Lattice-coupled Antiferromagnet on Frustrated Lattice

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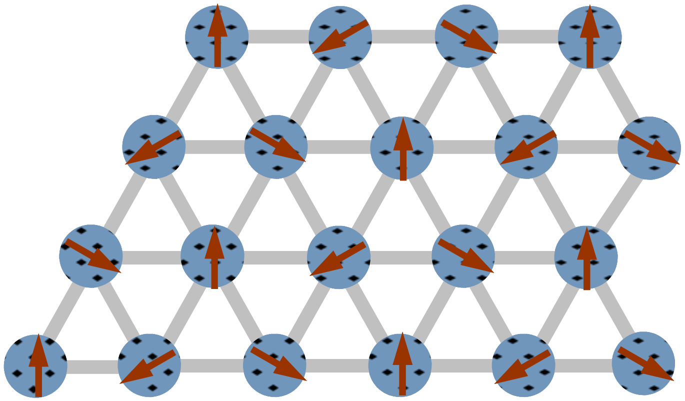
The lattice-coupled spin model

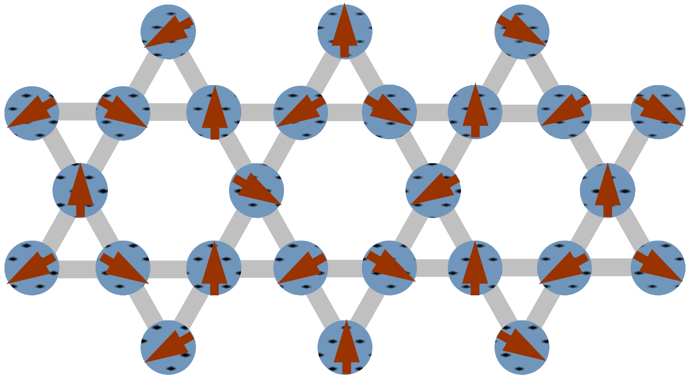
$$H = \sum_{\langle ij \rangle} \left[J_0 - J_1 \hat{e}_{ij} \bullet (u_i - u_j) \right] S_i \bullet S_j + \frac{K}{2} \sum_i u_i^2 \quad \textbf{(1)}$$

where $\hat{e}_{ij}$ is the unit vector, and u_i is the displacement vector of each ion. Minimizing the energy gives the condition relating the lattice positions with the spin:

$$\frac{K}{J_1} u_i = \langle f_i \rangle = \sum_{j \in i} \hat{e}_{ij} \langle S_i \bullet S_j \rangle \quad \textbf{(2)}$$

Triangular and Kagome Lattice





For these two types lattice structure, ground state spins possess the rotational symmetry, and the displacement becomes,

$$\langle f_i \rangle = \sum_k \langle S_k \bullet S_{-k} \rangle \sum_{j \in i} \hat{e}_{ij} e^{ik\cdot(r_j - r_i)} \equiv 0$$

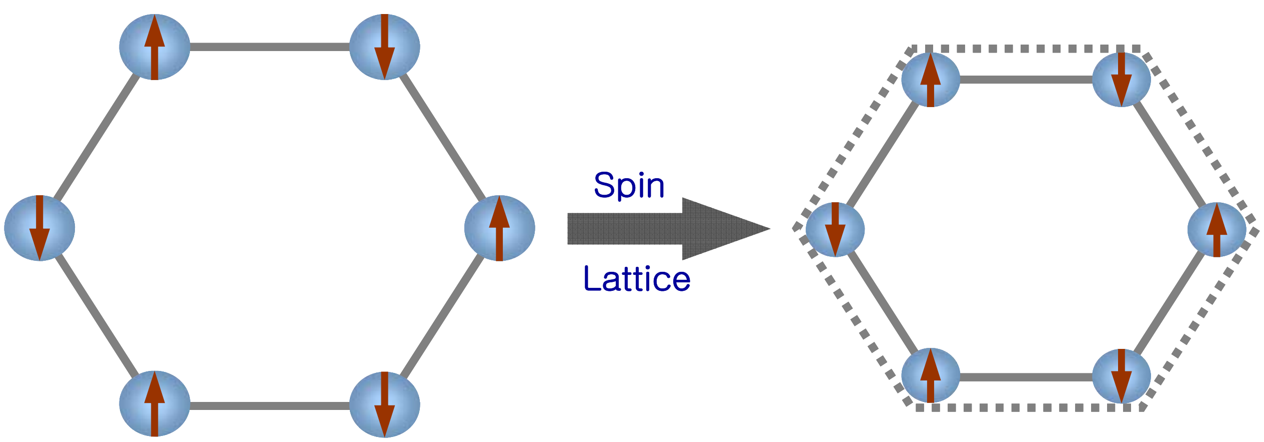
So, **the spin-lattice interaction does not lead to a static *lattice distortion*.**

A Single Hexagonal Chain

For a single hexagonal AFM chain coupled to the lattice, Eq.(2) gives

$$\langle f_i \rangle = \left[S(S+1) - \frac{S}{6} \sum_k \omega_k (n_B(k) + \frac{1}{2}) \right] \sum_{j \in i} \hat{e}_{ji} \qquad \textbf{(3)}$$

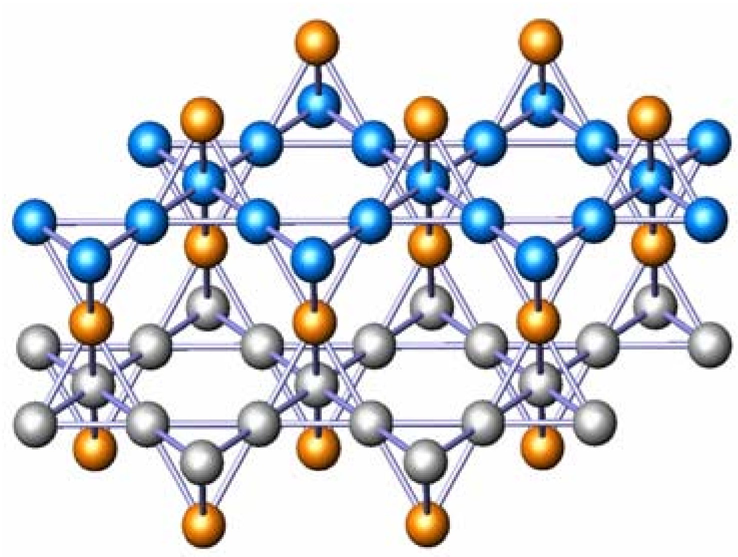
in the HP analysis. Eq.(3) imply that u_i all pointing inward to the center of the Hexagon.

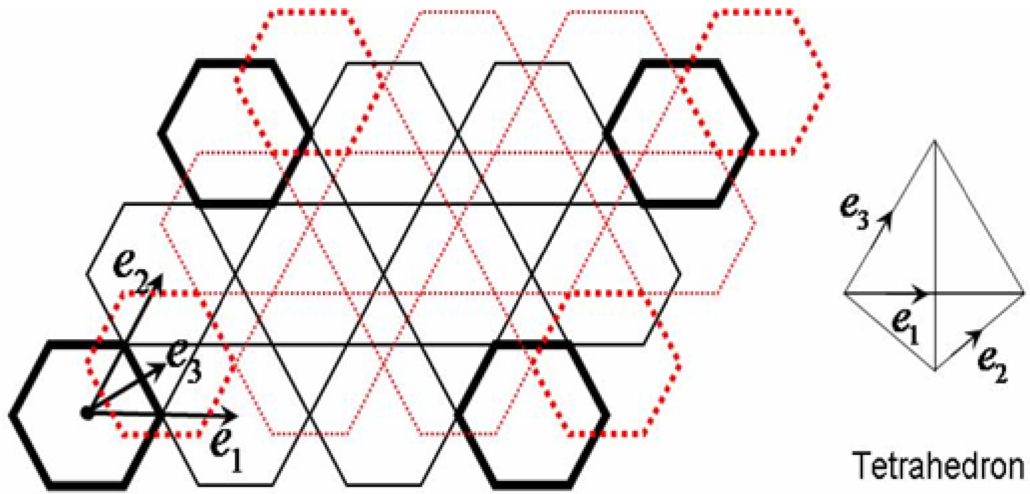


Pyrochlore Lattice

➢Lattice structure

Taking one Kagome plane as the basal, three vectors span the pyrochlore:

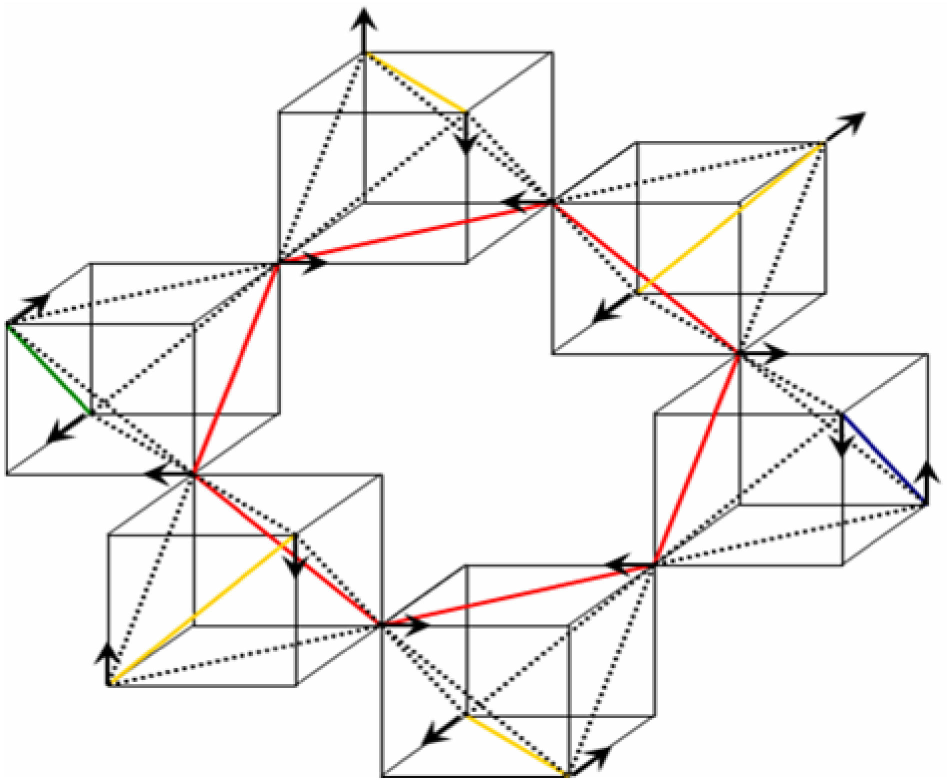




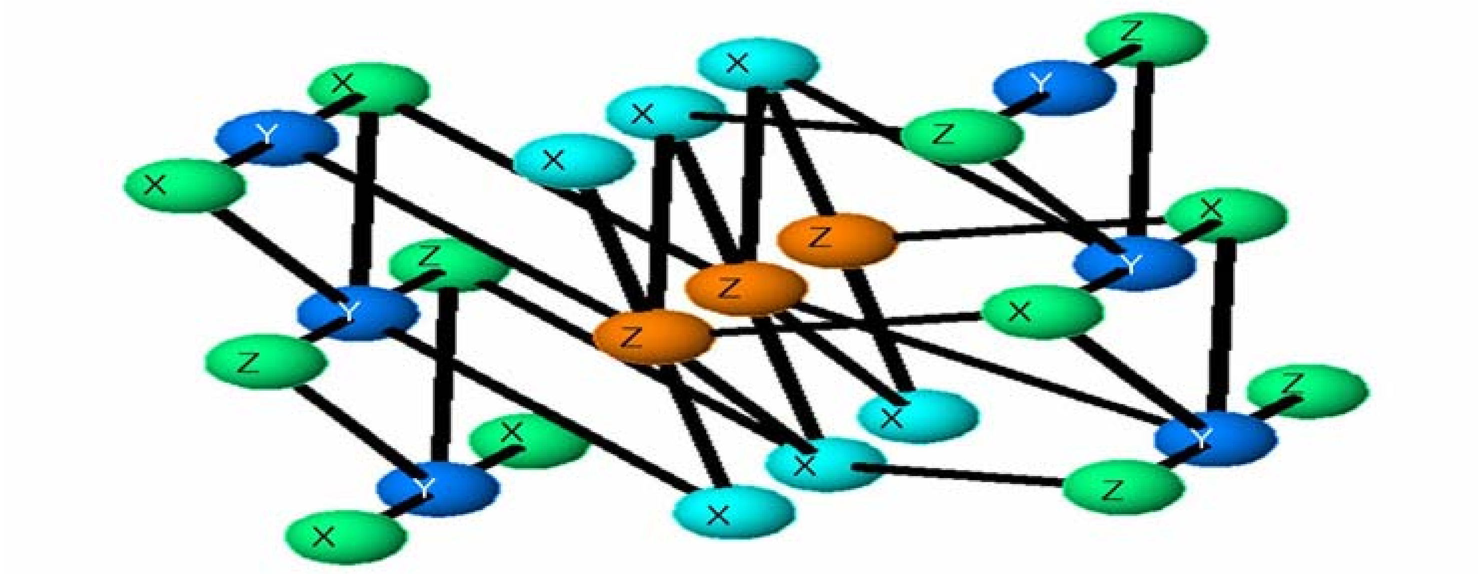
A unit cell has a 2x2x3 structure with eight hexagon.

➢The distortion of pyrochlore lattice

Requiring a uniform hexagon contraction throughout the whole pyrochlore lattice, Eq.(2) imposes the condition that the directors of the NN hexagons must be orthogonal:



➢Residual H-H interaction



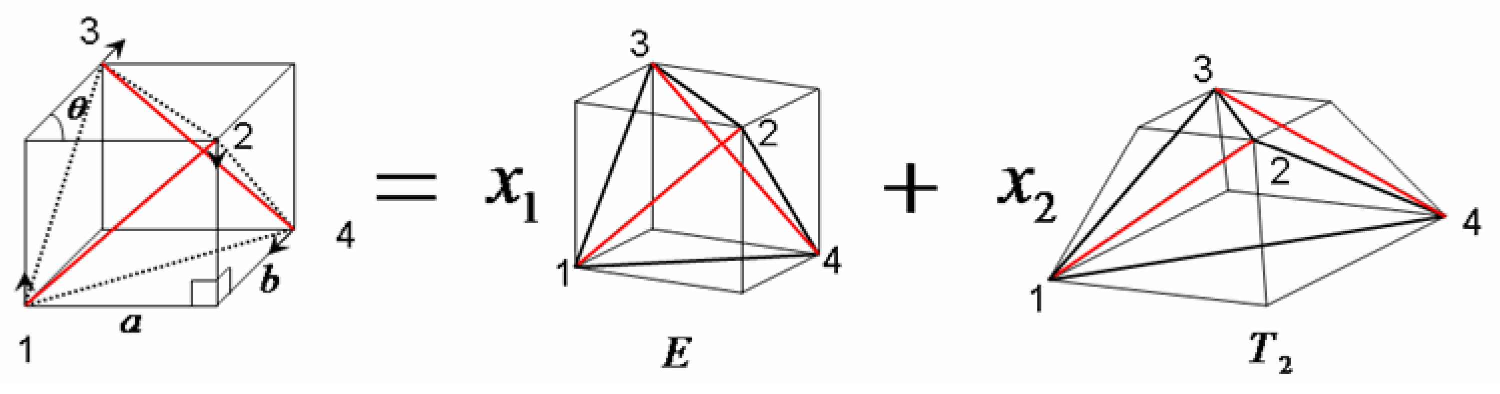
NN hexagon-hexagon interaction satisfies an AFM 3-states Potts model:

$$H_{3SP} = J_{eff} \sum_{\langle IJ \rangle} \delta(d_I, d_J)$$

Where directors take on three allowed orientations, X, Y, Z.

➢The distortion of an isolated tetrahedron

When the pyrochlore lattice undergoes the hexagon contraction, the resulting distortion for an isolated tetrahedron is not tetragonal (E), but is a linear combination of a doublet E and a triplet T_2 . The spin configuration is coplanar.



Summary

Employing the acoustic phonon model leads to the same conclusion:

- ***In triangular and Kagome lattices, spin-lattice coupling does not lead to a static deformation of the lattice, whether at the classical or quantum-mechanical level.***

- ***In pyrochlore lattice, spin-lattice coupling supports a particular pattern of lattice distortion, namely a hexagon contraction.***