КУРЧАТОВСКИЙ ИНСТИТУТ 75 ЛЕТ ДЛЯ СТРАНЫ И МИРА

НАЦИОНАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ ЦЕНТР «КУРЧАТОВСКИЙ ИНСТИТУТ»

Петербургский институт ядерной физики им. Б.П. Константинова
Национального исследовательского центра «Курчатовский институт»

Calculation of spin waves on magnetic structures using SpinW

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НИЦ «Курчатовский институт» - ПИЯФ.

Linear spin wave theory

1. Hamiltonian of the system:

$$H = \sum_{ij} J_{ij} \cdot \vec{S}_i \vec{S}_j$$

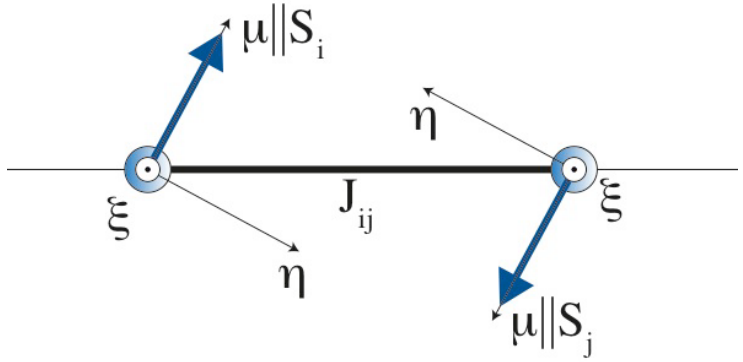
where S_i – spin vector operators, J_{ij} – 3x3 matrices describing pair coupling between spins.

2. Holstein-Primakoff transformation:

$$S_i^+(r_i) = \sqrt{2S} a_i = \sqrt{2S} b_i^+$$
$$S_i^-(r_i) = \sqrt{2S} a_i^+ = \sqrt{2S} b_i$$

local spin coordinate system: (ξ,η,μ)

$$S_i^\xi = \frac{1}{2}(S_i^+ + S_i^-)$$
$$S_i^\eta = \frac{1}{2i}(S_i^+ - S_i^-)$$
$$S_i^\mu = S_i - a_i^+ a_i = -S_i + b_i^+ b_i$$



3. After Fourier transformation we obtain bosonic Hamiltonian:

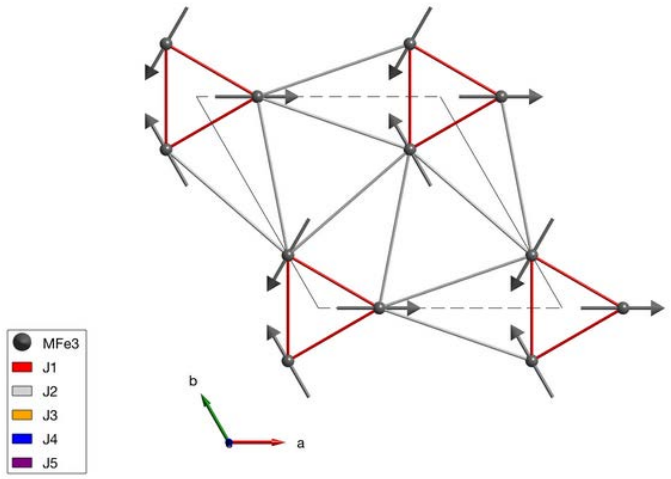
$$H = \sum_q \sum_{ij} A_{ij}(q)(a_{q,i}^+ a_{q,j} + b_{q,i}^+ b_{q,j}) + \sum_{ij} [B_{ij}(q) a_{q,i} b_{q,j} + h.c.]$$

where A_{ij}, B_{ij}– matrices, including the exchange parameters, spins and other parameters.

4. Spin wave energies:

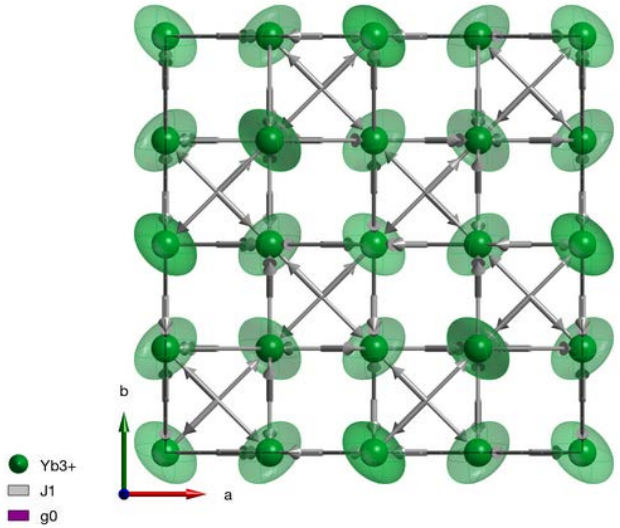
$$\omega^2(q) = (A + B)(A - B)$$

Linear spin wave theory



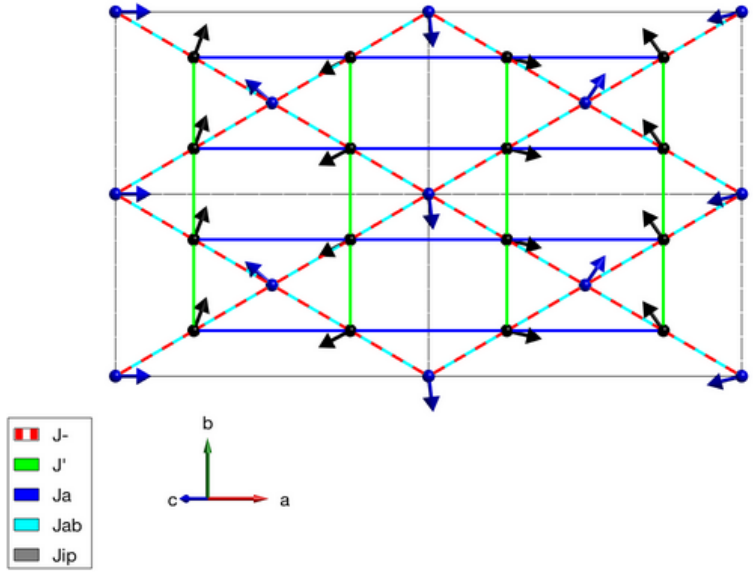
Model of $Ba_3NbFe_3Si_2O_{14}$ chiral compound. The magnetic ordering wave vector is k=(0,0, 1/7), the spins are lying in the ab-plane.

M. Loire, V. Simonet, S. Petit, K. Marty, P. Bordet, P. Lejay, J. Ollivier, M. Enderle, P. Steffens, E. Ressouche, A. Zorko, and R. Ballou, PRL 101, 247201 (2008)



The magnetic bonds of the ‘‘spin ice’’ compounds $Yb_2Ti_2O_7$.

Kate A. Ross, Lucile Savary, Bruce D. Gaulin, and Leon Balents, Phys. Rev. X 1, 021002 (2011)



Distorted kagome lattice in $KCu_3As_2O_7$.

G. J. Nilsen, Y. Okamoto, H. Ishikawa, V. Simonet, C. V. Colin, A. Cano, L. C. Chapon, T. Hansen, H. Mutka, and Z. Hiroi, Phys. Rev. B 89, 140412(R) (2014).

The spin Hamiltonian

$$H = \sum_{ij} J_{ij} \cdot \vec{S}_i \vec{S}_j + \sum_i A_i \vec{S}_i \vec{S}_i + \mu_B B \sum_i g_i \vec{S}_i$$

Heisenberg exchange:

$$J = \begin{bmatrix} J_x & 0 & 0 \\ 0 & J_y & 0 \\ 0 & 0 & J_z \end{bmatrix}$$

Dzyaloshinskii-Moriya exchange:

$$D = \begin{bmatrix} 0 & D_z & -D_y \\ -D_z & 0 & D_x \\ D_y & -D_x & 0 \end{bmatrix}$$

Spin operator:

$$S = \begin{bmatrix} S_x \\ S_y \\ S_z \end{bmatrix}$$

g-tensor:

$$g = \begin{bmatrix} g_x & 0 & 0 \\ 0 & g_y & 0 \\ 0 & 0 & g_z \end{bmatrix}$$

Easy-plane anisotropy:

$$A_{easy-plane} = \begin{bmatrix} -A_x & 0 & 0 \\ 0 & -A_x & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

External field:

$$B_{mag} = \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix}$$

Spin Wave Matlab library

https://wwwllb.cea.fr/logicielsllb/SpinWave/SW
by Sylvain Petit, Laboratoire Léon Brillouin

Matlab

https://www.psi.ch/spinw
by Sándor Tóth, Paul Scherrer Institut

SpinW is a Matlab library that can plot and numerically simulate magnetic structures and excitations of given spin Hamiltonian using classical Monte Carlo simulation and linear spin wave theory.

Crystal and Magnetic structures:
-definition of crystal lattice with arbitrary unit cell, using space group or symmetry operators

- definition of non-magnetic atoms and magnetic atoms with arbitrary moment size

Simulation of magnetic structures:
-simulation of magnetic excitations in general commensurate and incommensurate magnetic structures using linear spin-wave theory

-calculation of spin wave dispersion, spin-spin correlation functions

Magnetic interactions:
-definition of 1D, 2D and 3D magnetic structures

-representation of incommensurate structures using rotating coordinate system or complex basis vectors

Fitting spin wave spectra:
-possible to fit any parameter in the Hamiltonian

Linear spin wave theory for single-Q incommensurate magnetic structures
S. Toth and B. Lake J. Phys.: Condens. Matter 27, 166002 (2015).

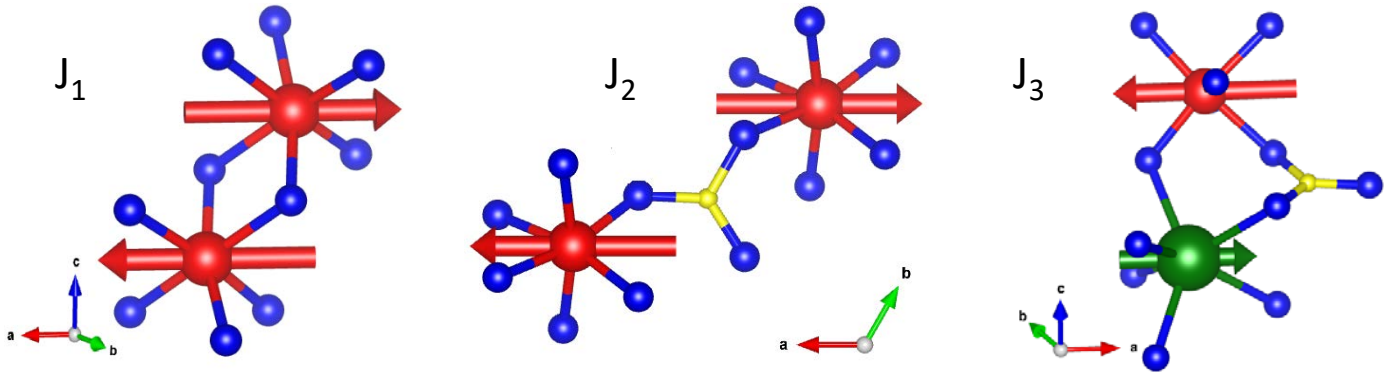
Modeling

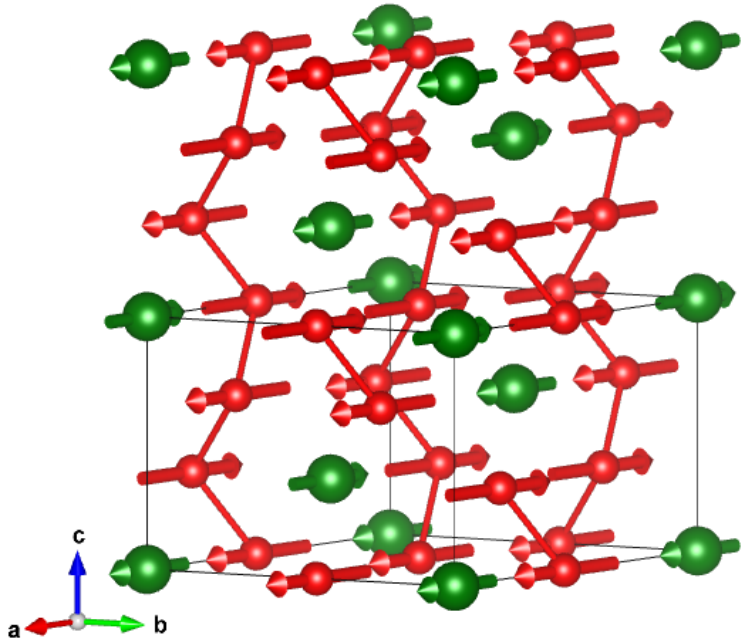
$$H = \sum_{ij} J_{ij} \cdot \vec{S}_i \vec{S}_j + \sum_i A_i \vec{S}_i \vec{S}_i + \mu_B B \sum_i g_i \vec{S}_i$$

1. Exchange paths and type of interaction

For example:

- Nd - Fe - O - B





Magnetic structure of $NdFe_3(BO_3)_4$, atoms of Nd are displayed in green, Fe - red. Space group R32, T_N=30K, k=[0 0 3/2].

Interaction	Distance (Å)	Value (meV)
J_1 Fe-Fe, intra-chain	3.185	0.71
J_3 Fe-Nd, nearest neighbors	3.788	0.04
J_2 Fe-Fe, inter-chain, nearest neighbors	4.409	0.17
and other interactions…		

I.V. Golosovsky, A.K. Ovsyanikov, D.N. Aristov, P.G. Matveeva, A.A. Mukhin, M. Boehm, L-P. Regnault, L.N. Bezmaternykh J. Magn. Magn. Mater. vol. 451, Pages 443-449 (2018)

Modeling

2. Literature or other methods

Absorption spectroscopy - energy levels, values of exchange parameters.

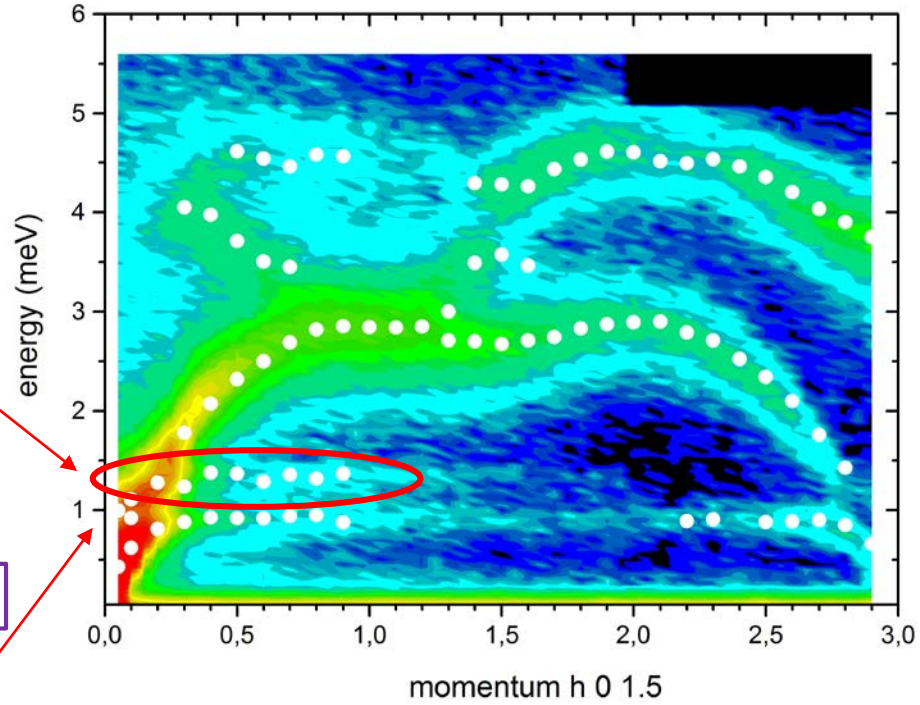
For example: transition between the exchange split levels of the Nd^{3}+ Kramers doublet at 1.08 meV.

	J1 Fe-Fe, meV	J2 Fe-Fe, meV	J3 Fe-R, meV	
Absorption spectroscopy	0.54	0.16	0.04	-
Neutron spectroscopy	0.71	0.17	0.04	and other interactions…

M. N. Popova, E. P. Chukalina et al., Phys. Rev. B 75, 224435 (2007).

Raman scattering - energy levels, values of exchange parameters, two magnon processes.

For example: transition between the exchange split levels of the Nd^{3}+ Kramers doublet at 1.23 meV.
Two-magnon scattering around 7.3 meV.



$NdFe_3(BO_3)_4$. Dispersion curves, measured on TAS ThALES at temperature 15 K along direction [h 0 1.5]

D. Fausti, A. A. Nugroho, and P. H. M. van Loosdrecht, S. A. Klimin, M. N. Popova, and L. N. Bezmaternykh, Phys. Rev. B 74, 024403, (2006)

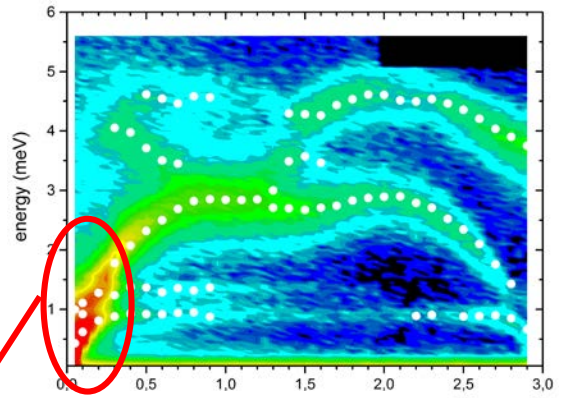
Modeling

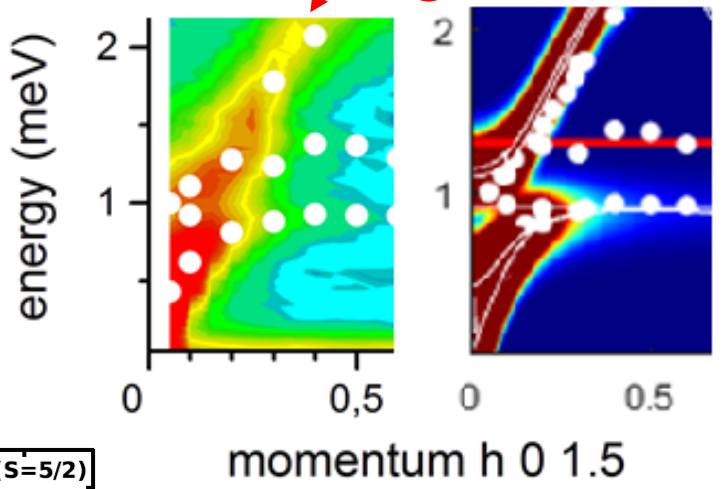
2. Literature or other methods

Quasi-optical Thz-spectroscopy - energy gaps.

For example: at q =0 have revealed several resonance modes at 1.21 meV and at 1.25 meV, which were associated with Nd-excitations, and the resonances of 0.42 meV and at zero energy, associated with excitations in Fe sublattice

A. M. Kuzmenko, A. A. Mukhin, V. Yu. Ivanovet al., JETP Lett. 94, 294, (2011).



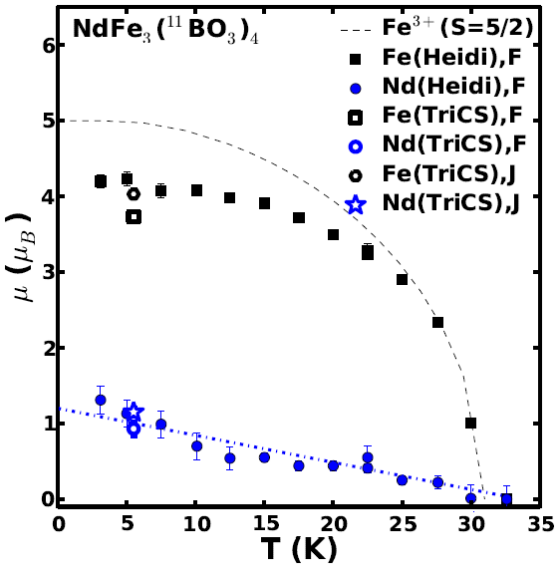


3. Average value of the spin moment

For example: $<S_{Fe}>\approx 2.0$ evaluated from the elastic neutron diffraction data at T=15K

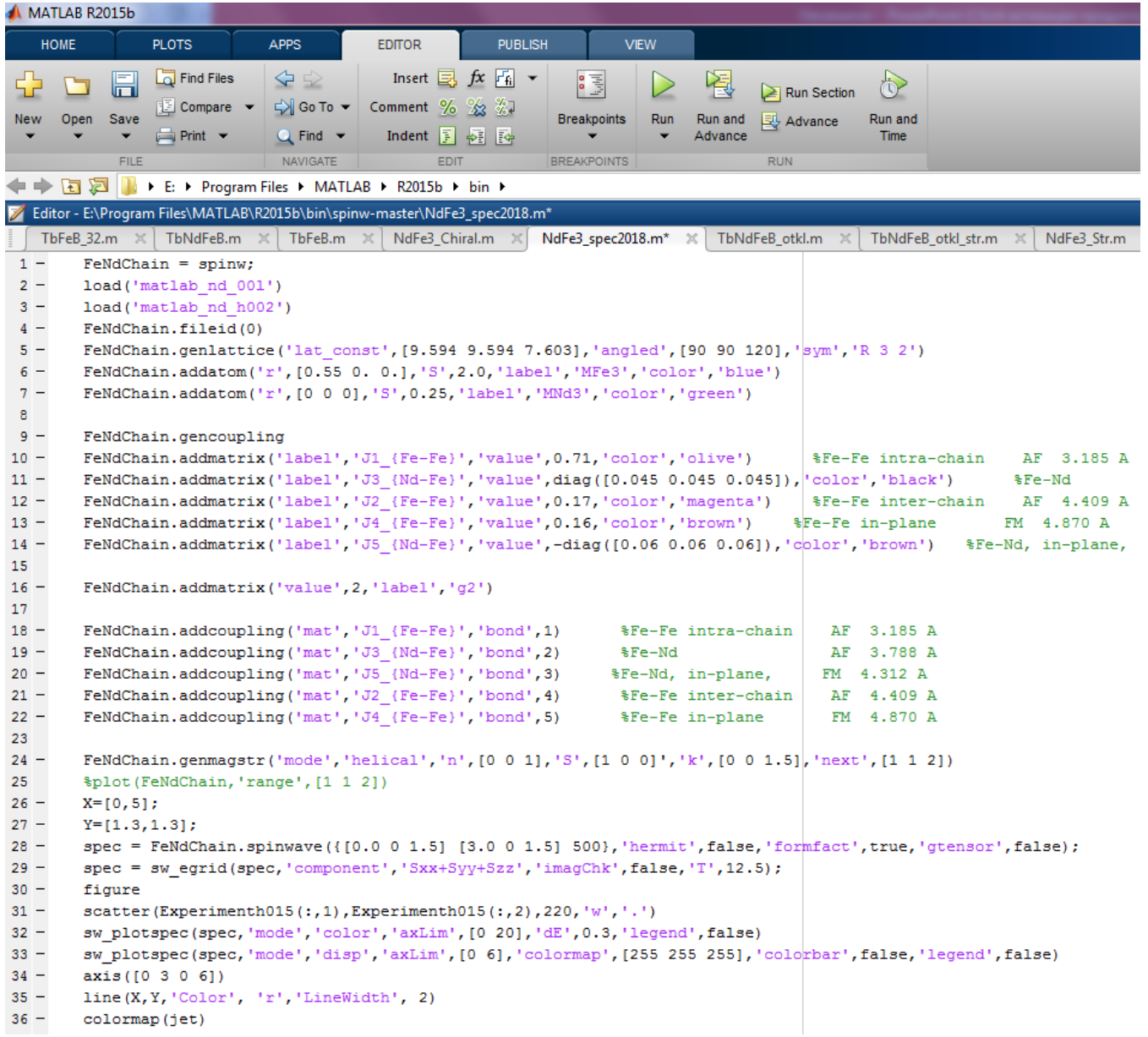
$$m_{Fe} = g_s \mu_\beta \langle S_{Fe} \rangle$$

where m_{Fe} – magnetic moment of Fe; $g_s = 2$ – g-factor; μ_β - Bohr magneton.

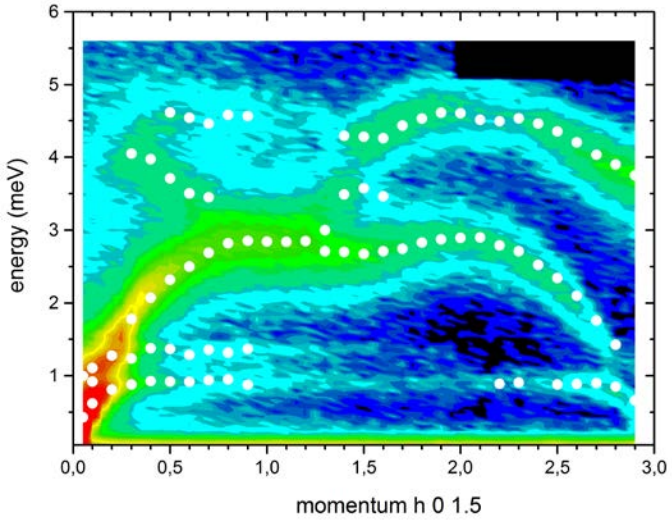


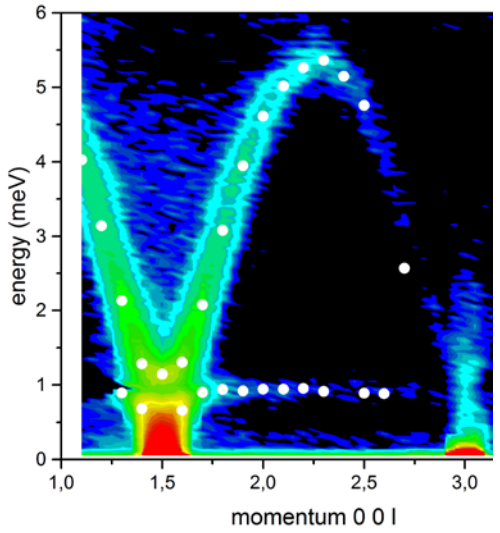
M. Janoschek, P. Fischer, J. Schefer, B. Roessli, V. Pomjakushin, M. Meven, V. Petricek, G. Petrakovskii, and L. Bezmaternikh, Phys. Rev. B 81, 094429 (2010).

Simulation

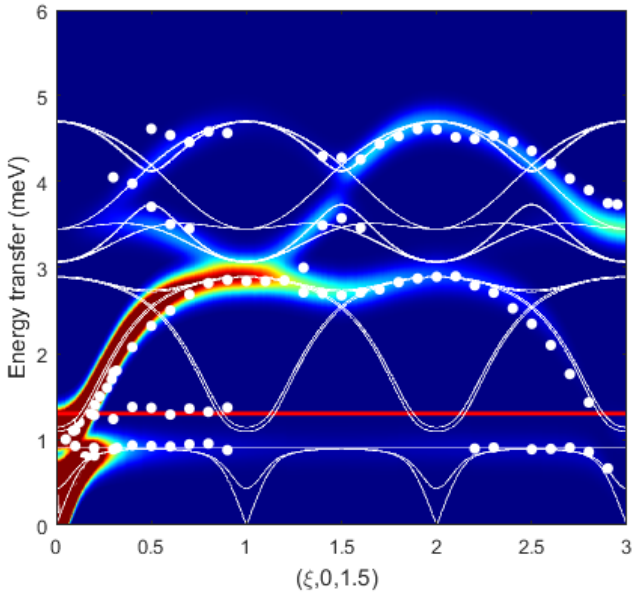

MATLAB R2015b
HOME
PLOTS
APPS
EDITOR
PUBLISH
VIEW
New
Open
Save
Find Files
Compare
Print
Go To
Find
Insert
Comment
Indent
Breakpoints
Run
Run and Advance
Run Section
Advance
Run and Time
FILE
NAVIGATE
EDIT
BREAKPOINTS
RUN
E: ▸ Program Files ▸ MATLAB ▸ R2015b ▸ bin ▸
Editor - E:\Program Files\MATLAB\R2015b\bin\spinw-master\NdFe3_spec2018.m*
TbFeB_32.m
TbNdFeB.m
TbFeB.m
NdFe3_Chiral.m
NdFe3_spec2018.m*
TbNdFeB_otkl.m
TbNdFeB_otkl_str.m
NdFe3_Str.m
1 FeNdChain = spinw;
2 load('matlab_nd_001')
3 load('matlab_nd_h002')
4 FeNdChain.fileid(0)
5 FeNdChain.genlattice('lat_const',[9.594 9.594 7.603],'angled',[90 90 120],'sym','R 3 2')
6 FeNdChain.addatom('r',[0.55 0. 0.],'S',2.0,'label','MFe3','color','blue')
7 FeNdChain.addatom('r',[0 0 0],'S',0.25,'label','MNd3','color','green')
8
9 FeNdChain.gencoupling
10 FeNdChain.addmatrix('label','J1_{Fe-Fe}','value',0.71,'color','olive') %Fe-Fe intra-chain AF 3.185 A
11 FeNdChain.addmatrix('label','J3_{Nd-Fe}','value',diag([0.045 0.045 0.045]),'color','black') %Fe-Nd
12 FeNdChain.addmatrix('label','J2_{Fe-Fe}','value',0.17,'color','magenta') %Fe-Fe inter-chain AF 4.409 A
13 FeNdChain.addmatrix('label','J4_{Fe-Fe}','value',0.16,'color','brown') %Fe-Fe in-plane FM 4.870 A
14 FeNdChain.addmatrix('label','J5_{Nd-Fe}','value',-diag([0.06 0.06 0.06]),'color','brown') %Fe-Nd, in-plane,
15
16 FeNdChain.addmatrix('value',2,'label','g2')
17
18 FeNdChain.addcoupling('mat','J1_{Fe-Fe}','bond',1) %Fe-Fe intra-chain AF 3.185 A
19 FeNdChain.addcoupling('mat','J3_{Nd-Fe}','bond',2) %Fe-Nd AF 3.788 A
20 FeNdChain.addcoupling('mat','J5_{Nd-Fe}','bond',3) %Fe-Nd, in-plane, FM 4.312 A
21 FeNdChain.addcoupling('mat','J2_{Fe-Fe}','bond',4) %Fe-Fe inter-chain AF 4.409 A
22 FeNdChain.addcoupling('mat','J4_{Fe-Fe}','bond',5) %Fe-Fe in-plane FM 4.870 A
23
24 FeNdChain.genmagstr('mode','helical','n',[0 0 1],'S',[1 0 0]','k',[0 0 1.5],'next',[1 1 2])
25 %plot(FeNdChain,'range',[1 1 2])
26 X=[0,5];
27 Y=[1.3,1.3];
28 spec = FeNdChain.spinwave({[0.0 0 1.5] [3.0 0 1.5] 500},'hermit',false,'formfact',true,'gtensor',false);
29 spec = sw_egrid(spec,'component','Sxx+Syy+Szz','imagChk',false,'T',12.5);
30 figure
31 scatter(Experimenth015(:,1),Experimenth015(:,2),220,'w','.')
32 sw_plotspec(spec,'mode','color','axLim',[0 20],'dE',0.3,'legend',false)
33 sw_plotspec(spec,'mode','disp','axLim',[0 6],'colormap',[255 255 255],'colorbar',false,'legend',false)
34 axis([0 3 0 6])
35 line(X,Y,'Color', 'r','LineWidth', 2)
36 colormap(jet)

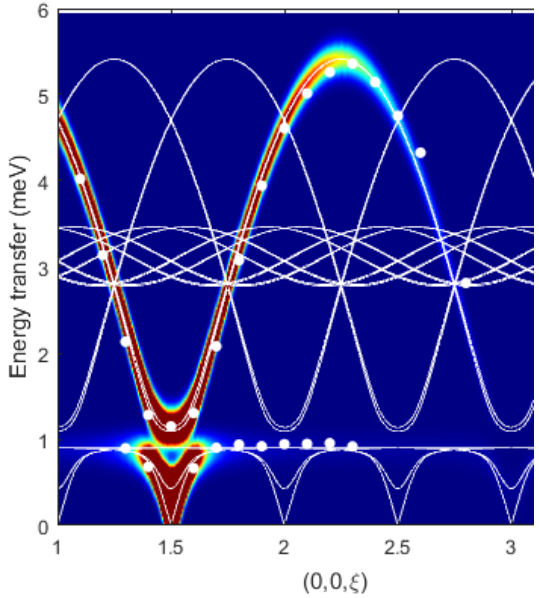
Simulation





Experimental maps of spin wave dispersion along [h 0 1.5] and along [0 0 l].
White spots correspond to the positions of the inelastic peaks.

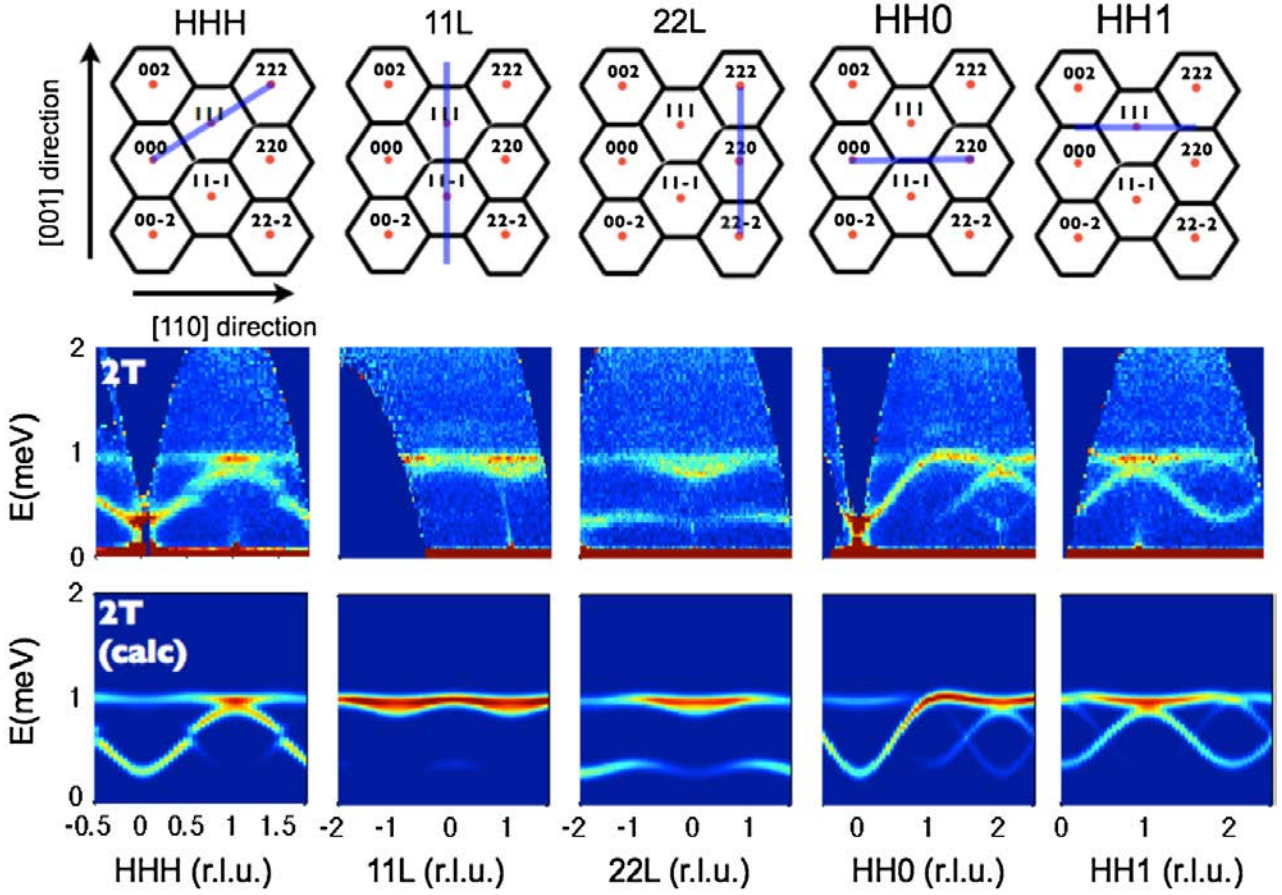


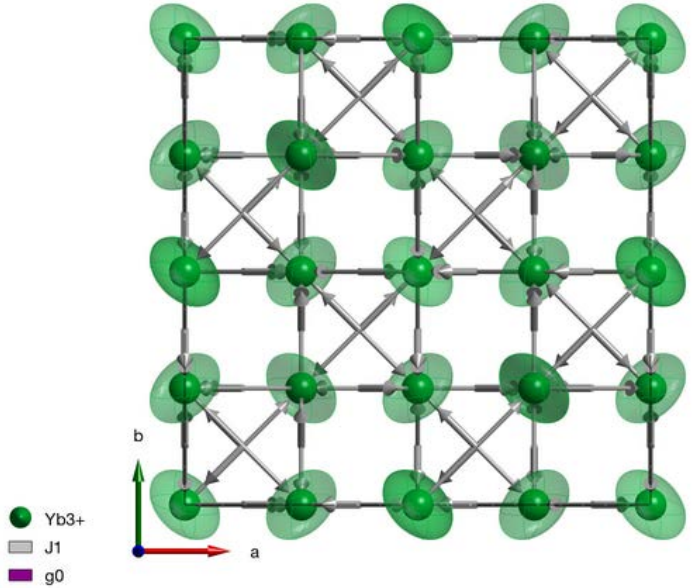


Calculation of spin wave dispersion along [h 0 1.5] and along [0 0 l].
White lines – the calculated dispersion curves.

Example - ‘‘spin ice’’ - $Yb_2Ti_2O_7$.

$$H = \sum_{ij} J_{ij} \cdot \vec{S}_i \vec{S}_j + \mu_B B \sum_i g_i \vec{S}_i$$





Magnetic structure of $Yb_2Ti_2O_7$.

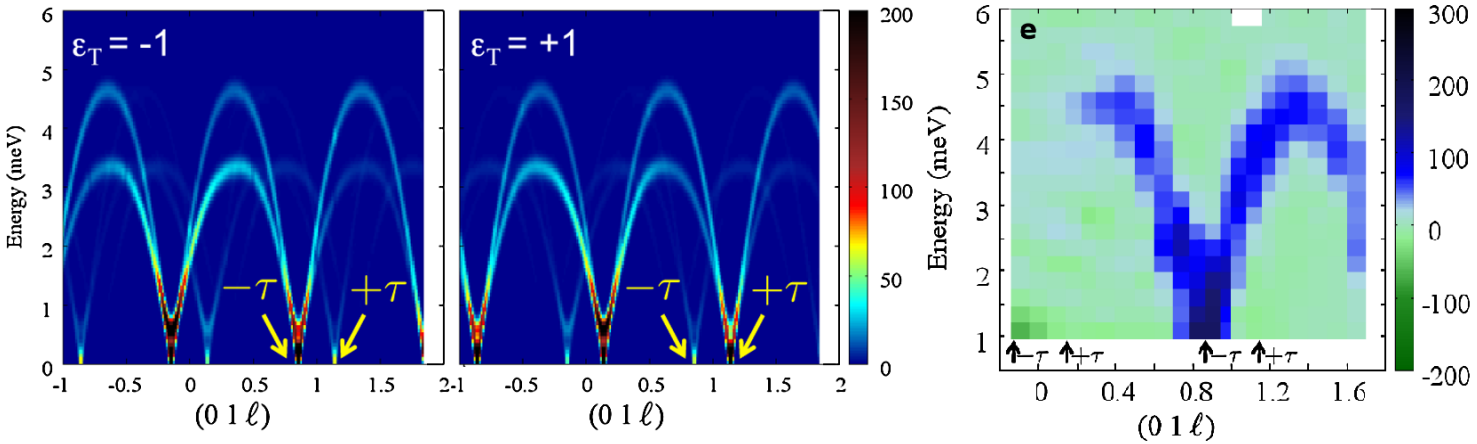
g-tensor to be g_{xy}=4.32, g_z=1.8

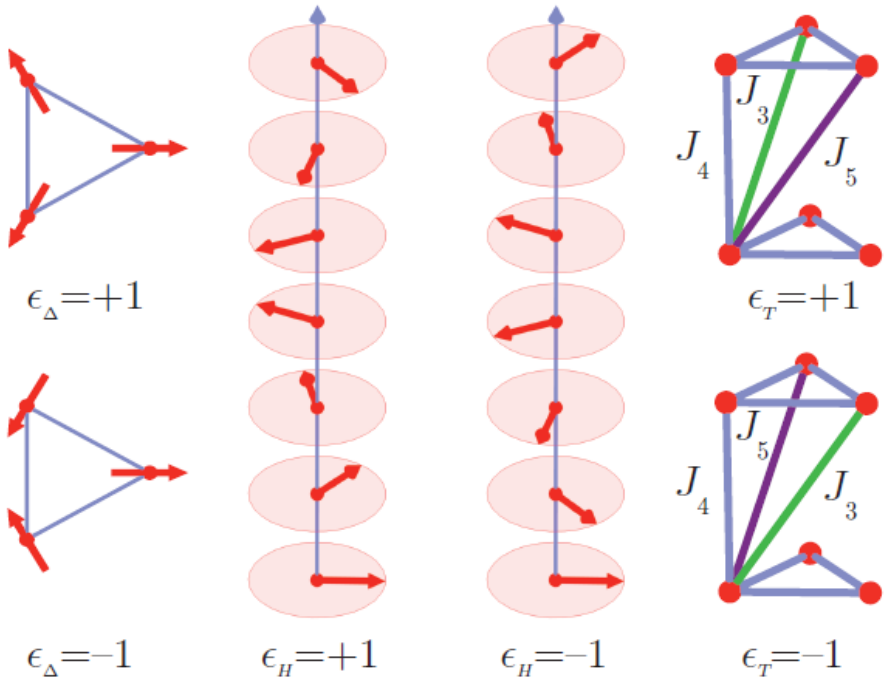
The magnetic bonds of the ‘‘spin ice’’ compounds Yb2Ti2O7. Kate A. Ross, Lucile Savary, Bruce D. Gaulin, and Leon Balents, Phys. Rev. X 1, 021002 (2011)

Example - $Ba_3NbFe_3Si_2O_{14}$ chiral compound

Space group P321.
The Neel temperature T_N=27 K with spins lying in the (a-b) plane and with the same 120 configuration on each trimer. This arrangement is helically modulated along the c axis with the period 1/τ=7.

Coupled chiral property: $\varepsilon_T = \varepsilon_\Delta \cdot \varepsilon_H$





Parity-Broken Chiral Spin Dynamics in Ba3NbFe3Si2O14 M. Loire, V. Simonet, S. Petit, et al., PRL 101, 247201 (2008)

Thank you for attention