Field dependence of spin wave dispersion in splay phase of the ferromagnetic pyrochlore Slabs

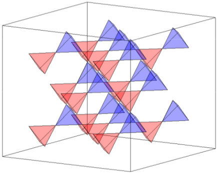
Project presentation By : Haraprasad Dhal

Project Guided By : Dr. V. Ravi Chandra

NISER,Bhubaneswar

April 26, 2023

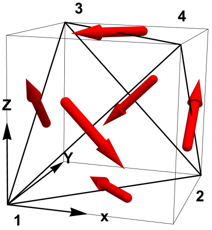
Pyrochlore lattice

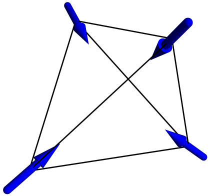


- Sixfold-coordinated structure whose underlying Bravais lattice is FCC,with four basis.primitive vectors:$\{(\frac{1}{2},\frac{1}{2},0),(0,\frac{1}{2},\frac{1}{2}),(\frac{1}{2},\frac{1}{2},0)\}$. Sublattice vectors:$[(0,0,0),(\frac{1}{4},\frac{1}{4},0),(0,\frac{1}{4},\frac{1}{4}),(\frac{1}{4},0,\frac{1}{4})]$. Spin sites lie on the corners of Tetrahedron
- Along [111]:stacking of Triangular and Kagome' Lattice planes.
- Along [100] and [110] ,square and rectangular lattice planes with bases.

Spin Hamiltonian

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

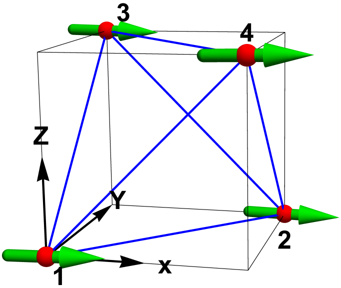




- DMI term for first two sublattices is $(\frac{-D}{\sqrt{2}}, \frac{D}{\sqrt{2}}, 0)\cdot(\mathbf{S}_{i1}\times\mathbf{S}_{i2})$
- $\hat{\mathbf{n}_\alpha}$ points to center of Tetrahedron
- $J = -1$ and $K \neq 0$: Splay phase:{(a,b,b),(a,b,-b),(a,-b,-b),(a,-b,b)}

Splay state

- $J = -1$ and $K \neq 0$: Splay phase:$\{$(a,b,b),(a,b,-b),(a,-b,-b),(a,-b,b)$\}$



Recap- Last semester

- Classical ground state for Bulk(full periodic boundary condition) in J,D,K model with non zero static magnetic field.
- V. V. Jyothis, Bibhabasu Patra, and V. Ravi Chandra. *Magnon bands in pyrochlore slabs with Heisenberg exchange and anisotropies*. 2022. DOI: 10.48550/ARXIV.2210.03548.
- Produced the magnon spectra in static magnetic field.
- Qualitative changes in spectra with different field direction and magnitude. Presence of Weyl points and change in position of these Weyl point with change in field direction.

Recap- Last semester

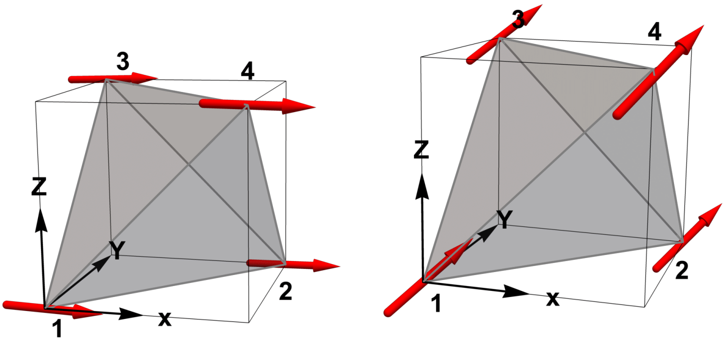


Figure: Classical ground state. $D = -K = 0.3$. left:$B = 0$. right:$B = 0.02$

Recap-Bulk spectra

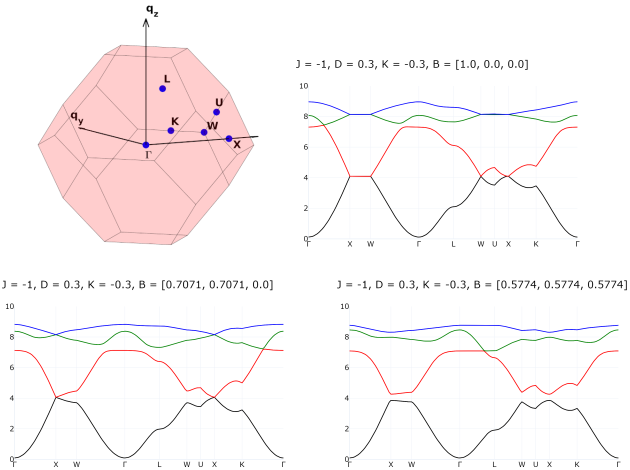


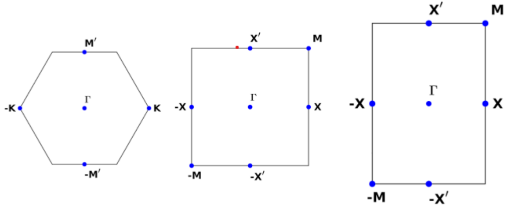
Figure: FCC BZ for pyrochlore. Y axis: $\omega_{\mathbf{q}}$ with magnitude of J and S set to 1. D$=-K=$0.3

Objectives-This semester

- Numerical computation of Classical ground state for slab geometry of Pyrochlore lattice.
- Calculation of magnon spectra for three different slab truncation [111],[100] and [110] with magnetic field.
- Calculation of magnon contribution to Thermal hall conductivity For Bulk and Slab geometries using the expressions from linear response theory.

Slab geometry

- Truncate in one direction. PBC in other two. The 2D Brillouin zone shown are for [111], [100] and [110] slab geometry.



For the three slab geometries mentioned we define effective 2D basis vectors $\mathbf{a_1}^{eff}$, $\mathbf{a_2}^{eff}$ and the stacking direction of layers $\mathbf{a}_s$, are defined in terms of FCC lattice vectors $\mathbf{a_i}$, as follows:

$$[111] : \mathbf{a_1}^{eff} = \mathbf{a_1} - \mathbf{a_3},\ \mathbf{a_2}^{eff} = \mathbf{a_2} - \mathbf{a_3},\ \mathbf{a_s} = \mathbf{a_1} \quad (1)$$

$$[100] : \mathbf{a_1}^{eff} = \mathbf{a_2},\ \mathbf{a_2}^{eff} = \mathbf{a_3} - \mathbf{a_1},\ \mathbf{a_s} = \mathbf{a_1} \quad (2)$$

$$[110] : \mathbf{a_1}^{eff} = -\mathbf{a_1} + \mathbf{a_2} + \mathbf{a_3},\ \mathbf{a_2}^{eff} = -\mathbf{a_2} + \mathbf{a_3},\ \mathbf{a_s} = \mathbf{a_3} \quad (3)$$

Classical Ground state

- We Write the Hamiltonian in Local spherical coordinates of classical Ground state configuration.
- Holstein-Primakoff transformation $(S^3_{i\alpha} = S - b^\dagger_{i\alpha} b_{i\alpha}, S^+_{i\alpha} = \sqrt{2S - b^\dagger_{i\alpha} b_{i\alpha}}\, b_{i\alpha})$.
- Coefficients of Linear terms vanish in Local Coordinate.

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

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

- We use these equations to solve for classical ground state configuration.
- For a Finite B we start from zero field solution guess and increase the field in small steps. We give guess as the solutions of Bulk angles repeated over each tetrahedron throughout the layers.

Diagonalization

- Spin Hamiltonian in momentum space has following form

$$\mathbf{H} = \varepsilon_0 + \sum_{\mathbf{q}}{}' \begin{bmatrix} (\mathbf{b}_{\mathbf{q}}^{\dagger})^T & (\mathbf{b}_{-\mathbf{q}})^T \end{bmatrix} H_{\mathbf{q}} \begin{bmatrix} \mathbf{b}_{\mathbf{q}} \\ \mathbf{b}_{-\mathbf{q}}^{\dagger} \end{bmatrix}, \; H_{\mathbf{q}} = \begin{bmatrix} \mathcal{A}_q & \mathcal{C}_q \\ \mathcal{C}_q^{\dagger} & \mathcal{A}_{-q}^T \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{f}_{\mathbf{q}} \\ \mathbf{f}_{-\mathbf{q}}^{\dagger} \end{bmatrix} = \Gamma_{\mathbf{q}} \begin{bmatrix} \mathbf{b}_{\mathbf{q}} \\ \mathbf{b}_{-\mathbf{q}}^{\dagger} \end{bmatrix}. \text{ paraunitary condition } \Gamma_{\mathbf{q}}^{\dagger} \sigma_3 \Gamma_{\mathbf{q}} = \sigma_3. \text{ Where } \sigma_3 = \begin{bmatrix} 1_{N\times N} & 0 \\ 0 & -1_{N\times N} \end{bmatrix}$$

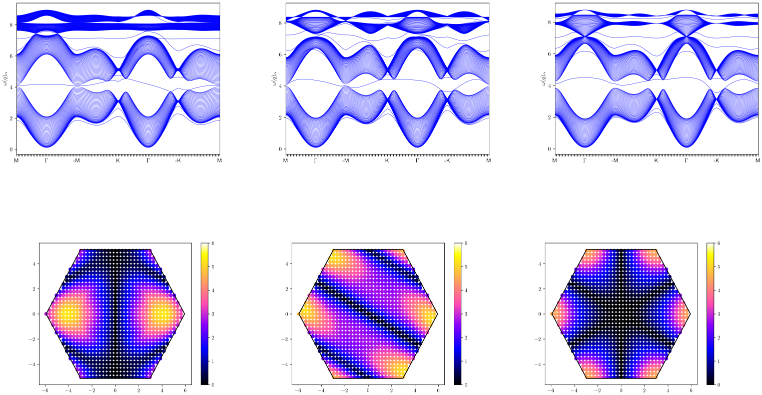
$$H = \epsilon_{zero\ point} + S \sum_{\mathbf{q},\alpha} [\omega_{\mathbf{q},\alpha} f_{\mathbf{q},\alpha}^{\dagger} f_{\mathbf{q},\alpha}]$$

- If N is the number of sublattices per site, $H_{\mathbf{q}}$ is $2N \times 2N$.
- $\mathbf{b}_{\mathbf{q}}$ and $\mathbf{b}_{\mathbf{q}}^{\dagger}$ are column vectors of $\{ b_{\mathbf{q}\alpha} \}$ and $\{ b_{\mathbf{q}\alpha}^{\dagger} \}$
- Reciprocity:

$$\mathcal{R}_{\mathbf{q}} = 2 \times \sum_{\alpha} |\omega_{\mathbf{q}\alpha} - \omega_{-\mathbf{q}\alpha}|$$

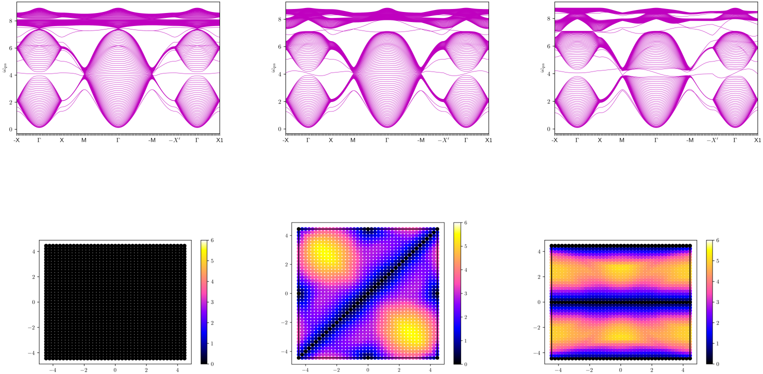
111 slab spectra

Figure: Spectrum for 111 slab, $D = -K = 0.3$. Field: left-100, middle-110, right-111. Field strength B=0.1. Data is for 40 layers.



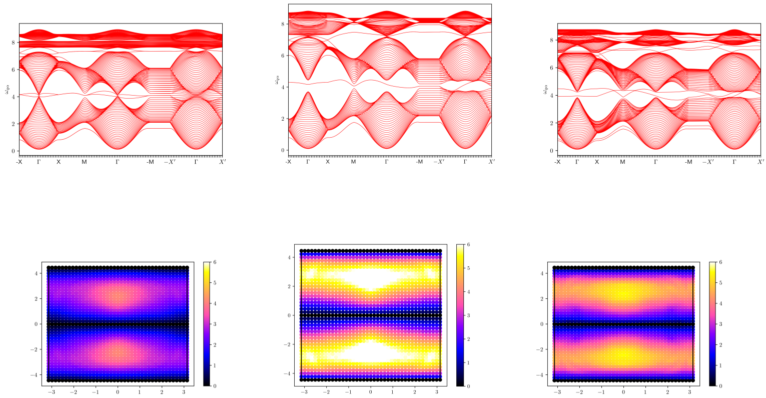
100 slab spectra

Figure: Spectrum for 100 slab, $D = -K = 0.3$. Field: left-100, middle-110, right-111. Field strength B=0.1



110 slab spectra

Figure: Spectrum for 110 slab, $D = -K = 0.3$. Field: left-100, middle-110, right-111. Field strength B=0.1



Edge State

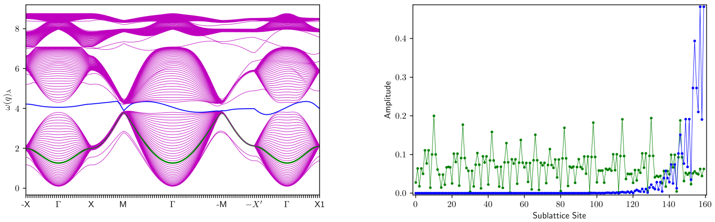
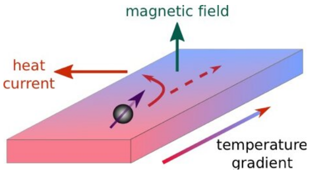
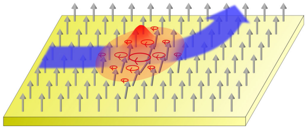


Figure: left: 100 slab spectrum with selected bands. $D = -K = 0.3$. field along 111. Right: Spin wave amplitude in real space. Data is for 40 layers.

Magnon Hall Effect





- $J^Q_\mu = -\sum_\nu k_{\mu\nu}\Delta_\nu T$
- Linear response Approach . Expressed by the Berry curvature associated with Bloch wave functions for spin-wave bands in the momentum space.
- Ryo Matsumoto, Ryuichi Shindou, and Shuichi Murakami. "Thermal Hall effect of magnons in magnets with dipolar interaction". In: *Phys. Rev. B* 89 (5 2014), p. 054420. DOI: 10.1103/PhysRevB.89.054420

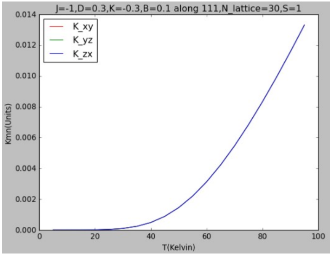
Magnon Hall effect

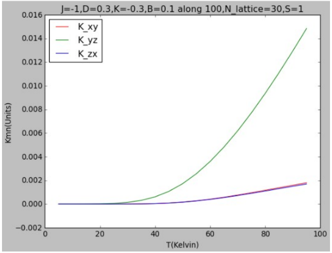
- $k_{xy} = \frac{k_B^2.T}{\hbar V}\sum_n \sum_{\mathbf{k}}\{\frac{\pi^2}{3} - c_2[g(E_{nk}/k_B.T)]\}\Omega^z_{n\mathbf{k}}$.
- $c_2(u) = (1+u)(ln\frac{1+u}{u})^2 - (lnu)^2 - 2Li_2(-u)$.
- Berry curvature Calculation:
  - Expressed in terms of velocity operator $\Delta_{\mathbf{q}} H_{\mathbf{q}}$
  - Loop metod:Berry phase associated with a loop enclosing an elementary. T. Fukui, Y. Hatsugai and H. Suzuki J. Phys. Soc. Jpn. J. Phys. Soc. Jpn. 74, 1674 (2005).Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances. plane in the Brillouin zone

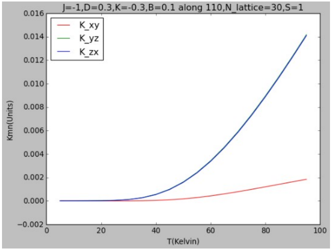
Material of interest: $Lu_2V_2O_7$

- For numerical Computation of $k_{\mu\nu}$ we use the value of J=8.22 meV.For comparison the value of k_B.T at room temperature is around 25 meV. M. Mena et al. "Spin-Wave Spectrum of the Quantum Ferromagnet on the Pyrochlore Lattice". In: *Phys. Rev. Lett.* 113 (4 July 2014), p. 047202. DOI: 10.1103/PhysRevLett.113.047202.
- Y. Onose et al. "Observation of the Magnon Hall Effect". In: *Science* 329.5989 (2010), pp. 297–299. DOI: 10.1126/science.1188260

Bulk Geometry Conductivity



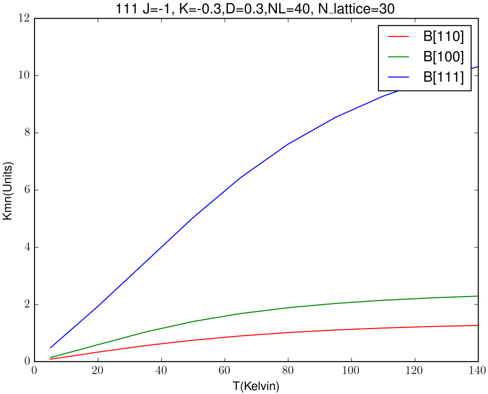




- Berry curvature data from Loop method.
- field along [111] : $k_{xy} \approx k_{yz} \approx k_{zx}$.
- field along [100] $k_{zx} \approx k_{xy}$
- field along [110] $k_{yz} \approx k_{zx}$

Figure: k_{mn} vs T. Y axis units in W/Km. $D = -K = 0.3$

Slab Geometry Conductivity



- 111 slab. $D = -K = 0.3$. Lattice size 30×30. Number of layers=40. Y axis units in W/Km.
- Berry curvature data from Loop method.
- Large values. $\mathbf{\Omega_{n,k}} = -\mathbf{\Omega_{n+N,k}}$

Summary

- The Luttinger Tisza analysis is robust for calculating the ground state for bulk cases, but not for slab geometry, where numerical optimization is relied upon instead.
- The reciprocity of the bulk spectrum follows directly from the invariance of the real space spinwave Hamiltonian under spatial inversion, but this is not true for slab geometry, where non-reciprocity is found in many instances.
- The slab geometry spectrum has Weyl point signatures, with the Weyl point positions varying depending on the slab truncation direction and magnetic field direction, and the number of edge states remaining invariant with slab geometry and field direction.
- The magnonic contribution to thermal hall conductivity was calculated using the results from linear response theory, and based on the qualitative and quantitative difference of spectrum and reciprocity signatures in different slab geometries and field directions, it is expected to be non-isotropic to truncation direction and field direction. Fixing Berry curvature calculations and the calculation of thermal hall conductivity are ongoing.

References

[1] V. V. Jyothis, Bibhabasu Patra, and V. Ravi Chandra. *Magnon bands in pyrochlore slabs with Heisenberg exchange and anisotropies*. 2022. DOI: 10.48550/ARXIV.2210.03548.

[2] Ryo Matsumoto, Ryuichi Shindou, and Shuichi Murakami. "Thermal Hall effect of magnons in magnets with dipolar interaction". In: *Phys. Rev. B* 89 (5 2014), p. 054420. DOI: 10.1103/PhysRevB.89.054420.

[3] M. Mena et al. "Spin-Wave Spectrum of the Quantum Ferromagnet on the Pyrochlore Lattice". In: *Phys. Rev. Lett.* 113 (4 July 2014), p. 047202. DOI: 10.1103/PhysRevLett.113.047202.

[4] Y. Onose et al. "Observation of the Magnon Hall Effect". In: *Science* 329.5989 (2010), pp. 297–299. DOI: 10.1126/science.1188260.

Thank you