Field dependence of spin wave dispersions of the splay phase of the ferromagnetic pyrochlore lattice

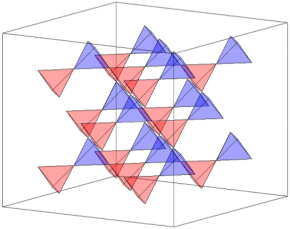
Project presentation By : Haraprasad Dhal

Project Guided By : Dr. V. Ravi Chandra

NISER,Bhubaneswar

November 30, 2022

Pyrochlore lattice



- Sixfold-coordinated structure whose underlying Bravais lattice is FCC,with four basis.primitive vectors:$\{(\frac{1}{2},\frac{1}{2},0),(0,\frac{1}{2},\frac{1}{2}),(\frac{1}{2},\frac{1}{2},0)\}$. Sublattice vectors:$[(0,0,0),(\frac{1}{4},\frac{1}{4},0),(0,\frac{1}{4},\frac{1}{4}),(\frac{1}{4},0,\frac{1}{4})]$
- Along [111]:stacking of Triangular and Kagom$e^{\prime}$ Lattice planes.
- Along [100] and [110] ,square and rectangular lattice planes with bases.

Spin Hamiltonian

$$H = \sum_{<i\alpha,j\beta>} J\mathbf{S}_{i\alpha} \cdot \mathbf{S}_{j\beta} + \sum_{<i\alpha,j\beta>} \mathbf{D}_{i\alpha,j\beta} \cdot \mathbf{S}_{i\alpha} \times \mathbf{S}_{j\beta} + K \sum_{i\alpha} (\mathbf{S}_{i\alpha} \cdot \hat{\mathbf{n}}_{\alpha})^2 - \sum_{i\alpha} \mathbf{S}_{i\alpha} \cdot \mathbf{B} \tag{1}$$

- $\mathbf{D}_{i\alpha,j\beta}$ are DMI vectors.DMI term for first two sublattices is $(\frac{-D}{\sqrt{2}}, \frac{D}{\sqrt{2}}, 0) \cdot (\mathbf{S}_{i1} \times \mathbf{S}_{i2})$.The rest of the vectors are determined by lattice symmetry.
- $\hat{\mathbf{n}}_{\alpha}$ points from the site to the centre of the tetrahedron

Method

- Assumption:Spin state are Translation invariant.
- We write the Hamiltonian in terms of local spherical coordinates of sub lattices,$\mathbf{e}_\alpha^m$, $(\mathbf{e}_\alpha^1, \mathbf{e}_\alpha^2, \mathbf{e}_\alpha^3)=(\theta_\alpha, \phi_\alpha, r_\alpha)$.The e_α^3 points along the classical spin direction. Represent Hamiltonian in terms of spin Ladder operators.
- $$S_{i\alpha}^+ = S_{i\alpha}^1 + iS_{i\alpha}^2 = (S_{i\alpha}^-)^\dagger$$

$$\begin{aligned}\mathbf{H} = \sum_{i\alpha,j\beta} [&J_{i\alpha;j\beta}^{33} S_{i\alpha}^3 S_{j\beta}^3 + J_{i\alpha;j\beta}^{++} S_{i\alpha}^+ S_{j\beta}^+ + J_{i\alpha;j\beta}^{--} S_{i\alpha}^- S_{j\beta}^- + J_{i\alpha;j\beta}^{+-} S_{i\alpha}^+ S_{j\beta}^- \\ &+ J_{i\alpha;j\beta}^{-+} S_{i\alpha}^- S_{j\beta}^+ + J_{i\alpha;j\beta}^{+3} S_{i\alpha}^+ S_{j\beta}^3 + J_{i\alpha;j\beta}^{3+} S_{i\alpha}^3 S_{j\beta}^+ + J_{i\alpha;j\beta}^{-3} S_{i\alpha}^- S_{j\beta}^3 \\ &+ J_{i\alpha;j\beta}^{3-} S_{i\alpha}^3 S_{j\beta}^-] - \sum_{i\alpha} \left[\mathcal{B}^3 S_{i\alpha}^3 + \mathcal{B}^+ S_{i\alpha}^+ + \mathcal{B}^- S_{i\alpha}^-\right] \quad (2)\end{aligned}$$

Method

- Holstein-Primakoff Transformation $(S^3_{i\alpha} = S - b^\dagger_{i\alpha} b_{i\alpha}, S^+_{i\alpha} = \sqrt{2S - b^\dagger_{i\alpha} b_{i\alpha}} b_{i\alpha})$ and Keep terms up to second order. The first order terms are:

$$\sum_{i\alpha} \sqrt{2S} \left[\sum_{j\beta} S[J^{+3}_{i\alpha;j\beta} + J^{3+}_{j\beta;i\alpha}] - \mathcal{B}^+ \right] b_{i\alpha} = 0 \tag{3}$$

$$\sum_{i\alpha} \sqrt{2S} \left[\sum_{j\beta} S[J^{-3}_{i\alpha;j\beta} + J^{3-}_{j\beta;i\alpha}] - \mathcal{B}^- \right] b^\dagger_{i\alpha} = 0 \tag{4}$$

- Coefficients of $b_{i\alpha}$ vanish for the local axis.Hence first order terms vanish.We derive the result by setting the derivatives of Hamiltonian in equation 2 with respect to $S^1_{i\alpha}$ and $S^2_{i\alpha}$ to zero in the ground state configuration

Method

- We write the Hamiltonian in Momentum space.
- $$\mathbf{H} = \varepsilon_0 + \sum_{\mathbf{q}}{}' \begin{bmatrix} (\mathbf{b}_{\mathbf{q}}^{\dagger})^T & (\mathbf{b}_{-\mathbf{q}})^T \end{bmatrix} \begin{bmatrix} \mathcal{A}_q & \mathcal{C}_q \\ \mathcal{C}_q^{\dagger} & \mathcal{A}_{-q}^T \end{bmatrix} \begin{bmatrix} \mathbf{b}_{\mathbf{q}} \\ \mathbf{b}_{-\mathbf{q}}^{\dagger} \end{bmatrix} \tag{5}$$

  Where,

$$\varepsilon_0 = NS(S+1)\sum_{\alpha\beta} \tilde{J}^{33}_{\alpha\beta}(0) + 2S\sum_{\mathbf{q}\alpha}{}' \eta_{\mathbf{q}}[\tilde{J}^{+-}_{\alpha\alpha}(\mathbf{q}) - \tilde{J}^{-+}_{\alpha\alpha}(\mathbf{q})] + \sum_{\mathbf{q}\alpha} \mathcal{B}^3_\alpha$$

$$[\mathcal{A}_{\mathbf{q}}]_{\alpha\beta} = -\eta_{\mathbf{q}} \left[S\sum_{\beta'}[\tilde{J}^{33}_{\alpha\beta'}(0) + \tilde{J}^{33}_{\beta'\alpha}(0)] + \mathcal{B}^3_\alpha \right] \delta_{\alpha\beta}$$

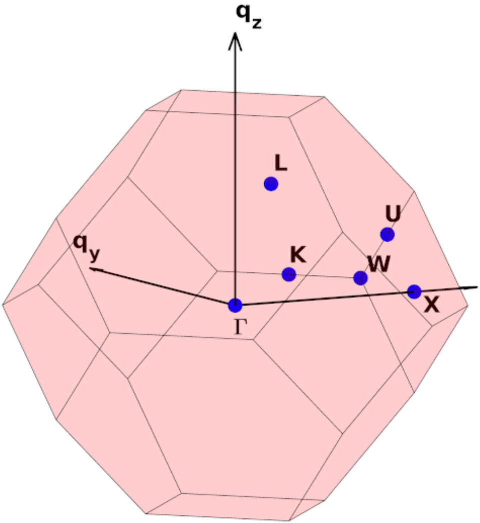
$$+2S\eta_{\mathbf{q}}[\tilde{J}^{+-}_{\beta\alpha}(\mathbf{q}) - \tilde{J}^{+-}_{\alpha\beta}(-\mathbf{q})]$$

$$[\mathcal{C}]_{\alpha\beta} = 2S\eta_{\mathbf{q}}[\tilde{J}^{--}_{\alpha\beta}(-\mathbf{q}) - \tilde{J}^{--}_{\beta\alpha}(\mathbf{q})] \tag{6}$$

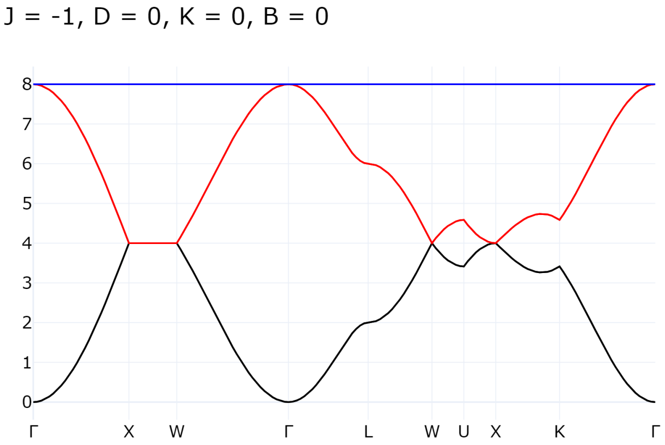
Method

- Splay phase:{(a,b,b),(a,b,-b),(a,-b,-b),(a,-b,b)}
- We carry the minimization starting with guess value as result from zero field.As we increase the field slowly, we use the guess value as result of previous field.Check that hessian is positive definite and linear terms vanish.
- Bogoliubov Transformation.We Follow the detail method given in J. Colpa's Paper(J.H.P. Colpa. "Diagonalization of the quadratic boson hamiltonian". In: Physica A: Statistical Mechanics and its Applications 93.3 (1978), pp. 327–353. issn: 0378-4371)

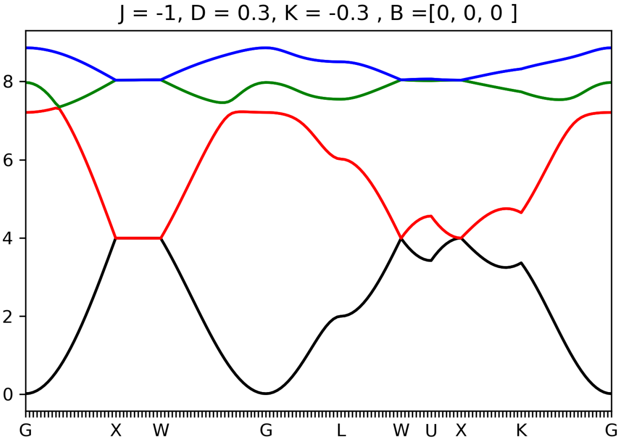
Brillouin zone FCC Lattice

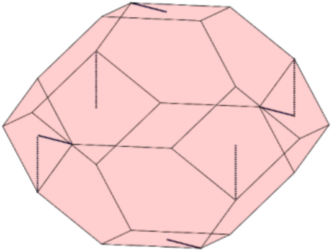


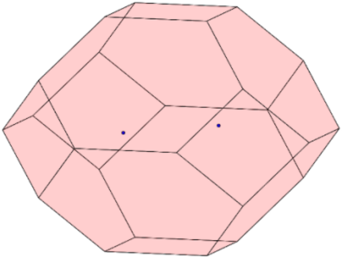
Spectrum Without DMI and Anisotropy



Spectrum With DMI and Anisotropy

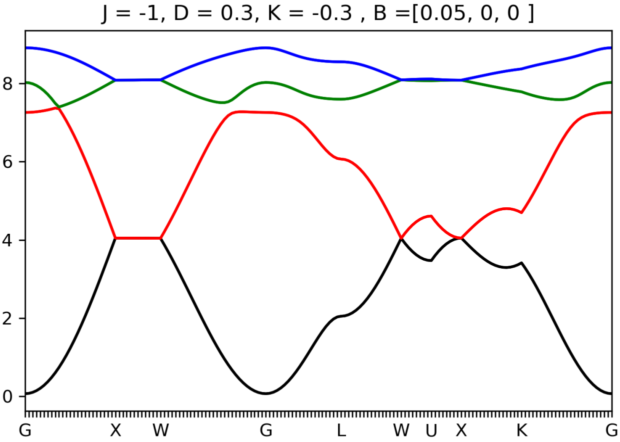






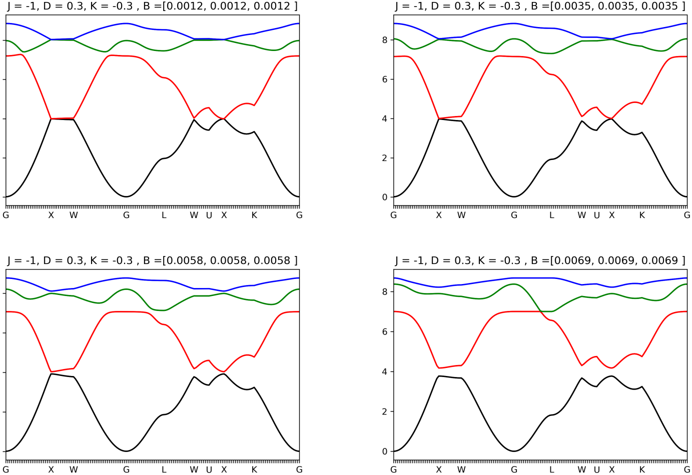
- There is a point degeneracy between band 2 and 3 on the path between G and X.The corresponding **q** point on the Brillouin zone is [2.2619,0,0].

Field along [100]



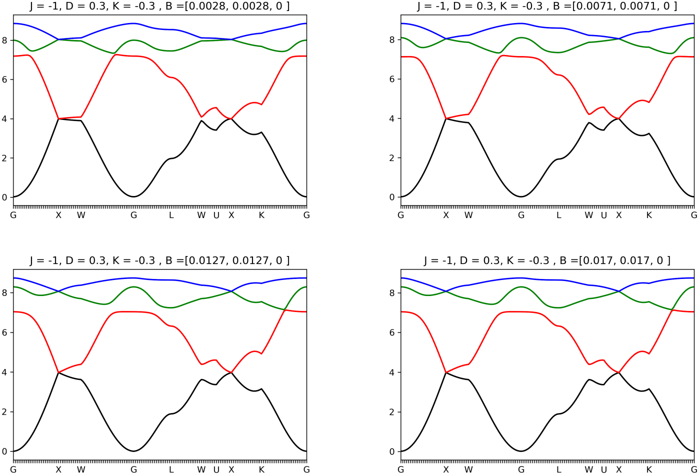
Field along [111]

Figure: B=0.002,0.006,0.01,0.012 respectively

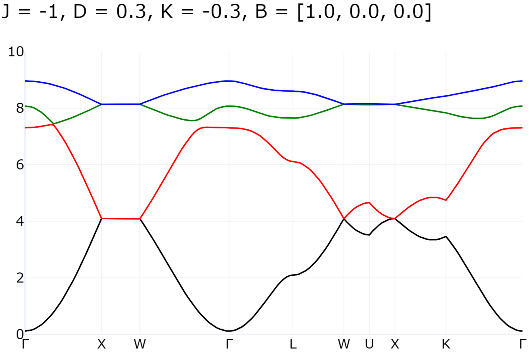


Field along [110]

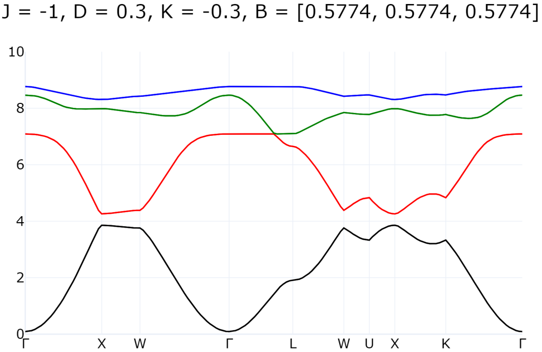
Figure: B=0.004,0.01,0.018,0.024 respectively



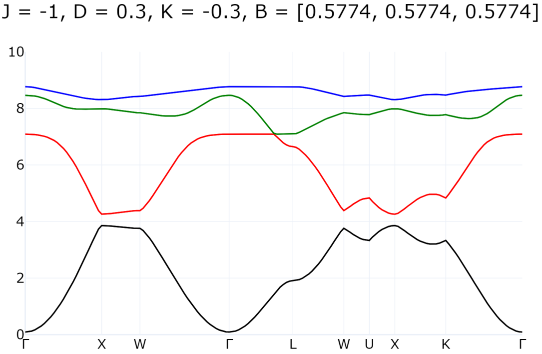
Field Rotation:[100]$\rightarrow$ [110]



Field Rotation:[111]$\rightarrow$ [100]



Field Rotation:[111]$\rightarrow$ [110]



Conclusion and Future Calculation

- Change in Magnetic Field,Qulitative Change in Magnon Spectra except for [100].All of [100],[111],[110] have weyl points at different positions.By Changing the direction we get weyl points at different positions in BZ for the system.
- Code stabilized.We will proceed to calculation of Slab Geometries.
- In bulk Minimization was over 8 Variables.In slab geometry minimization over 8N variables for N layers.
- Magnon spectrum and Berry curvature calculation in slab geometries with presence of external field,Which will lead to calculation of Thermal hall conductivity due to magnonic excitation as they are the two main ingredients for the calculation.