Chiral Spin States in the Pyrochlore Heisenberg Magnet

Jung Hoon Kim & Jung Hoon Han

Department of Physics, Sungkyunkwan University, Korea

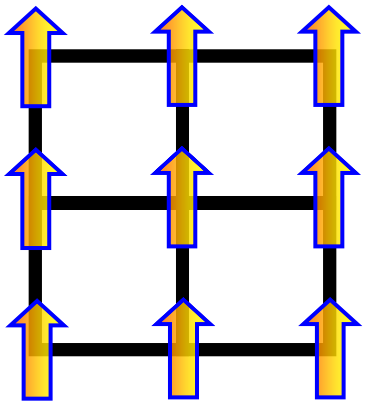
PRB 78, 180410(R) (2008)

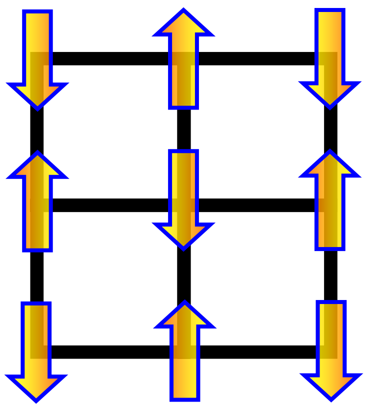
Introduction

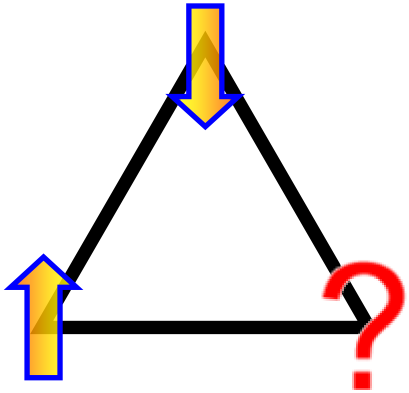
- We would like to better understand the quantum ground state of the spin-1/2 Heisenberg Hamiltonian on the pyrochlore lattice

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

➡ Can lead to exotic phases and completely different ground states

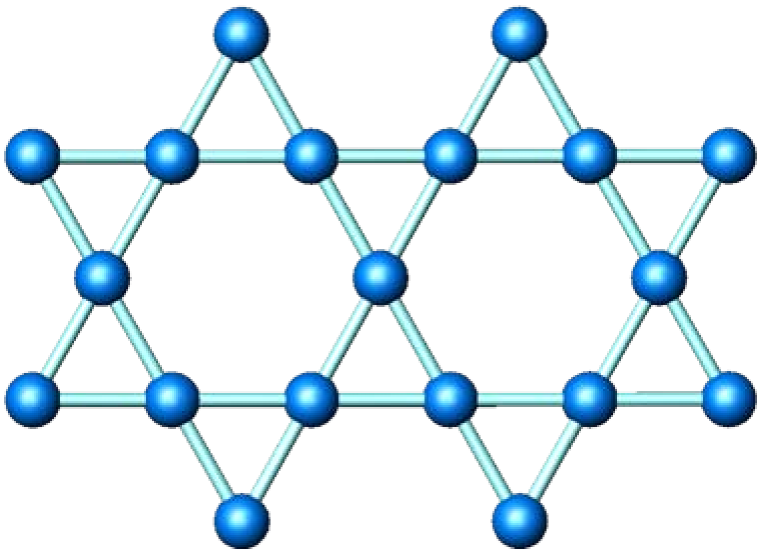




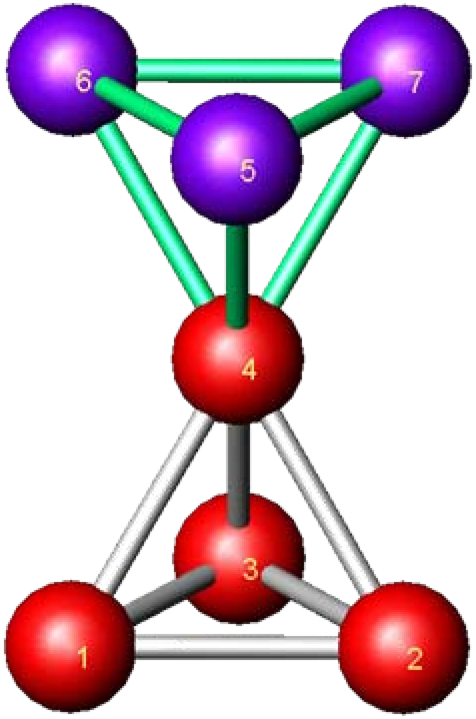


Introduction (2)

- Highly Frustrated Systems



Kagome Lattice



Pyrochlore Lattice

Mean–field Analysis

- Solve the Heisenberg Hamiltonian within fermionic mean-field theory

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

J = exchange interaction

S_i = spin operator at site i

- Rewrite spin operators as fermion bilinears

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

$$S_i \cdot S_j \quad \Rightarrow \quad (f_i^\dagger \boldsymbol{\sigma} f_i)(f_j^\dagger \boldsymbol{\sigma} f_j)$$

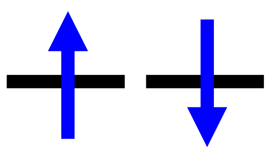
Terms of 4 interacting fermions

Mean-field Analysis

- Apply mean-field theory (consider hopping terms only : $\langle f_j^\dagger f_i \rangle$)

$$H = -\sum_{\langle ij \rangle} \chi_{ij}^* \sum_\sigma f_{j\sigma}^\dagger f_{i\sigma} - \sum_{\langle ij \rangle} \chi_{ij} \sum_\sigma f_{i\sigma}^\dagger f_{j\sigma} \quad \text{where } \chi_{ij} = \langle \textstyle\sum_\sigma f_{j\sigma}^\dagger f_{i\sigma} \rangle$$

- Interested in spin-1/2 systems

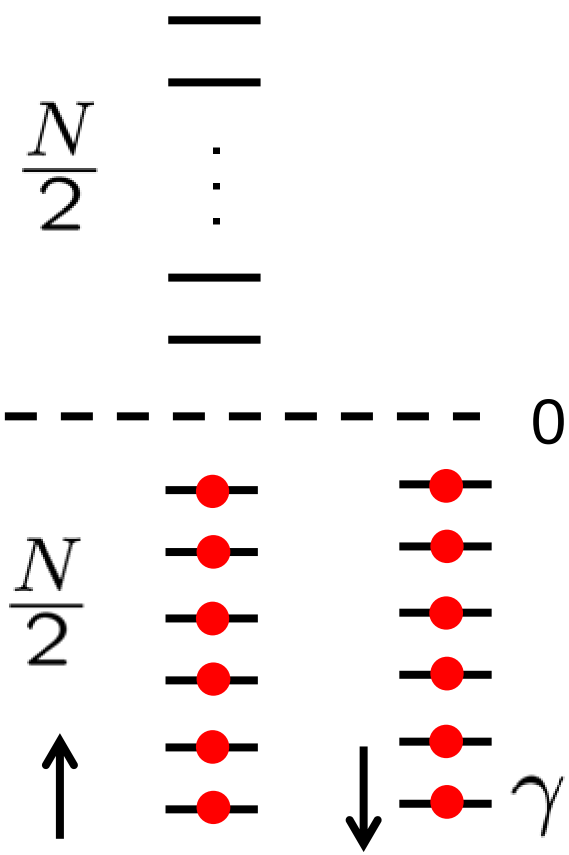
- Allowed states  ⇨ constraint : $f_{i\uparrow}^\dagger f_{i\uparrow} + f_{j\downarrow}^\dagger f_{j\downarrow} = 1$

$$\sum_i \lambda_i \left(\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} - 1 \right) \quad : \text{ chemical potential}$$

$$H_{MF} = -\sum_{\langle ij \rangle} \chi_{ij}^* \sum_\sigma f_{j\sigma}^\dagger f_{i\sigma} + \sum_i \left(\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} - 1 \right)$$

Mean-field Analysis

- For the half-filled case :



- Project out doubly occupied states by Gutzwiller projection

$$e.g.\quad \text{for } i=1,\ u_{11}u_{11}f^\dagger_{1\uparrow}f_{1\downarrow}$$
$$u_{12}u_{12}f^\dagger_{2\uparrow}f_{2\downarrow}$$

$$|GS\rangle = \prod_\sigma \gamma^\dagger_{\frac{N}{2}\sigma}\cdots\gamma^\dagger_{2\sigma}\gamma^\dagger_{1\sigma}|0\rangle$$

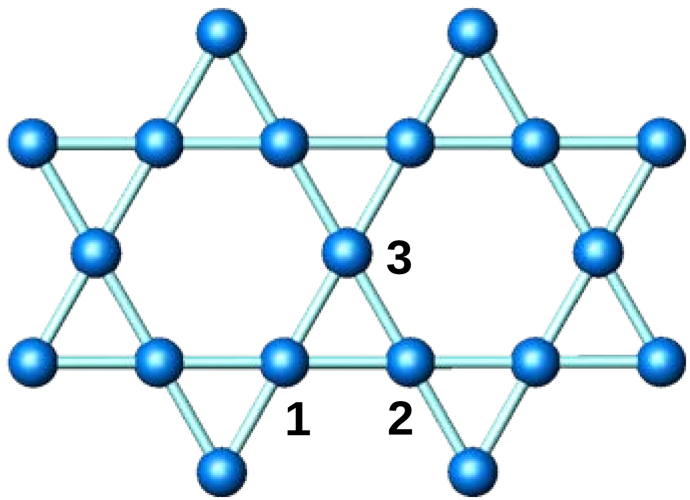
$$\gamma^\dagger_{1\sigma} = \sum_i u_{1i}f^\dagger_{i\sigma},\ \gamma^\dagger_{2\sigma} = \sum_i u_{2i}f^\dagger_{i\sigma}$$

$$|GS\rangle = \sum_s \psi_s|s\rangle + \sum_d \psi_d|d\rangle$$

Tractable by numerical analysis (Variational Monte Carlo)

Flux States – Kagome

- Possible flux states (Kagome) :

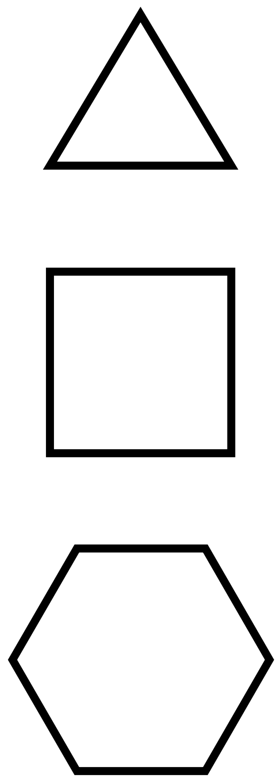


$$\prod_{\triangle} \chi_{ij} = \chi_{12}\chi_{23}\chi_{31} = \chi e^{i\Phi}$$

Φ : flux $\rightarrow$ gauge invariant

- Rokhsar's theorem

Rokhsar PRL 65, 1506 (1990)



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

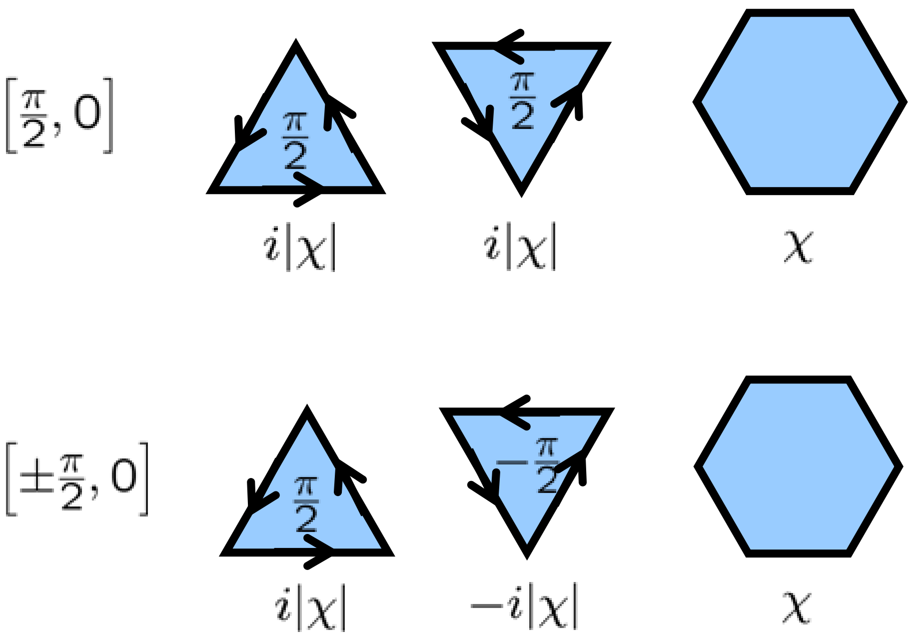
$$\Phi = \pi$$

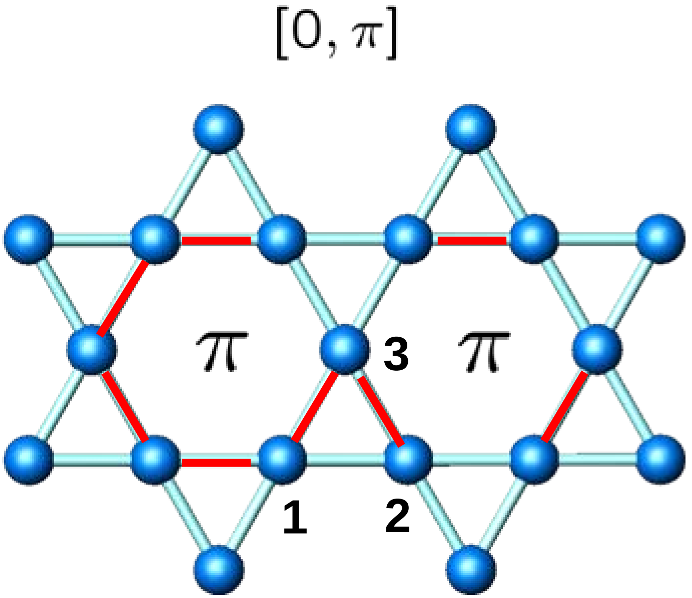
$$\Phi = 0$$

Flux States – Kagome

- Possible flux states (Kagome) :

Ran *et al.* PRL 98, 117205
Hermele *et al.* arxiv:0803.1150v2

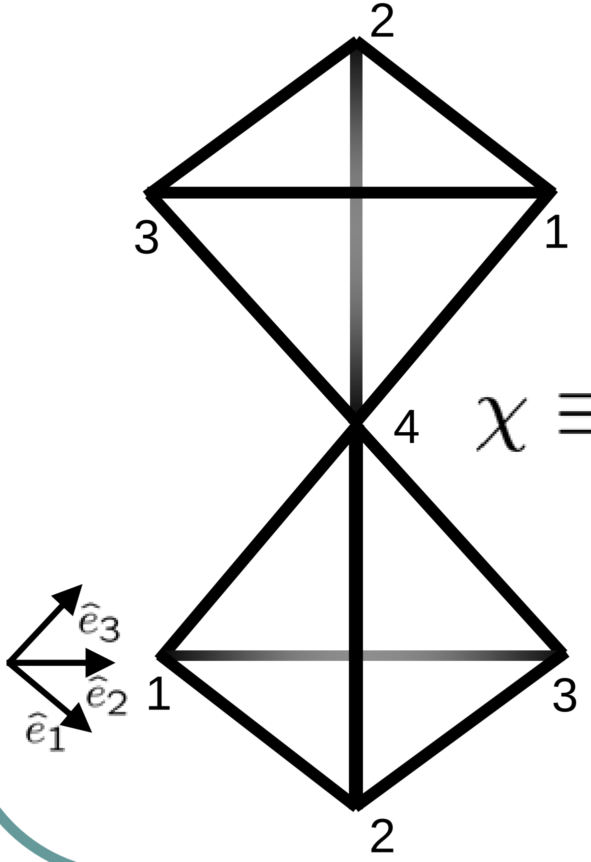




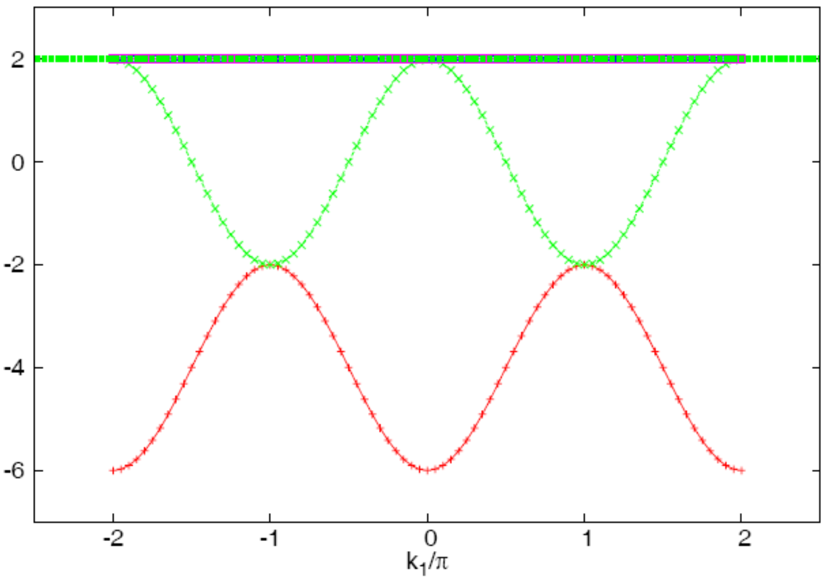
Flux States – Pyrochlore

- [0, 0, 0]-flux state

Jung Hoon Kim and Jung Hoon Han
arXiv 0807.2036

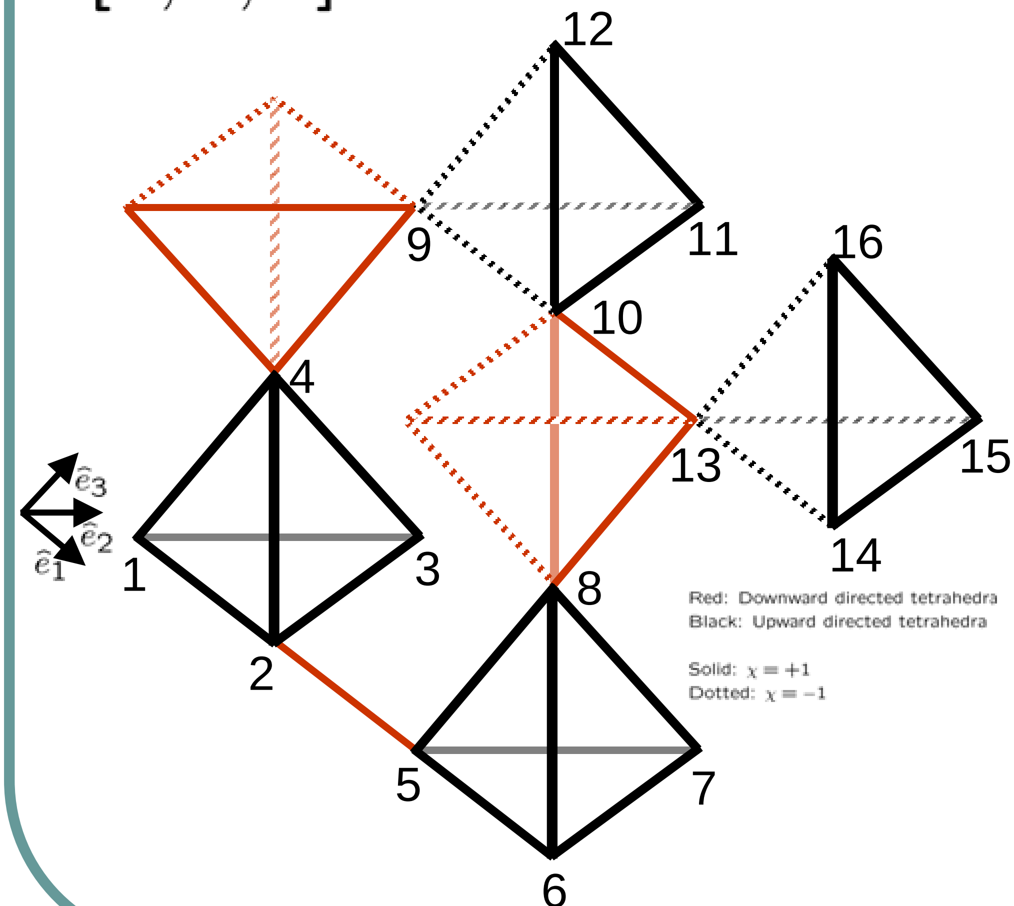


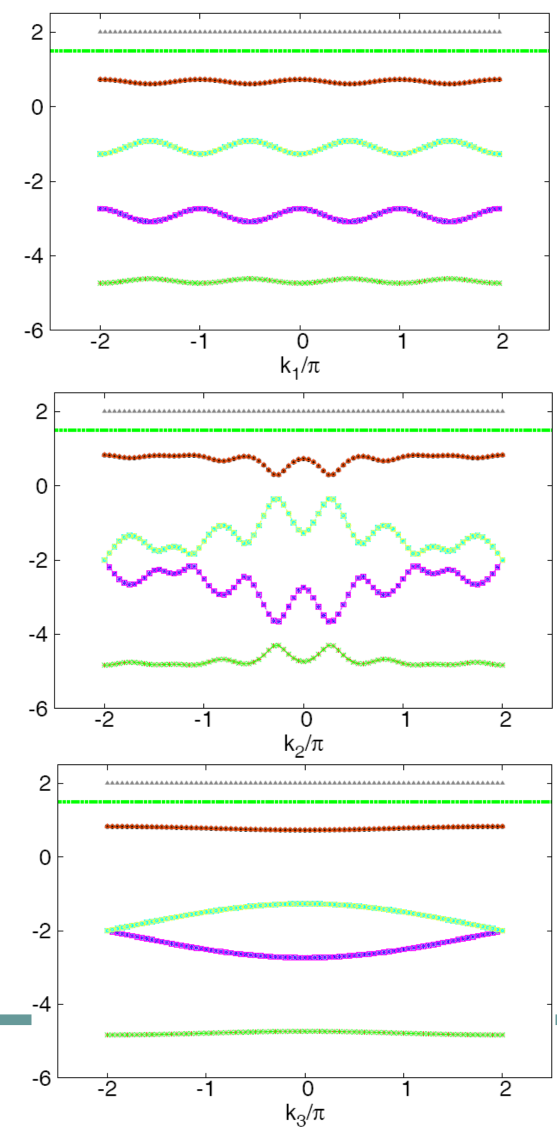
$\chi \equiv 1$



Flux States – Pyrochlore

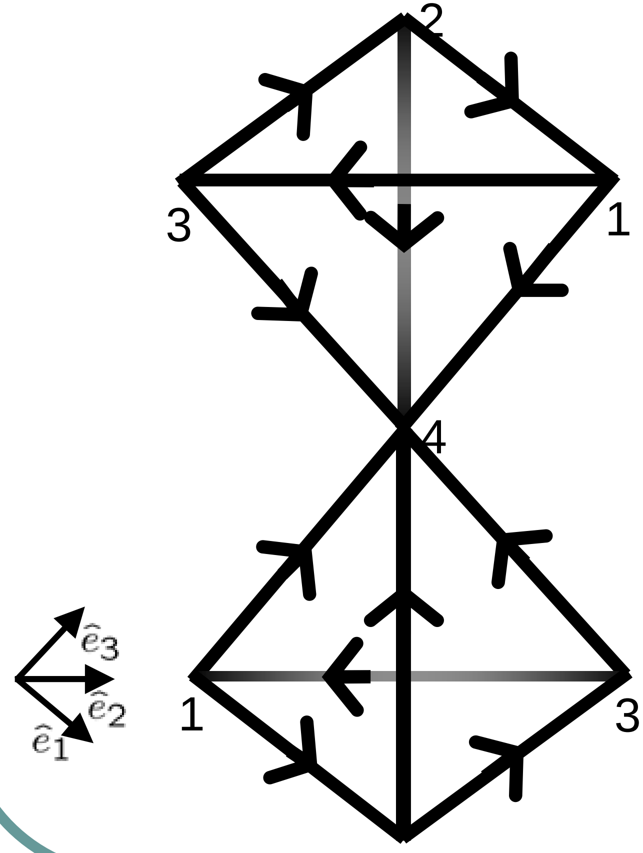
- $[0, 0, \pi]$-flux state

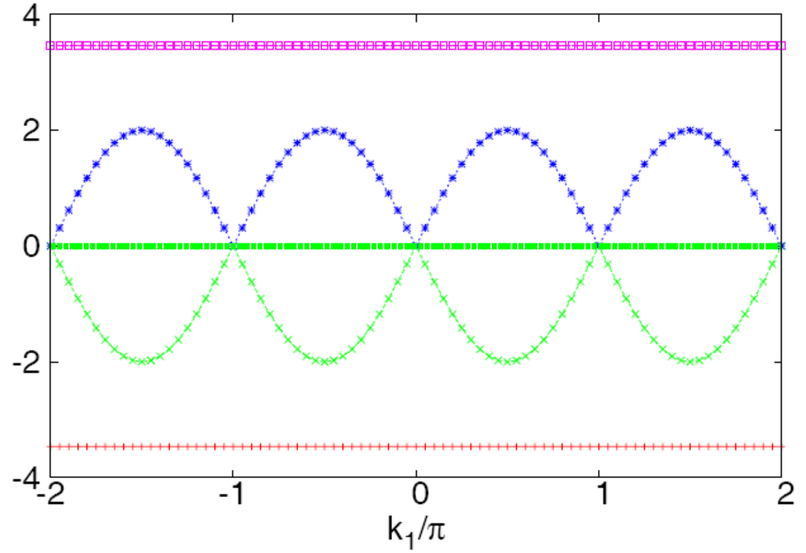


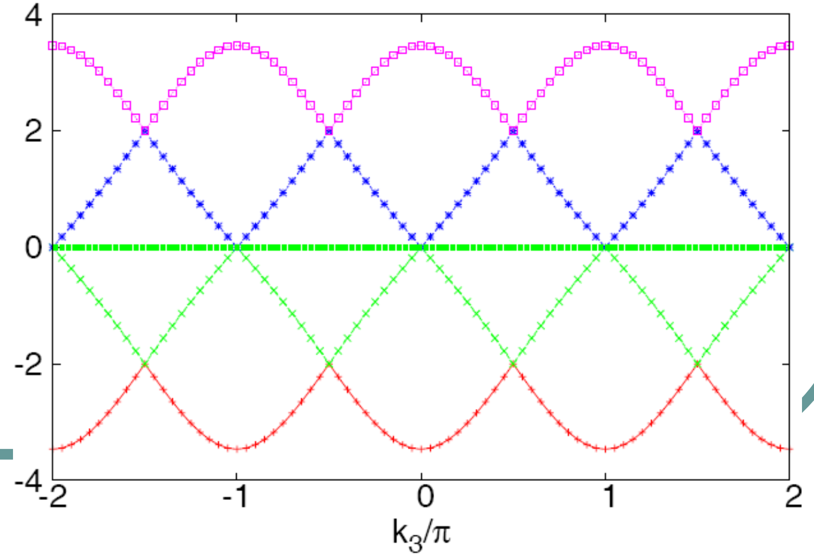


Flux States – Pyrochlore

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

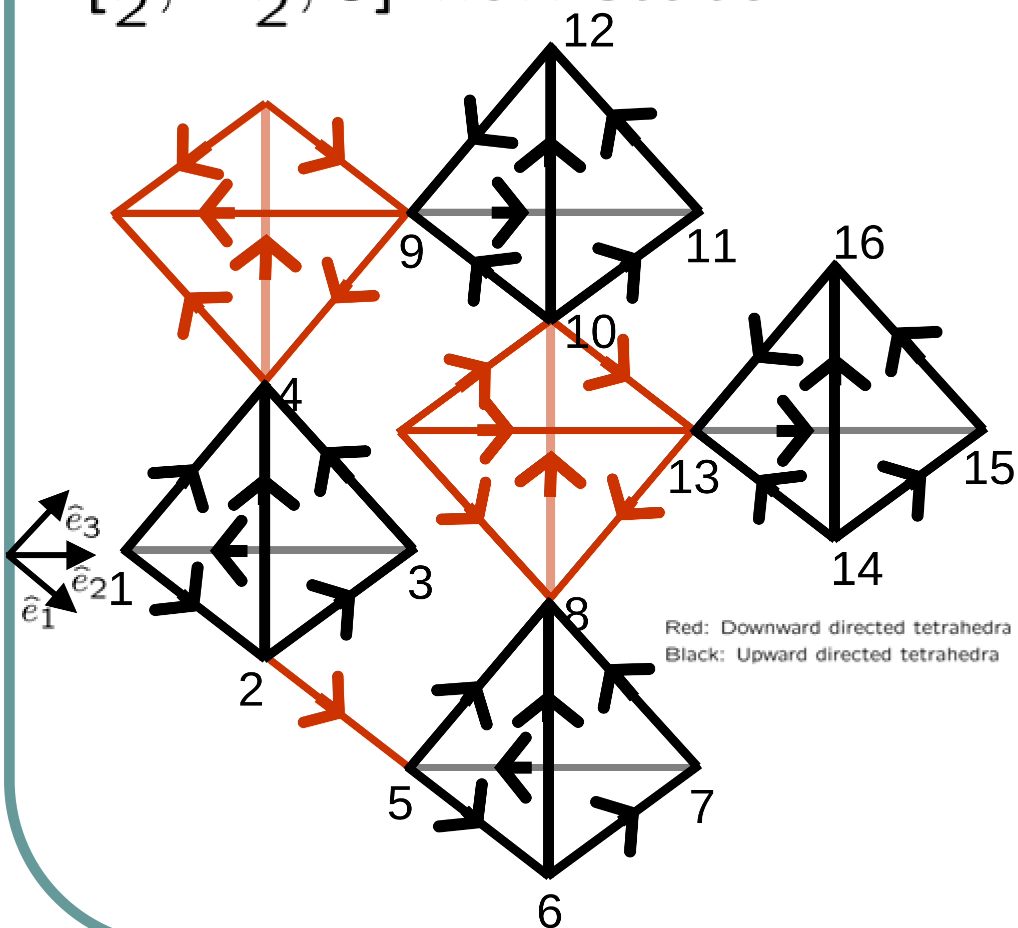


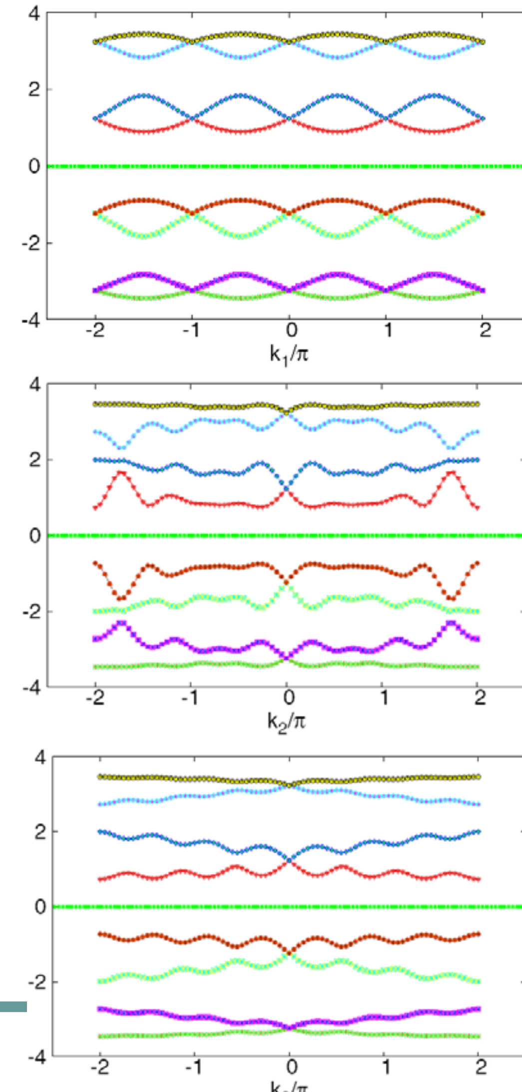




Flux States – Pyrochlore

- $[\frac{\pi}{2}, -\frac{\pi}{2}, 0]$-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.
- Although the [π/2,π/2,0]-flux state had the lowest energy, the [π/2,–π/2,0]-flux state is the more stable state, as can be seen from the band structure.
- Due to the rapid decrease of the spin-spin correlation and small lattice sizes considered, it was hard to distinguish between a power law and exponential decay of the spin-spin correlation function.
- The two flux states, [π/2,π/2,0] and [π/2,–π/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).