Magnetic structure and excitations in vanadates, \( \text{BaV}_{10}\text{O}_{15} \) and \( \text{CoV}_2\text{O}_4 \)

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4\textsuperscript{th} year research seminar
Outline

- **Introduction**
  - Frustrated magnetism, spin and orbital degrees of freedom
  - neutron scattering basics
- **BaV\textsubscript{10}O\textsubscript{15}**
  - Background
  - Experimental data – Diffraction and Inelastic
  - Results – Magnetic ground state and excitations
  - Conclusions
- **CoV\textsubscript{2}O\textsubscript{4}**
  - Background
  - Experimental data – Diffraction and Inelastic
  - Results – Magnetic Structure and linear spin wave calculation
  - Conclusions
What is Frustration?

Antiferromagnetically interacting spins

Triangular (2D)  Tetrahedral (3D)

- When a system is geometrically frustrated, absence of a unique ground state gives a finite entropy at absolute zero temperature.
- Some materials may have many nearly-degenerate ground states (a spin glass), or may retain dynamic disorder (a quantum spin liquid).
- Orbital degree of freedom can lift the degeneracy and drive the system into a particular ground state or reduce the frustration.
What is Frustration?

Most degenerate- and thus most frustrated-lattice Readily realizable in three dimensions or less is one made up with corner sharing tetrahedra, the pyrocholre lattice.

Figure 3. The entropy $S$ of the spin-ice compound dysprosium titanate Dy$_2$Ti$_2$O$_7$ as a function of temperature $T$. At high $T$, $S = k_B \ln 2$ per spin, the same as for free spins. Cooling the system causes the entropy to drop as correlations develop between spins. An unfrustrated magnet follows the plot’s schematic red line down to zero entropy because the system assumes a unique ground state. In spin ice, geometrical frustration creates an exponentially large number of degenerate ground states. The large degeneracy manifests itself in a non-vanishing entropy, which is close to the value that Linus Pauling predicted for ordinary water ice. (Adapted from ref. 5.)
Frustrated magnets

• Lies in two fundamental enterprises in condensed matter physics.

• On the applied side, the instabilities exhibited by frustrated magnets open a window on richness of nature realized in different materials.

• On the fundamental side is the search for principles that help organize the variety of behavior we observed around us.
Jahn–Teller effect

- Any nonlinear molecule with a spatially degenerate electronic ground state will undergo a geometrical distortion that removes that degeneracy, because the distortion lowers the overall energy of the species.

- The Jahn–Teller effect is most often encountered in octahedral complexes of the transition metals.

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</table>

**w**: weak Jahn–Teller effect ($t_{2g}$ orbitals unevenly occupied),
**s**: strong Jahn–Teller effect expected ($e_g$ orbitals unevenly occupied), **blank**: no Jahn–Teller
Neutron Scattering

Why neutron?

1. **Zero net charge** makes neutron to penetrate deep inside the sample without being scattered by the electrons like X-ray, hence measuring bulk properties.

2. Its internal **magnetic moment** interact with the unpaired electrons spins in an atom via dipole-dipole interaction enabling direct measurement of magnetic moments.

3. Due to **large neutron mass**, when moderated with water or liquid hydrogen, the kinetic energy becomes comparable to that of many elementary excitations in a solid.

Maxwell distribution of thermal neutron

\[
\begin{align*}
\text{T} &= 293K \\
\text{E} &= 25.3 \text{ meV} \\
\lambda &= 1.798\text{Å}
\end{align*}
\]
What we measure

nuclear scattering

\[ \frac{d^2\sigma}{d\Omega_f dE_f} = N \frac{k_f}{k_i} b^2 S(\vec{Q}, \omega) \]

\[ S(\vec{Q}, \omega) = \frac{1}{2\pi\hbar N} \sum_{\nu} \int_{-\infty}^{\infty} dt \langle e^{-i\vec{Q} \cdot \vec{r}_\nu(0)} e^{i\vec{Q} \cdot \vec{r}_\nu(t)} \rangle e^{-i\omega t} \]

\[ = \frac{1}{2\pi\hbar N} \int_{-\infty}^{\infty} dt \langle \rho_{\vec{Q}}(0) \rho_{-\vec{Q}}(t) \rangle e^{-i\omega t} \]

\[ \rho_{\vec{Q}}(t) = \sum_l e^{i\vec{Q} \cdot \vec{r}_l(t)} \]

magnetic scattering

\[ \frac{d^2\sigma}{d\Omega_f dE_f} = \frac{N k_f}{\hbar k_i} p^2 e^{-2W} \sum_{\alpha,\beta} \left( \delta_{\alpha,\beta} - \hat{Q}_\alpha \hat{Q}_\beta \right) S^{\alpha,\beta}(\vec{Q}, \omega) \]

\[ S^{\alpha,\beta}(\vec{Q}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_l e^{i\vec{Q} \cdot \vec{r}_l} \langle S^\alpha_0(0) S^\beta_l(t) \rangle \]

\[ pS = \left( \frac{\gamma r_0}{2} \right) g_f(\vec{Q}) S \]

The scattering cross section, the actual number measured by the detector, is proportional to the scattering function, \( S(Q, \omega) \) which is the Fourier transform of time dependent pair correlation function of either atomic density or spin component.
Neutron scattering

- **Elastic Neutron Scattering (Neutron diffraction)**
  - Reveals the crystal structure.
  - Reveals the microscopic magnetic structure

  Instruments – Powder and single crystal diffractometer

- **Inelastic Neutron Scattering**
  - To study atomic and molecular motion as well as magnetic and crystal field excitations.

  Instruments – Triple axis spectrometer

  Time of flight spectrometer
Elastic Neutron Scattering

Inelastic Neutron Scattering

Source - http://neutron.magnet.fsu.edu/neutron_scattering.html
Neutron diffraction

Powder Diffractometer

Single Crystal Diffractometer

HB2A, HFIR

RESI, FRM II

Bragg’s law

\[ n\lambda = 2d\sin\theta \]
Triple axis spectrometer

It allows measurement of the scattering function at any point in energy and momentum space physically accessible by the spectrometer.

$$|Q|^2 = |k_i|^2 + |k_f|^2 - 2 |k_i||k_f|\cos(2\theta)$$

$$\hbar\omega = E_f - E_i = \frac{\hbar^2}{2m_n} (k_i^2 - k_f^2)$$
Time of Flight measurement

The time of flight spectrometer, as can be expected from its name, determines neutron energy by measuring its time of flight from one point to another.

The beams are monochromated using several choppers rotating at different frequencies allowing only neutrons at certain velocity can pass through.

Since we know the distance between the sample and detectors and can measure the time for neutron to fly from the sample to the detector, we then can calculate the energy of scattered neutrons.

The direction of momentum can be figured out from the detector angle.

Time-of-flight method is powerful in that it can map out the huge Q-E space at a time.
Spin waves

- Propagating disturbances in the ordering of magnetic materials. These low-lying collective excitations occur in magnetic lattices with continuous symmetry.

- Spin waves are the analog for magnetically ordered systems of lattice waves in solid systems; and just as a quantized lattice wave is called a “phonon”, a quantized spinwave is called a “magnon”.
Animations are Created by IDL code written by Prof. Seunghun Lee
Frustrated magnet $\text{BaV}_{10}\text{O}_{15}$
Introduction – BaV$_{10}$O$_{15}$

$V^{3+}(3d^2)$ | $V^{2+}(3d^3)$

\[ \begin{align*}
4 & : 1 \\
\end{align*} \]

V ions surrounded by oxygen in octahedral fashion

face-, edge-, corner- sharing

mixed valence

t2g orbital ground state
z=0: V5 boat
z=1/4: 180° rotation

due to small overlap between z=0 and z=-1/4, considered as bi-layer structure stacked in ABAB fashion with B shifted along a

C.Bridges et. al., PRB 74, 024426 (2006)
J.Miyazaki et. al., PRB 79 180410(R) (2009)
Bulk Properties

- Structural phase transition at 123 K (Cmce → Pbca)
- Opening of charge gap
- Magnetic phase is unknown

KAJITA et al., PRB 81, 060405R 2010
**Strength of interaction**

- **which connection is strong?**
  - depends on the amount of orbital overlap

- **In octahedrally coordinated 3d ions case**
  - corner < edge < face

  *Green ions: V3a(light), V3b(dark)*

  *Yellow ions: Oxygen*


**example of V3 ions interaction**
Strength of interaction

- **which connection is strong?**
  - depends on the amount of orbital overlap

- **In octahedrally coordinated 3d ions case**
  - corner < edge < face


*Green ions: V3a(light), V3b(dark)*
*Yellow ions: Oxygen*

example of V3 ions interaction
Interactions (face and edge sharing bonds)

$0.3 < z < 0.7$

$-0.2 < z < 0.3$
Experiments

- ARCS, SNS
  - Time of Flight neutron scattering measurement
  - $T=4\text{K}$ with $E_i=65\text{meV}$
  - $k_i//c$ with rotation angle -10 to 40 deg.

- HB2A, HFIR
  - Neutron powder diffractometer
  - $T=4\text{K}$ with Wavelength 1.538 A

- RESI, FRM II
  - Single Crystal Diffractometer
  - $T=4\text{K}$ with wavelength 1 A
Magnetic excitations

- **H**:
  - Band 1: almost dispersionless, 5~6 meV
  - Band 2: flat, ~13 meV

- **K**:
  - Band 1: highly dispersive, 0-10 meV
  - Band 2: flat, ~13 meV

- **L**:
  - Band 1: 0-13 meV, highly dispersive
  - not consistent with bi-layer stacked along c
Powder Diffraction

Cmca $\rightarrow$ Pbca
V1(RED) $\rightarrow$ V1 (Red)
V2(Blue) $\rightarrow$ V2a, V2b(Blue, Sky)
V3(Green) $\rightarrow$ V3a, V3b(Green, Dark Green)

: mirror symmetry is lost
### Single Crystal Data

#### Magnetic peaks

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**RESI, FRM II**

-Single Crystal Diffractometer

-\(T = 4\text{K}\) with wavelength 1 Å
Representational Analysis

\[ \Gamma_{mag} = \sum_{\Gamma_i} n_i \Gamma_i \quad \Gamma_i - Irreducible \ representation \]

\[ S^{kv} = \sum_{L} \sum_{\lambda} C_{L}^{kL} \psi_{\lambda}^{kL} \]

Spin of the \( n^{th} \) cell \( S_{ni} = \exp(it_{n})S_{oi} \)
Representational Analysis

\[ \Gamma_{mag} = \sum_{\Gamma_i} n_i \Gamma_i \]

\( \Gamma_i \) — Irreducible representation

Magnetic structure

\[ m_j = \sum_L \sum_\lambda C_L^{kL\nu} \psi_\lambda^{kL\nu} e^{-2\pi i \mathbf{k} \cdot \mathbf{t}} \]

The propagation vector

\[ \mathbf{V}_j = \mathbf{V}_i \exp(-2\pi i \mathbf{k} \cdot \mathbf{r}) \]

\[ \mathbf{V}_j = \mathbf{V}_i \exp \left( -2\pi i \begin{pmatrix} 0 & 0 & 0 \\ 0.5 & 0 \end{pmatrix} \right) = \mathbf{V}_i \exp[-3\pi i] = -\mathbf{V}_i \]

\[ \mathbf{V}_j = \mathbf{V}_i \exp \left( -2\pi i \begin{pmatrix} 0 & 0 & 0 \\ 0.5 & 0 \end{pmatrix} \right) = \mathbf{V}_i \exp[-2\pi i] = \mathbf{V}_i \]

\[ \mathbf{V}_j = \mathbf{V}_i \exp \left( -2\pi i \begin{pmatrix} 0 & 0 \end{pmatrix} \right) = \mathbf{V}_i \exp[-\pi i] = -\mathbf{V}_i \]

\[ \mathbf{V}_j = \mathbf{V}_i \exp \left( -2\pi i \begin{pmatrix} 0 & 0 \end{pmatrix} \right) = \mathbf{V}_i \exp[-0\pi i] = \mathbf{V}_i \]
Refining the magnetic structure - Basis functions

80 Magnetic V atoms

\[ \Gamma_{mag} = 6\Gamma_1 + 6\Gamma_2 \]
\[ \Gamma_1, \Gamma_2 - 2 \text{ Dimensional} \]

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- C. Bridges Thesis 2002
Refining the magnetic structure

- Refining the Magnetic structure by carrying out all the possibilities is very hard, due to enormous possibilities.

- We approached the refinement in two ways.
Refining the magnetic structure

1. Trimer with tetramer

There are 4 basis vectors that is pointing in a-direction. BV1, BV4, BV7, BV10

   a.) All bonds with in all tetramers in unit cell are satisfied

   \[ \Gamma_1 \] - BV1 and BV 10
   \[ \Gamma_2 \] - BV4 and BV 7

   b.) Some bonds within tetramers does not satisfy

   Other combinations of BV1, BV4, BV7, BV10

Shimizu et. al. PRB 84, 064421 (2011)
Trimer with tetramer - All bonds within all tetramers in unit cell are satisfied
**Trimer with tetramer** - All bonds within all tetramers in unit cell are satisfied

$\Gamma_1$

Corner sharing bond along C, not satisfied or ferromagnetic
Trimer with tetramer - Some bonds within tetramers do not satisfy (-0.5 2 1)
Refining the magnetic structure

2. Non trimer model – All five V atoms are ordered

Here we assumed that chain along c-direction is always satisfied.
This allows us to restrict number of combinations in the basis vectors.

For eg.:

<table>
<thead>
<tr>
<th>Direction</th>
<th>Combination</th>
</tr>
</thead>
<tbody>
<tr>
<td>a direction</td>
<td>V3 (BV1) + V3B (BV4) + V3 (BV7) + V3B (BV10)</td>
</tr>
<tr>
<td>b direction</td>
<td>V3 (BV5) + V3B (BV2) + V3 (BV11) + V3B (BV8)</td>
</tr>
<tr>
<td>c direction</td>
<td>V3 (BV6) + V3B (BV3) + V3 (BV12) + V3B (BV9)</td>
</tr>
</tbody>
</table>
Non Trimer models – All five V atoms are ordered
Non Trimer models – All five V atoms are ordered
Linear spinwave calculation - Tetramer

\[ H = \sum J_{ii} S_i \cdot S_j \]
Linear spinwave calculation - Tetramer

\[ J_2 = 7.5 \text{ meV}; \]
\[ J_1 = 0.3 \times J_2; \]
\[ J_3 = 0.6 \times J_2; \]
Interactions – Non Trimer

- **FS**: $2.65713$
- **ES**: $2.53601$
- **J1**: $2.95476$
- **J2**: $2.96233$
- **J3**: $3.01432$
- **J4**: $3.01874$
- **J5**: $2.52781$
- **J6**: $3.01874$
- **J7**: $2.96233$
- **J8**: $2.53601$
- **J9**: $3.14098$
- **J10**: $2.95476$
- **J3B**: $3.09923$
- **J4B**: $3.00006$
- **J5B**: $3.07713$
- **J7B**: $2.79118$
- **J9B**: $3.12234$
- **J10B**: $2.72243$
- **J4**: $2.72243$
- **J7**: $3.08665$
- **J9**: $2.94994$
- **J10**: $3.00006$
- **J4B**: $2.79118$
- **J9B**: $3.12234$
- **J10B**: $2.72243$

0.3<z<0.7
Interactions – Non Trimer

-0.2 < z < 0.3
Non Trimer models – All five V atoms are ordered – Spin waves

- Chain along c-direction with one face sharing and one edge sharing bonds can satisfy the L dependence of the excitations.
- Also, along a-direction it is mostly disconnected and thus can produce the flat modes observed along H.
- The reason for highly dispersive mode along K, is still a question and our hypothesis is frustrated bonds some how create a similar chain along b direction which might be connected to face sharing bond along c direction.
Summary and future work

• We have examined the magnetic structure of BaV10O15 using Single Crystal and powder diffraction data.

• Our analysis shows that Trimer model with only V1 and V2a atoms ordered, cannot reproduce our diffraction data.

• Frustrated model with all five atoms ordered can reasonably reproduce our both single crystal and powder diffraction data.

• We will continue our analysis to find the best Hamiltonian for this system.
• Our future experiments consists of,
  1. Field dependence of the excitations
  2. Inelastic experiment to see whether there is any high energy modes.
Spinel $\text{CoV}_2\text{O}_4$
Spinel Family

• Spinel is an important class of mixed-metal oxides, which has the general chemical composition of $\text{AB}_2\text{O}_4$.

• When the shape of the orbital is changed by an external stimulus, the magnetic, electric, elastic, and optical properties may also be altered.

• Spinel oxides with the general formula $\text{AB}_2\text{O}_4$ provide a fertile playground for studying the interplay between these degrees of freedom.
Spinel Family

Kismarahrenja, Dissertation 2010

Table 2: The physical properties of transition-metal spinel vanadate.

<table>
<thead>
<tr>
<th></th>
<th>(\rho) at RT</th>
<th>structural transition and</th>
<th>magnetic ordering and</th>
<th>comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co(_2)O(_4)</td>
<td>(6 \times 10^{-3})</td>
<td>no transition</td>
<td>ferrimagnetic</td>
<td>Time decaying behaviour observed at low temperature.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ t_{2g} \]
\[ e_g \]
\[ t_{2u} \]
\[ e_u \]

Mn\(^{3+}\), tetrahedral, high spin, \(e_g, t_{2u}, 3\)
Magnetic moment = 5.91 \(\mu_B\), free electrons = 5

Fe\(^{3+}\), tetrahedral, high spin, \(e_g, 3\), \(t_{2u}, 3\)
Magnetic moment = 4.89 \(\mu_B\), free electrons = 4

Co\(^{3+}\), tetrahedral, high spin, \(e_g, 4\), \(t_{2u}, 3\)
Magnetic moment = 3.87 \(\mu_B\), free electrons = 3

V\(^{3+}\), octahedral, high spin, \(e_u, 0\), \(t_{2g}, 2\)
Magnetic moment = 2.82 \(\mu_B\), free electrons = 2

Graph showing Magnetic Transition Temperature (K) vs. \(1/R_{\rho A} (\text{A}^{-1})\).
MnV$_2$O$_4$: Magnetic structure
FeV₂O₄: Magnetic structure
Magnetic excitations in MnV$_2$O$_4$

**TABLE 1.** The optimal parameters used to calculate spin wave dispersions of MnO$_4$ (Fig. 2b) and MnV$_2$O$_4$ (Fig. 3) ($J$ and $B$ are in meV).

<table>
<thead>
<tr>
<th></th>
<th>$\lambda_{1s}$</th>
<th>$\lambda_{2s}$</th>
<th>$\lambda_{2g}$</th>
<th>$\beta_0^{1s}$</th>
<th>$\beta_0^{2s}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO$_4$</td>
<td>2.7(1)</td>
<td>19(1)</td>
<td>-1.1(7)</td>
<td>0.1(3)</td>
<td>0.28(3)</td>
</tr>
<tr>
<td>MnV$_2$O$_4$</td>
<td>2.8(2)</td>
<td>9.8(9)</td>
<td>3.0(8)</td>
<td>-0.6(4)</td>
<td>-0.8(4)</td>
</tr>
</tbody>
</table>
**CoV$_2$O$_4$: Structure (Cubic with $a = 8.41$ Å)**

A-site ($\text{Co}^{2+}$, $S=3/2$) forms a diamond lattice while B-site ($\text{V}^{3+}$, $S=1$) forms a pyrochlore lattice. $\text{V}^{3+}$ ions are Jahn-Teller active.
CoV$_2$O$_4$: Detailed structure

CoV$_2$O$_4$: A Spinel Approaching the Itinerant Electron Limit


TABLE I. Room temperature crystallographic data for CoV$_2$O$_4$.

<table>
<thead>
<tr>
<th>Space Group</th>
<th>Fd$ar{3}$m (No. 227)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a (Å)</td>
<td>8.4073(1)</td>
</tr>
<tr>
<td>Z</td>
<td>8</td>
</tr>
<tr>
<td>Atom Positions, $U_{iso}$</td>
<td>Co 0.375, 0.00670(13)</td>
</tr>
<tr>
<td>(x = y = z)</td>
<td>V 0, 0.00568(12)</td>
</tr>
<tr>
<td>V (Å$^3$)</td>
<td>594.251(12)</td>
</tr>
<tr>
<td>$\rho_{cal}$ (g/cm$^3$)</td>
<td>5.026</td>
</tr>
<tr>
<td>$\mu$ (mm$^{-1}$)</td>
<td>11.497</td>
</tr>
<tr>
<td>Data Collection Range (deg)</td>
<td>8.06 &lt; $\theta$ &lt; 61.47</td>
</tr>
<tr>
<td>Reflections Collected</td>
<td>7124</td>
</tr>
<tr>
<td>Independent Reflections</td>
<td>260[$R_{int}$ = 0.097]</td>
</tr>
<tr>
<td>Parameter Refined</td>
<td>8</td>
</tr>
<tr>
<td>$R_1$, $wR_2$ (F$_o$ &gt; 4$\sigma$F$_o$)</td>
<td>0.0370, 0.1035</td>
</tr>
<tr>
<td>$R_1$, $wR_2$ (All Data)</td>
<td>0.0398, 0.1015</td>
</tr>
<tr>
<td>Goodness-of-Fit</td>
<td>1.112</td>
</tr>
</tbody>
</table>

$Fd\bar{3}m$ $O_h^7$ $m\bar{3}m$ Cubic

No. 227 $F$ 4/$d$ 3 2/m

Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 2
CoV$_2$O$_4$: Magnetism

CoV$_2$O$_4$ shows a ferrimagnetic transition at $T = 145$ K. And there may be two additional transitions at $T = 60$ and 90 K (spin re-orientation ?).
Experiments

• E5, HZB
  - Single Crystal Diffractometer
  - T= 4K with wavelength 1 A

• HB1A, HFIR
  - Thermal Triple axis spectrometer
  - T=4K with E_f=65meV
Temperature dependence of nuclear + magnetic peaks
No structural transition
Refinement – 200 K (nuclear)
Refinement – 115 K (magnetic)

<table>
<thead>
<tr>
<th></th>
<th>Co</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$2.58227 \mu_B$</td>
<td>$-0.68620 \mu_B$</td>
</tr>
</tbody>
</table>
Refinement – 75 K (magnetic)

<table>
<thead>
<tr>
<th>Co</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.95270 $\mu_B$</td>
<td>-0.82596 $\mu_B$</td>
</tr>
</tbody>
</table>
Refinement – 10 K (magnetic)

<table>
<thead>
<tr>
<th></th>
<th>Co</th>
<th>V</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3.27383 $\mu_B$</td>
<td>-0.87081 $\mu_B$</td>
</tr>
</tbody>
</table>
Refinement – Magnetic Structure

<table>
<thead>
<tr>
<th>Temp (K)</th>
<th>Co Moment ($\mu_B$)</th>
<th>V Moment ($\mu_B$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>115 K</td>
<td>2.582(1)</td>
<td>0.686(1)</td>
</tr>
<tr>
<td>75 K</td>
<td>2.952(2)</td>
<td>0.825(1)</td>
</tr>
<tr>
<td>10 K</td>
<td>3.273(2)</td>
<td>0.870(1)</td>
</tr>
</tbody>
</table>
Magnetic excitations
Linear Spinwave calculation

\[ \mathcal{H} = \sum_{i,j} J_{\text{Co-V}} \mathbf{S}_{i,\text{Co}} \cdot \mathbf{S}_{j,\text{V}} + \sum_{i,j} J_{\text{Co-Co}} \mathbf{S}_{i,\text{Co}} \cdot \mathbf{S}_{j,\text{Co}} + \sum_{i,j} J_{\text{V-V}} \mathbf{S}_{i,\text{V}} \cdot \mathbf{S}_{j,\text{V}} + \sum_i D_{\text{Co}} (S_{i,\text{Co}}^z)^2 + \sum_i D_{\text{V}} (S_{i,\text{V}}^z)^2 \]

\( J_{\text{Co-Co}} \), \( J_{\text{V-V}} \) and \( J_{\text{Co-V}} \) are nearest neighbor interactions. \( D_{\text{Co}} \) and \( D_{\text{V}} \) are the single ion anisotropy for Co and V along z direction.

A good fit with the observed magnetic excitations were obtained when \( J_{\text{Co-V}} = 1.3 \text{ meV} \), \( J_{\text{V-V}} = -2.7 \text{ meV} \), \( J_{\text{Co-Co}} = -4.1 \text{ meV} \), \( D_{\text{V}} = -0.32 \text{ meV} \) and \( D_{\text{Co}} = -0.02 \text{ meV} \).
Linear Spinwave calculation

$J_{\text{Co-Co}} = 1.3 \text{ meV}$, $J_{\text{V-V}} = -2.7 \text{ meV}$, $J_{\text{Co-Co}} = -4.1 \text{ meV}$

$D_{\text{V}} = -0.32 \text{ meV}$, $D_{\text{Co}} = -0.02 \text{ meV}$. 
Linear Spinwave calculation

\[ J_{co-v} = 1.3 \text{ meV}, \ J_{v-v} = -2.7 \text{ meV}, \ J_{co-co} = -4.1 \text{ meV} \]
\[ D_v = -0.32 \text{ meV}, \ D_{co} = -0.02 \text{ meV}. \]
Summary and future work

• CoV$_2$O$_4$ does not show any structural transition as observed in MnV$_2$O$_4$ and FeV$_2$O$_4$.

• Single crystal data can be successfully refined with a collinear ferrimagnetic structure.

• Collinear ferrimagnetic structure can be used to reproduce inelastic data using a Hamiltonian with nearest neighbor interactions and single ion anisotropy.

• Origin of the anomaly around 40 K is yet to be understood.
THANK YOU!