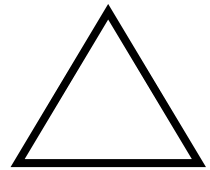
Flux States – Rokshar's Rule

Rokhsar PRL 65, 1506 (1990)

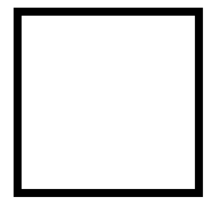


$$\prod_{\triangle} \chi_{ij} = \chi_{12}\chi_{23}\chi_{31} = \chi e^{i\Phi}$$

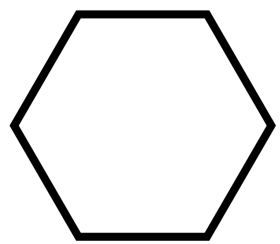
Φ : (physical) flux



$$\Phi = \frac{\pi}{2}$$



$$\Phi = \pi$$



$$\Phi = 0$$

VMC work on Kagome

In the fermionic representation of spins,

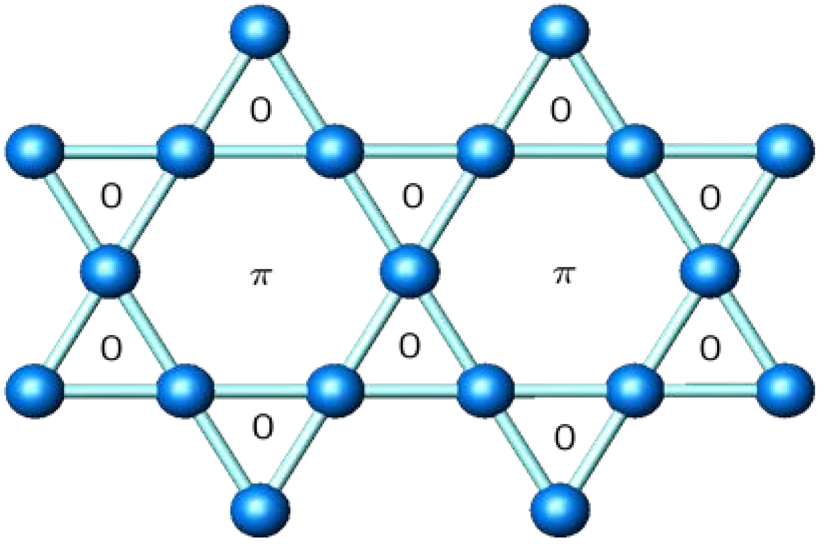
$$\chi_{ijk} = \langle \mathbf{S}_i \cdot \mathbf{S}_j \times \mathbf{S}_k \rangle =$$

$$\frac{1}{2i} \times (\langle (f_{i\sigma}^{+} f_{k\sigma})(f_{k\sigma}^{+} f_{j\sigma})(f_{j\sigma}^{+} f_{i\sigma}) \rangle$$

$$-\langle (f_{i\sigma}^{+} f_{j\sigma})(f_{j\sigma}^{+} f_{k\sigma})(f_{k\sigma}^{+} f_{i\sigma}) \rangle) \sim \sin(\Phi)$$

If Rokhsar's Rule was right, maximal chirality should be obtained for triangle-based lattices (Kagome, pyrochlore)

VMC work on Kagome



Nonchiral SL with π flux through hexagons had lowest VMC energy

Effective field theory is one of Dirac spinons

Had Rokhsar's rule prevailed, one would arrive at sCSL

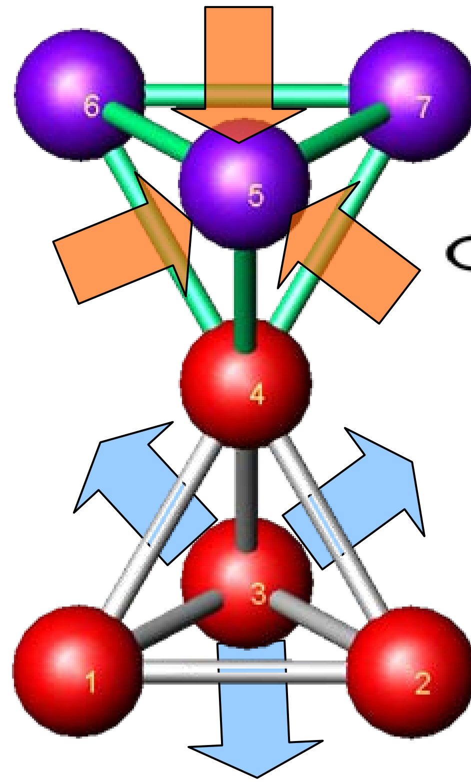
Mean-field analysis on pyrochlore

$$H = -\sum_{\langle ij \rangle} \chi_{ij} \sum_{\sigma} f^{\dagger}_{i\sigma} f_{j\sigma}$$

where $\chi_{ij} = \langle \sum_{\sigma} f^{\dagger}_{j\sigma} f_{i\sigma} \rangle$

Self-consistent mean-field solution gives chiral spin liquid ground state

π/2-flux through triangles,
0-flux through hexagons



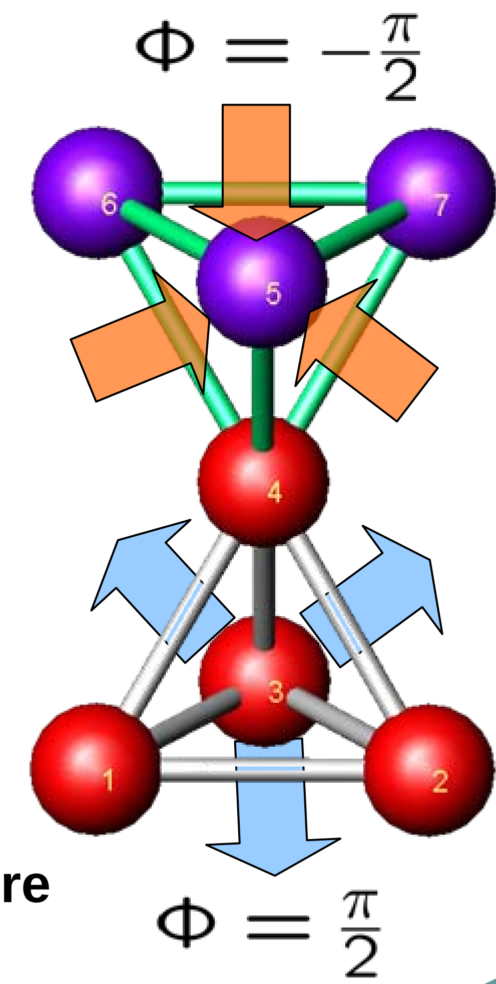
$\Phi = -\frac{\pi}{2}$

$\Phi = \frac{\pi}{2}$

VMC work on pyrochlore

TABLE I. Energy per site of various states obtained from VMC depending on the number of up tetrahedra L in each direction. The two chiral states have much lower energies than the nonchiral states. Statistical uncertainties lie below the digits shown. Boundary conditions, aPBC or PBC, used in the calculation are listed.

L	$[0,0,0]$	$[\frac{\pi}{2},\frac{\pi}{2},0]$	$[\frac{\pi}{2},-\frac{\pi}{2},0]$	$[0,0,\pi]$
	aPBC	aPBC	PBC	PBC
2	−0.372	−0.478	−0.466	−0.374
4	−0.374	−0.459	−0.456	−0.375



- **VMC ground state is *chiral* for the pyrochlore**

VMC work on pyrochlore

Average flux through each triangle can be calculated within VMC

Amount of flux is reduced from mean-field value pi/2

CSL state with long-range ordered chiralities

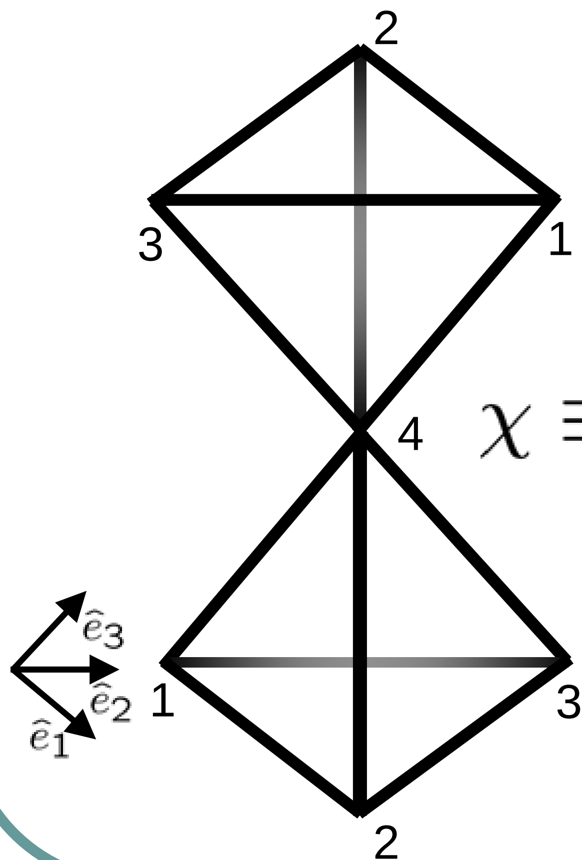
TABLE III. The real and imaginary parts of the averages of $\langle s_+|\psi\rangle/\langle s|\psi\rangle$ and the flux (in units of $\pi/2$) through the triangle for $[\frac{\pi}{2},\frac{\pi}{2},0]$ (left three columns) and $[\frac{\pi}{2},-\frac{\pi}{2},0]$ (right three columns).

L	η_{123}	$\|\chi_{123}\|$	$\|\Phi_{123}\|$	η_{123}	$\|\chi_{123}\|$	$\|\Phi_{123}\|$
2	0.376	0.356	0.483	0.368	0.325	0.461
4	0.314	0.358	0.542	0.312	0.358	0.544

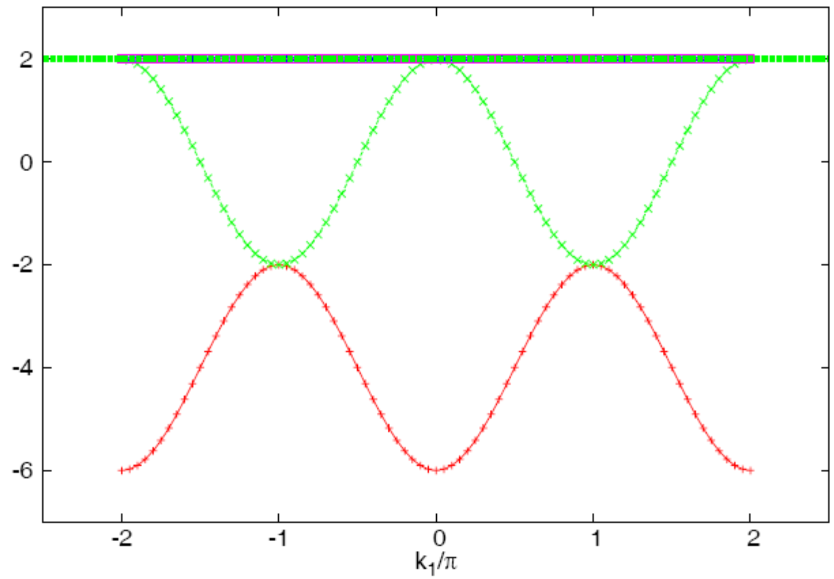
Flux States – Pyrochlore

- [0, 0, 0]-flux state

Jung Hoon Kim and Jung Hoon Han
arXiv 0807.2036

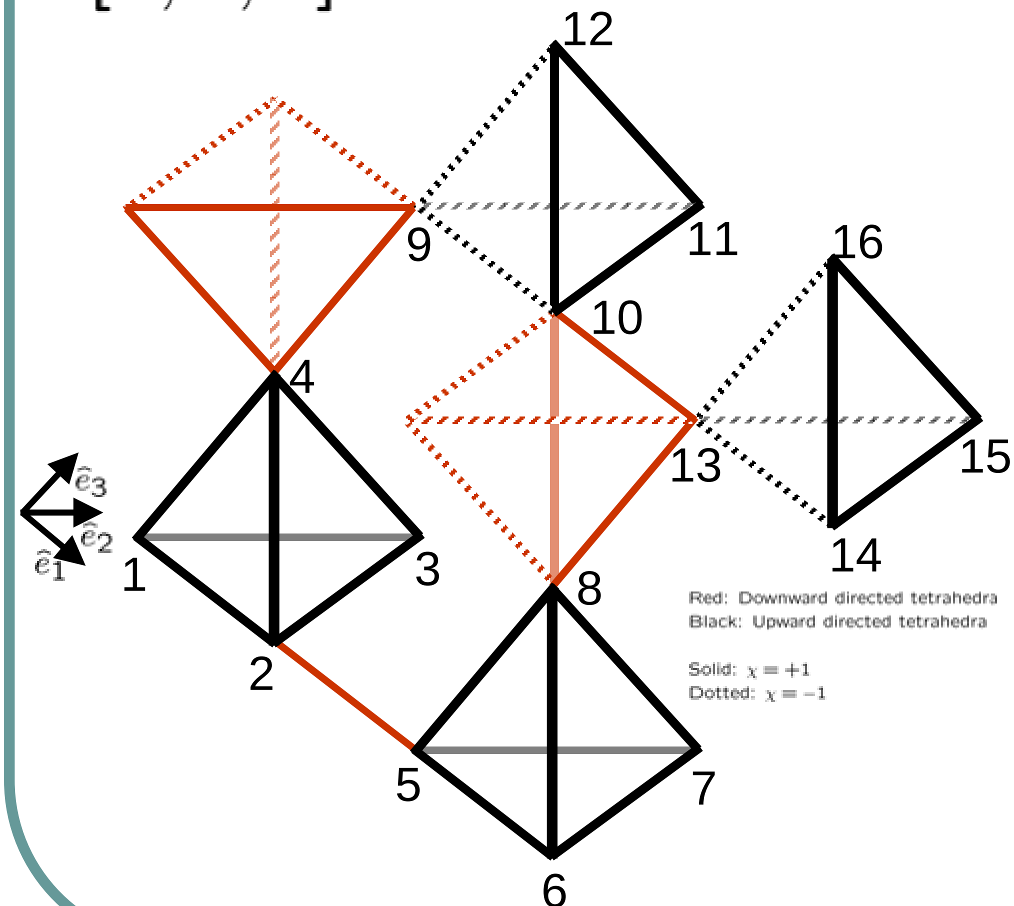


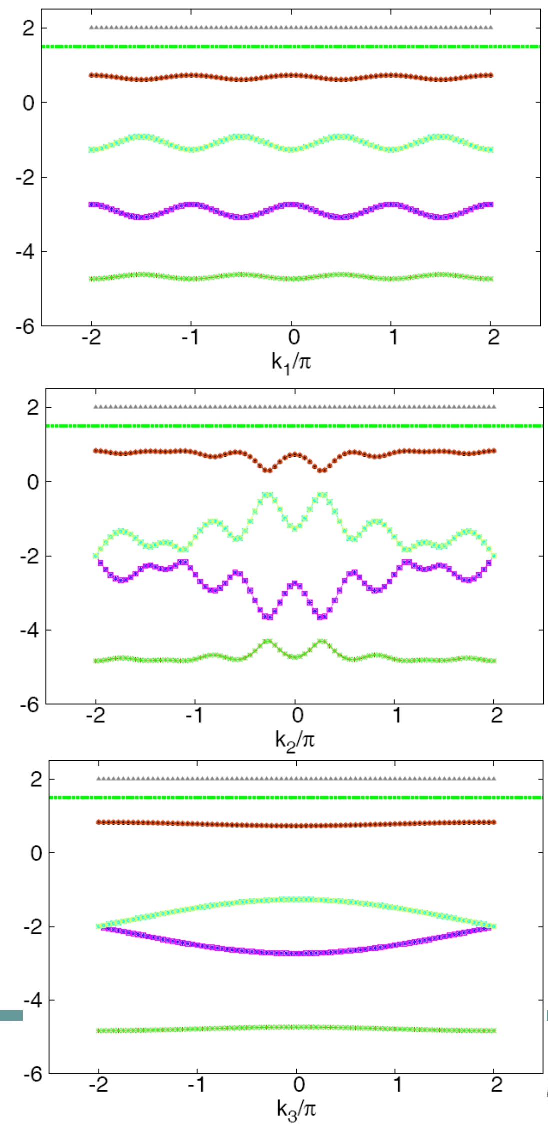
$$\chi \equiv 1$$



Flux States – Pyrochlore

- $[0, 0, \pi]$-flux state





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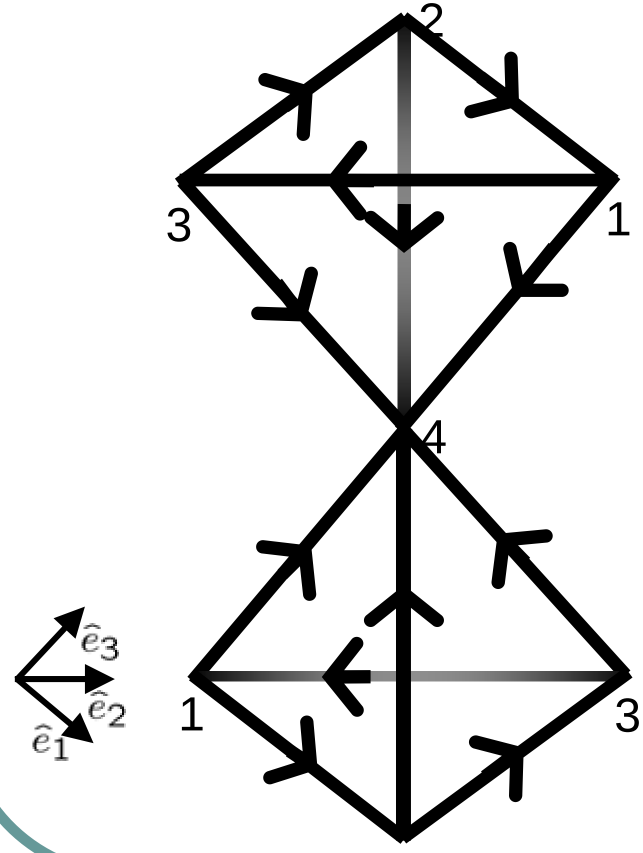
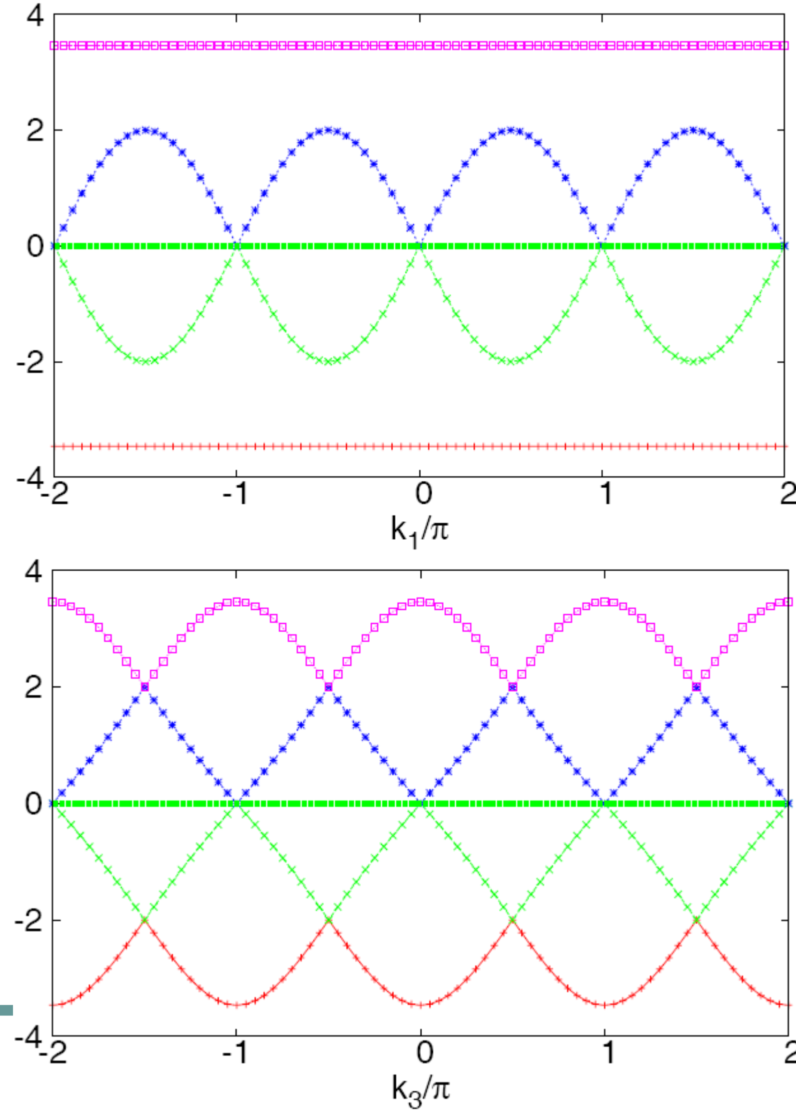
Flux States – Pyrochlore

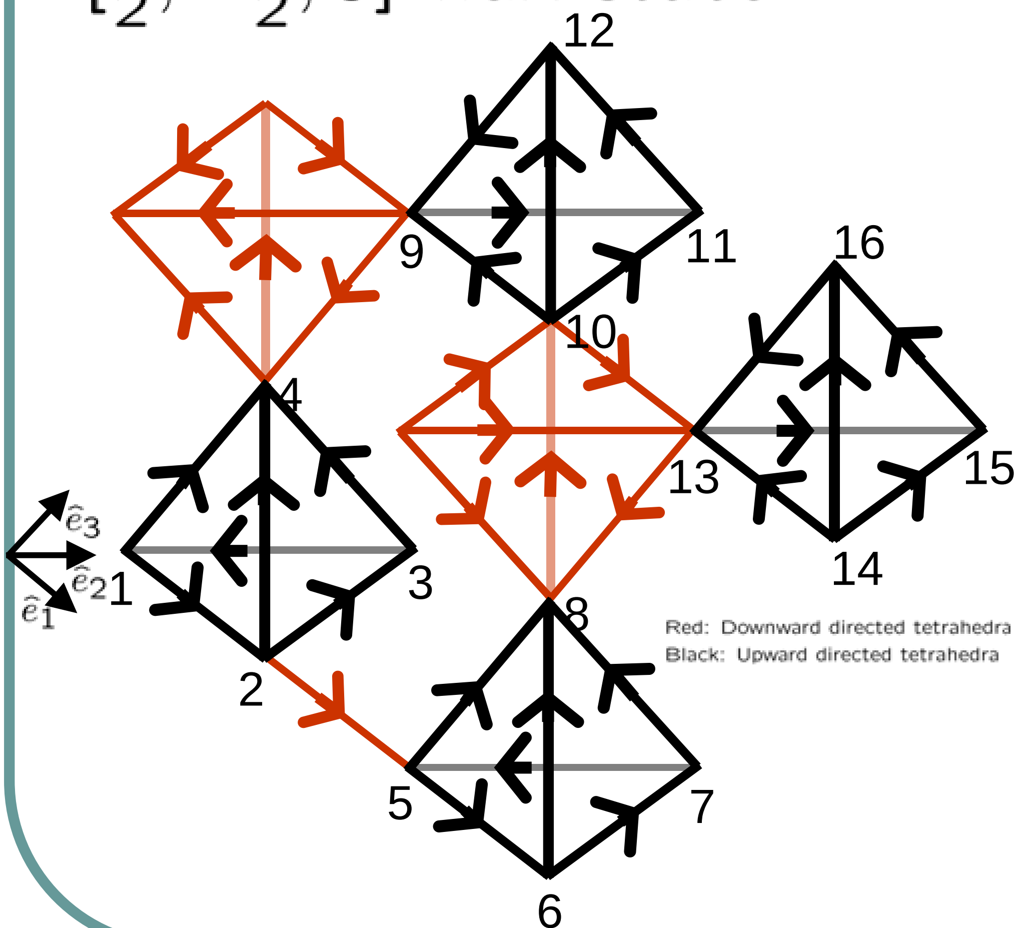
- $[\frac{\pi}{2}, \frac{\pi}{2}, 0]$-flux state

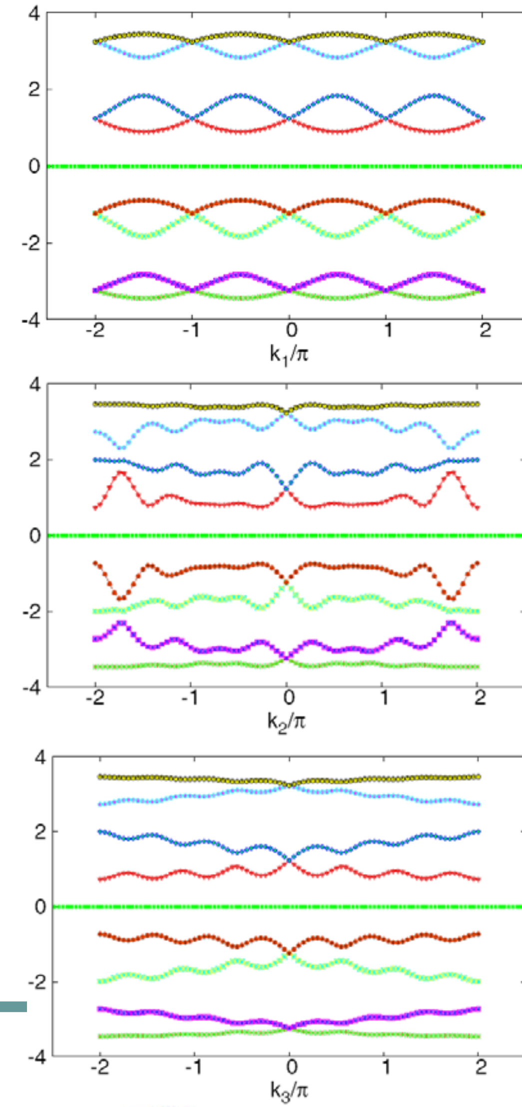




Flux States – Pyrochlore

- $[\frac{\pi}{2}, -\frac{\pi}{2}, 0]$-flux state





Summary

- Fermionic mean-field theory and variational Monte Carlo techniques have been employed to understand the nature of the ground state of the spin-1/2 Heisenberg model on the pyrochlore lattice.

- From VMC calculations, of the four different flux states considered, the [π/2,π/2,0]-flux state had the lowest energy.

- The two flux states, [π/2,π/2,0] and [π/2,$-\pi$/2,0], have non-zero expectation values of the scalar chirality, $\langle S_i \cdot S_j \times S_k \rangle$, showing that they are indeed chiral flux states (*i.e.* states with broken time-reversal symmetry).

- Dimer instability found previously contrasts with T-breaking state found here

- Resolving contending views will require new ideas (maybe some ED)

PRB 78, 180410(R) 2008

See also :
F. J. Burnell, Shoibal Chakravarty, and S. L.Sondhi, arXiv:0809.0528v1.