Mdanse 2018 neutron school

INTRODUCTION TO SPIN WAVES

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[1] P.W. Anderson, Phys. Rev. 83, 1260 (1951)

[2] R. Kubo, Phys. Rev. 87, 568 (1952)

[3] T. Oguchi, Phys. Rev 117, 117 (1960)

[4] D.C. Mattis, *Theory of Magnetism I*, Springer Verlag, 1988

[5] R.M. White, *Quantum Theory of Magnetism*, Springer Verlag, 1987

[6] A. Auerbach, *Interacting electrons and Quantum Magnetism*, Springer Verlag, 1994.

Introduction

Neutrons = one of the best tools to investigate condensed matter

Lattice & Magnetic response

- Structure
- Dynamics

Aim of the school : present a numerical « toolbox » to help

design/understand/interpret

Neutron instruments
Neutron experiments
Neutron data

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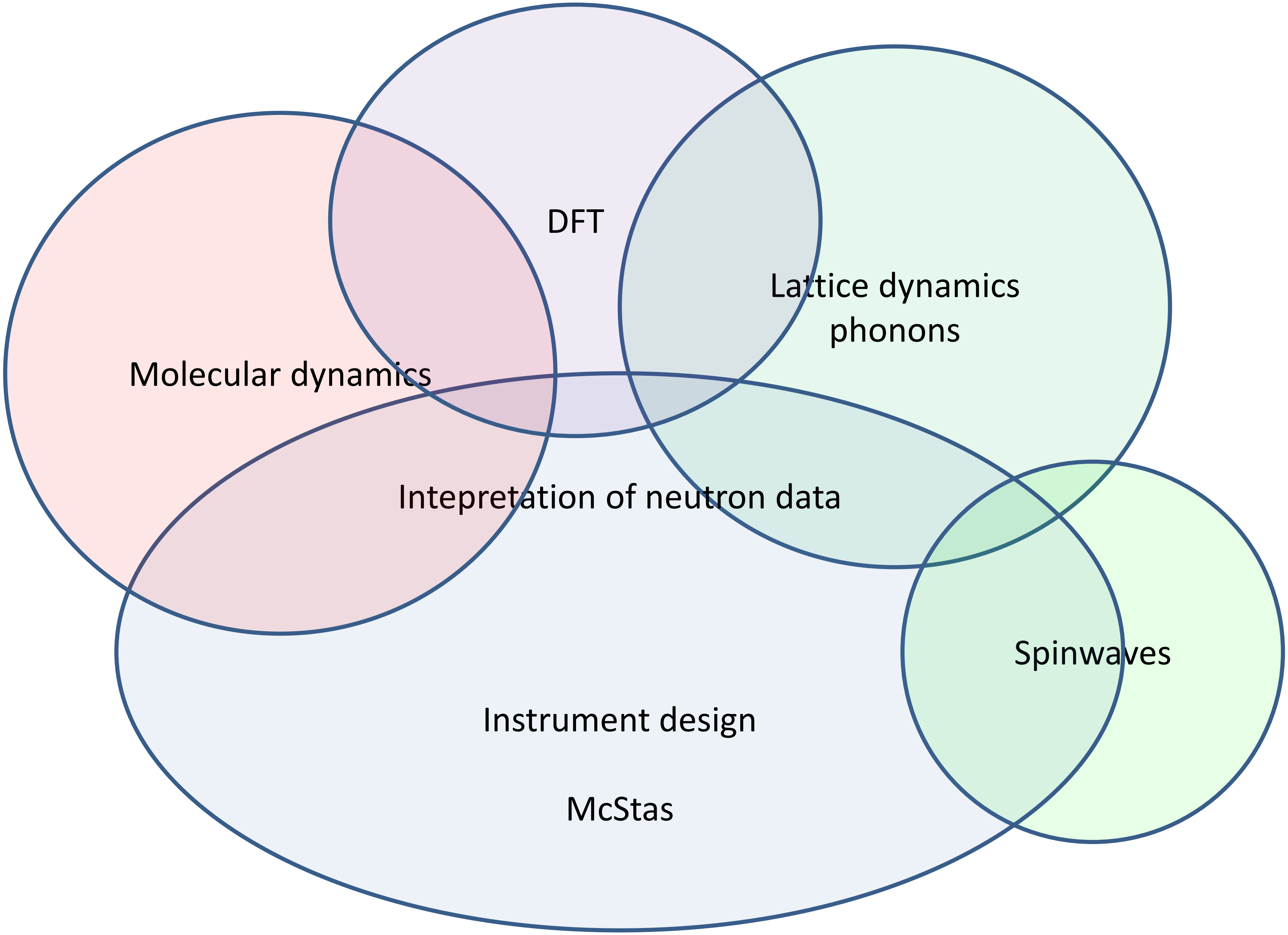
Introduction



Heisenberg Model
(exchange interactions between 3d spins):

$$\mathcal{H} = \frac{1}{2}\sum_{m,i,n,j} \mathbf{S}_{m,i}\mathcal{J}_{m,i,n,j}\mathbf{S}_{n,j} + \sum_{n,m} B_{n,m}O_{n,m}$$

$$\begin{array}{rcl} O_{20} & = & 3S_z^2 \\ O_{22} & = & S_x^2 - S_y^2 \\ O_{2-2} & = & S_xS_y + S_yS_x \\ O_{2-1} & = & S_zS_x + S_xS_z \\ O_{21} & = & S_zS_y + S_yS_z \\ \ldots & & \end{array}$$

+

Anisotropy (single ion, easy plane, easy axis)

Why are spin waves important ?

1. The Heisenberg Hamiltonian is relevant in a number of magnets.

2. Today's physics goes beyond the Néel paradigm and the theory is quite complicated ! Trick: "push" the system back to a Néel order, measure the spin spin waves and determine the exchange couplings.

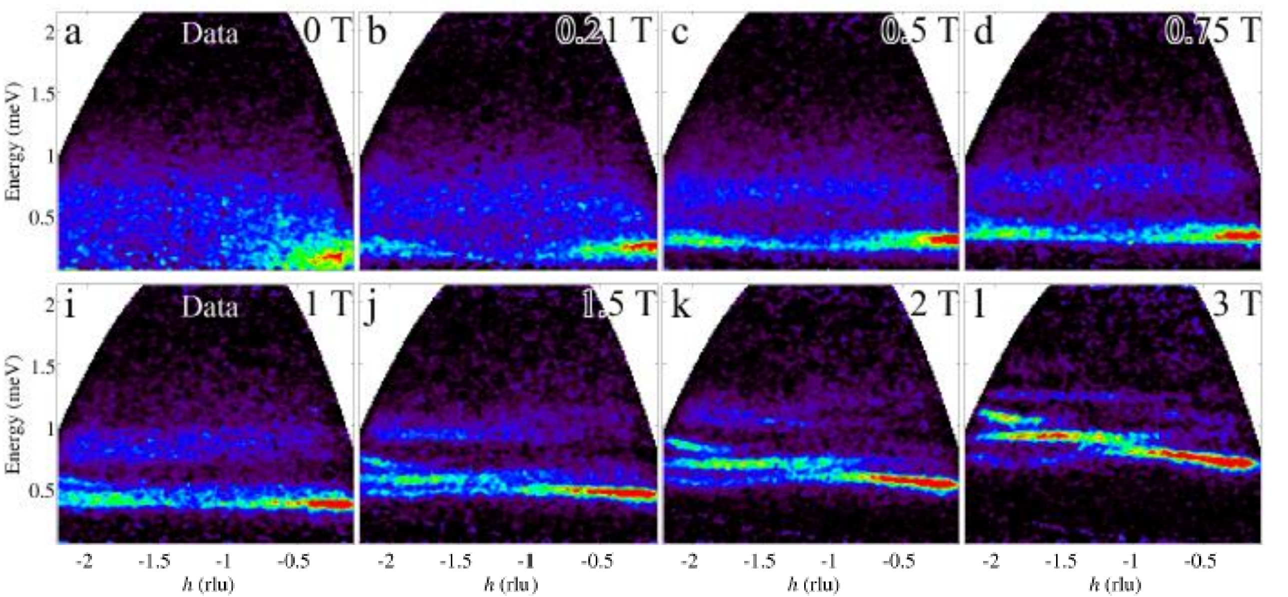
3. Examples : standard magnets, multiferroics, 1D systems, spin liquids ...

Introduction

Applying a magnetic field on the pyrochlore magnet $Yb_2Ti_2O_7$ kills the continuum and restores « classical » spinwaves

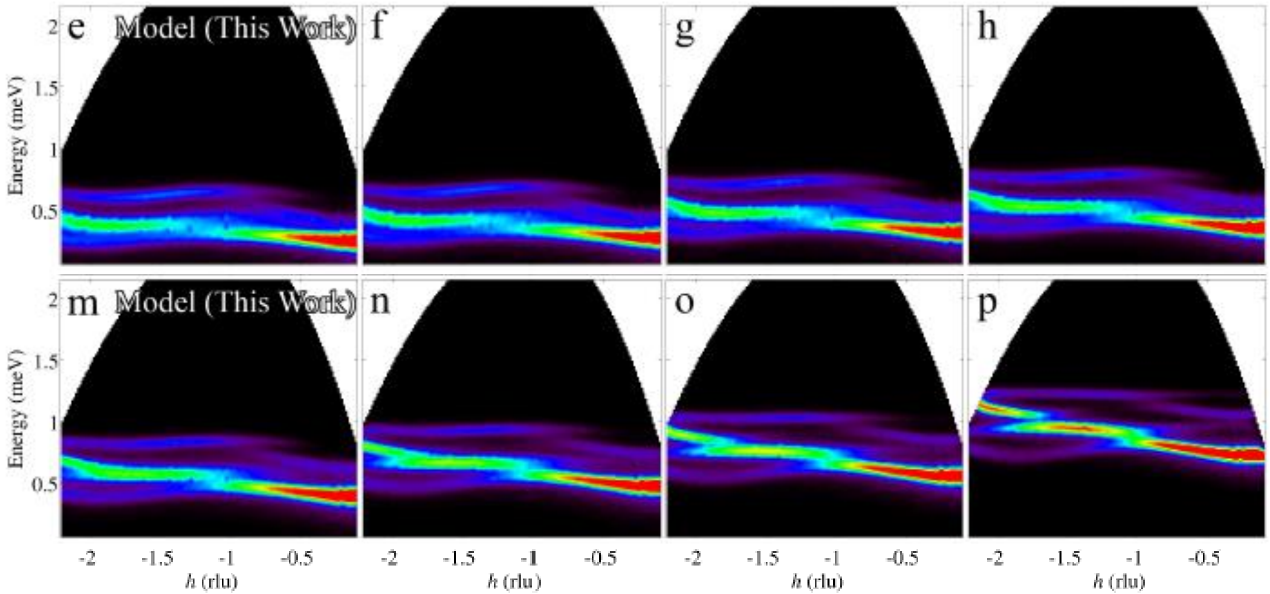
PRL 119, 057203 (2017) PHYSICAL REVIEW LETTERS week ending 4 AUGUST 2017

Quasiparticle Breakdown and Spin Hamiltonian of the Frustrated Quantum Pyrochlore $Yb_2Ti_2O_7$ in a Magnetic Field



Introduction

The spin wave theory successfully explains the high field spectrum but fails at zero field



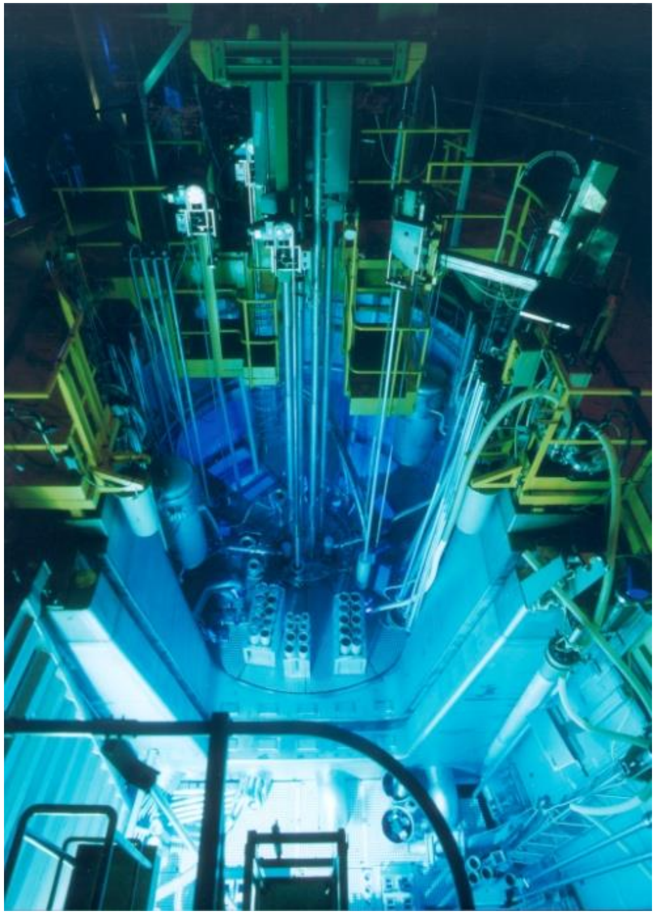
How to observe spin waves ?

Neutron scattering.

ILL, LLB, Munich, PSI, ISIS …

And ESS in the future !!

THz, IR spectroscopy



Part 1 : neutron cross section

Cross section

- The spins (and orbital motion) of unpaired electrons create a dipolar field.
- The spin of the neutron interacts with this field.

$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{k_f}{k_i}(\gamma r_o)^2 \sum_{m,n} \int_{-\infty}^{+\infty} dt \sum_{a,b} \langle S_m^a \left(\delta_{a,b} - \frac{\mathbf{Q}^a\mathbf{Q}^b}{\mathbf{Q}^2}\right) S_n^b(t)\, e^{i\mathbf{Q}\,\mathbf{R}_m}\, e^{-i\mathbf{Q}\,\mathbf{R}_n(t)}\rangle\, e^{-i\omega t}$$

Cross section

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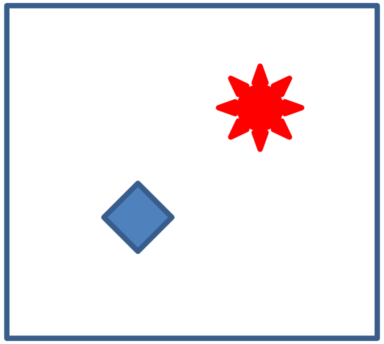
$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{k_f}{k_i}(\gamma r_o)^2 \sum_{i,j} e^{i\mathbf{Q}\,(\mathbf{R}_i^o-\mathbf{R}_j^o)} \sum_{\ell,\ell'} f_\ell(\mathbf{Q})\, f^*_{\ell'}(\mathbf{Q})\, e^{i\mathbf{Q}\,(\mathbf{r}_\ell-\mathbf{r}_{\ell'})}\, e^{-W_\ell-W_{\ell'}}$$

$$\times\int_{-\infty}^{+\infty} dt\, \langle \sum_{a,b} S^a_{i\ell} \left(\delta_{a,b}-\frac{\mathbf{Q}^a\mathbf{Q}^b}{\mathbf{Q}^2}\right) S^b_{j\ell'}(t)\rangle\, e^{-i\omega t}$$

1. Spins reside on a lattice
2. Decoupled from atomic displacements

$$\mathbf{R}_m(t) = \mathbf{R}_i^o + \mathbf{r}_\ell$$



Cross section

Classical radius of electrons

$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{k_f}{k_i}\,(\gamma r_o)^2 \sum_{i,j} e^{i\mathbf{Q}\,(\mathbf{R}_i^o-\mathbf{R}_j^o)} \sum_{\ell,\ell'} f_\ell(\mathbf{Q})\; f_{\ell'}^*(\mathbf{Q})\; e^{i\mathbf{Q}\,(\mathbf{r}_\ell-\mathbf{r}_{\ell'})}\; e^{-W_\ell-W_{\ell'}}$$
$$\times \int_{-\infty}^{+\infty} dt\, \langle \sum_{a,b} S_{i\ell}^a \left(\delta_{a,b} - \frac{\mathbf{Q}^a\mathbf{Q}^b}{\mathbf{Q}^2}\right) S_{j\ell'}^b(t)\rangle\; e^{-i\omega t}$$

Cross section

Unit cell position

Classical radius of electrons

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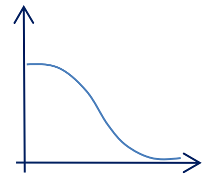
Cross section

Form factor of unpaired electrons in a given orbital (tabulated)



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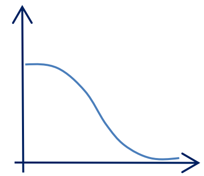
Cross section

Form factor of unpaired electrons in a given orbital (tabulated)

Atomic positions within the unit cell



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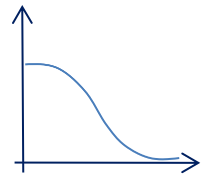

Atomic positions within the unit cell

Debye-waller factor (thermal motion of the ions)

Unit cell position

Classical radius of electrons

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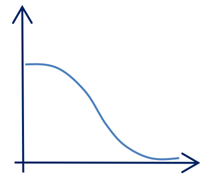

Unit cell position

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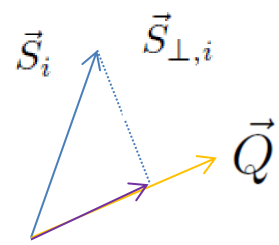

- Spin-spin correlation function
- spin components perp to Q (dipolar interaction)

$$\sum_{a,b} S_m^a \left(\delta_{a,b} - \frac{\mathbf{Q}^a \mathbf{Q}^b}{\mathbf{Q}^2} \right) S_n^b(t) = \mathbf{S}_{\perp,m} \cdot \mathbf{S}_{\perp,n}(t)$$

Frozen spins (Cross section)

$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{k_f}{k_i}(\gamma r_o)^2 \sum_{i,j} e^{i\mathbf{Q}\,(\mathbf{R}_i^o-\mathbf{R}_j^o)} \sum_{\ell,\ell'} f_\ell(\mathbf{Q})\, f^*_{\ell'}(\mathbf{Q})\, e^{i\mathbf{Q}\,(\mathbf{r}_\ell-\mathbf{r}_{\ell'})}\, e^{-W_\ell-W_{\ell'}}$$

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Assume frozen spins (independent on time)

Frozen spins (Cross section)

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Assume frozen spins (independent on time)

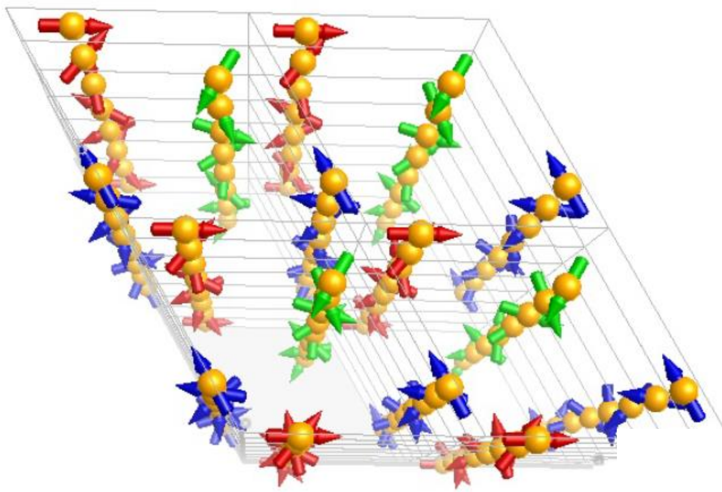
$$\downarrow$$

$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \frac{k_f}{k_i}\,(\gamma r_o)^2 \sum_{i,j} e^{i\mathbf{Q}\,(\mathbf{R}_i^o-\mathbf{R}_j^o)} \sum_{\ell,\ell'} f_\ell(\mathbf{Q})\; f_{\ell'}^*(\mathbf{Q})\; e^{i\mathbf{Q}\,(\mathbf{r}_\ell-\mathbf{r}_{\ell'})}\; e^{-W_\ell-W_{\ell'}}\; \langle \mathbf{S}_{\perp,i\ell}\; \mathbf{S}_{\perp,j\ell'}\rangle\; \delta(\omega)$$

$$= \frac{k_f}{k_i}\,(\gamma r_o)^2\, |\sum_{i,\ell} e^{i\mathbf{Q}\,(\mathbf{R}_i^o+\mathbf{r}_\ell)}\; f_\ell(\mathbf{Q})\; e^{-W_\ell}\; \mathbf{S}_{\perp,i\ell}|^2\; \delta(\omega)$$

This is noting but the magnetic structure factor

Frozen spins (Cross section)



Crystalline and magnetic structures

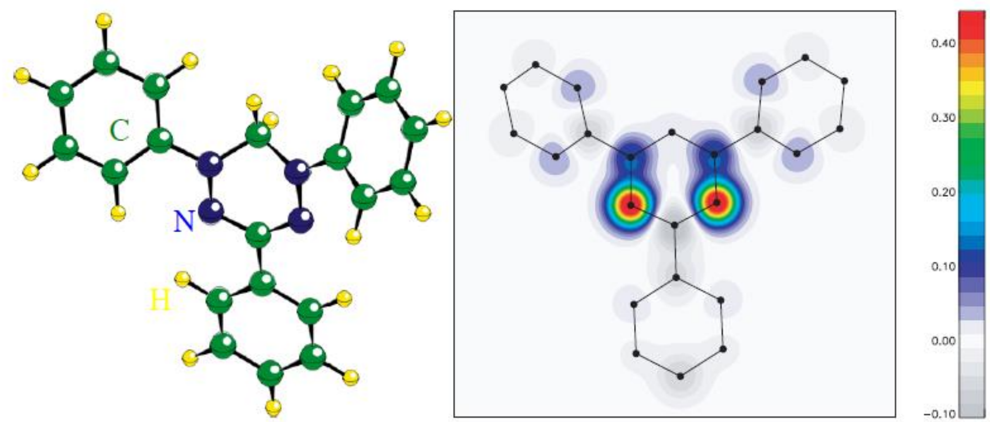
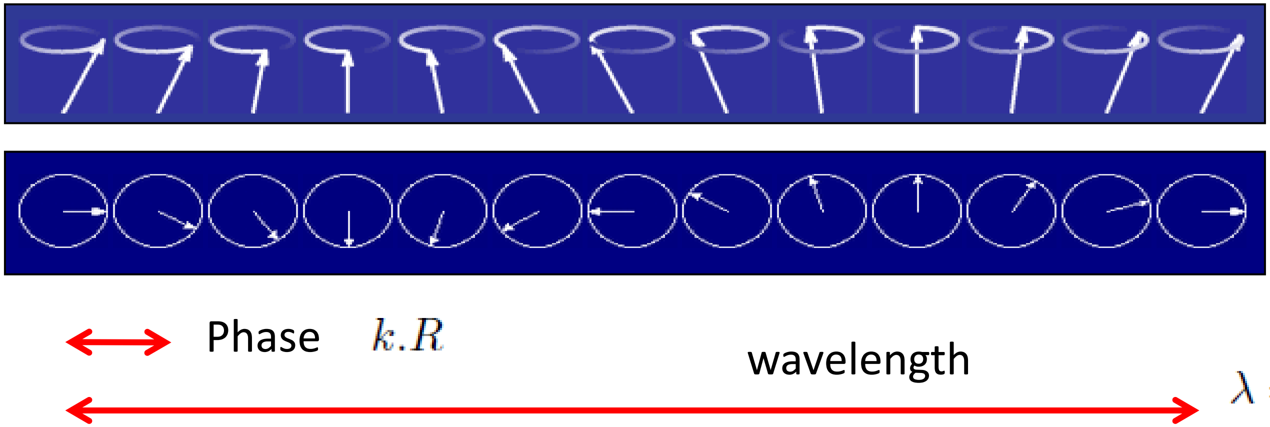


Fig. 4. View of the TPV molecule (left) and experimental magnetization distribution (right) as measured by polarized neutron diffraction.

Part 2 : theory of spin waves

Spins are no more frozen

Physical picture



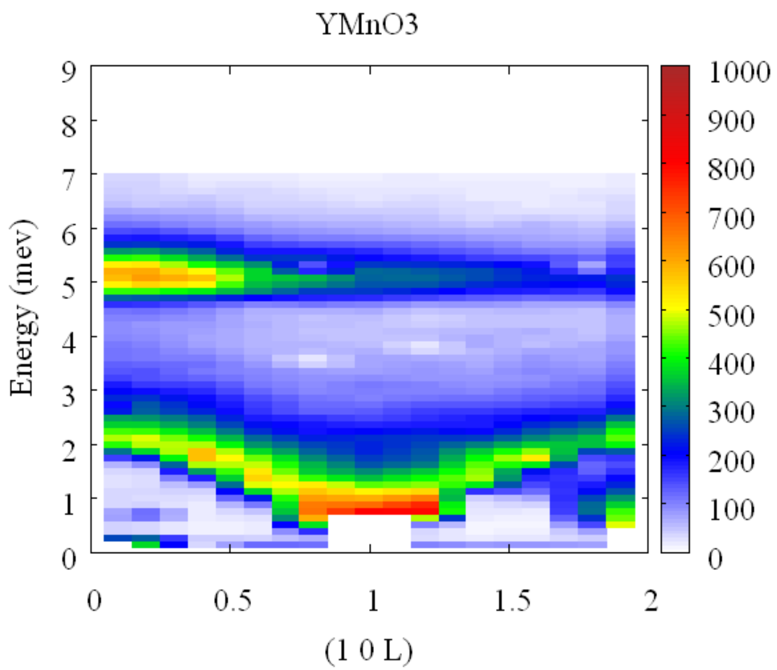
$$\lambda = \frac{2\pi}{k}$$

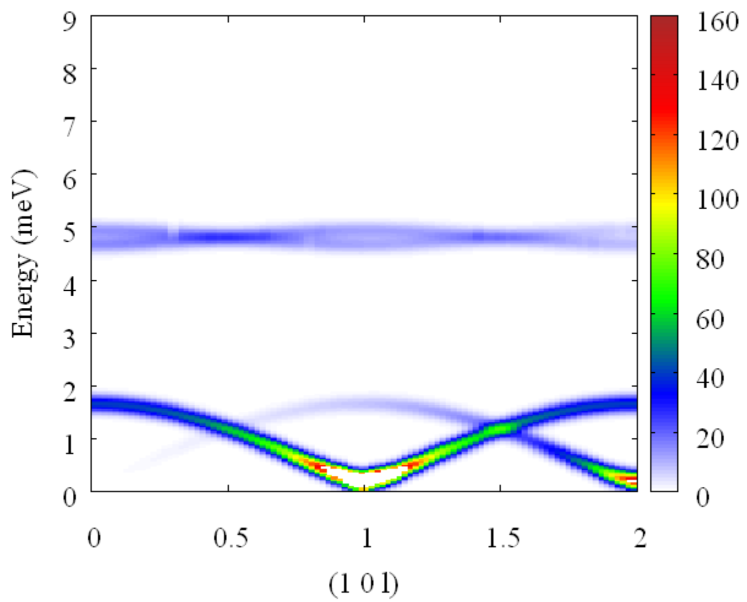
1. Spin waves are precession modes of the spins around the ordered structure (conventional magnets).

2. INS allows to measure the dispersion of those modes

3. With the help of a model, it becomes possible to determine exchange couplings, anisotropies, … but we need a theory for that !

Physical picture

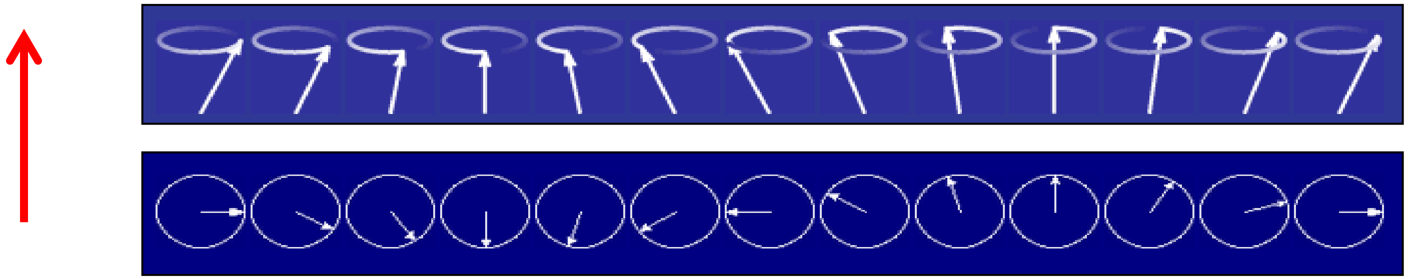




Spin wave response (showing the dispersion) in the multiferroic material $YMnO_3$
Right panel shows the modeling

Flavor of the theory

1. Describe the ground state in a « simple » mean field approximation



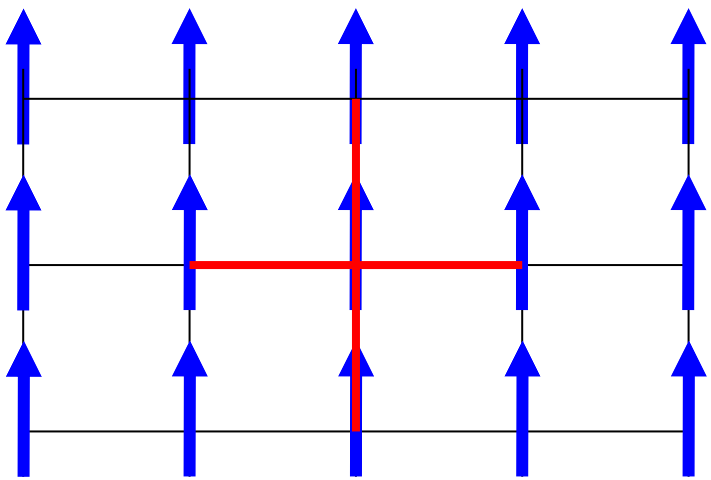
2. Describe deviations away from local magnetization, keep small deviations only

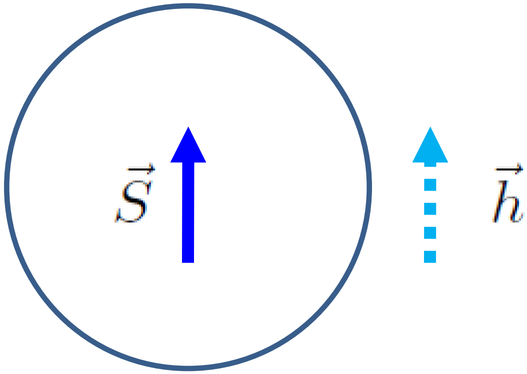
3. Periodic in time and space : Fourier transform

4. Final solution involves some « diagonalization » to obtain « eigen modes »

Mean field

Heisenberg Hamiltonian $\mathcal{H} = \frac{1}{2} \sum_{m,n} \mathbf{S}_m \mathcal{J}_{m,n} \mathbf{S}_n$ $\rightarrow$ $\boxed{\mathcal{H} = \sum_{m} \mathbf{S}_m \left(\sum_{n} \mathcal{J}_{m,n} \langle \mathbf{S}_n \rangle \right)}$

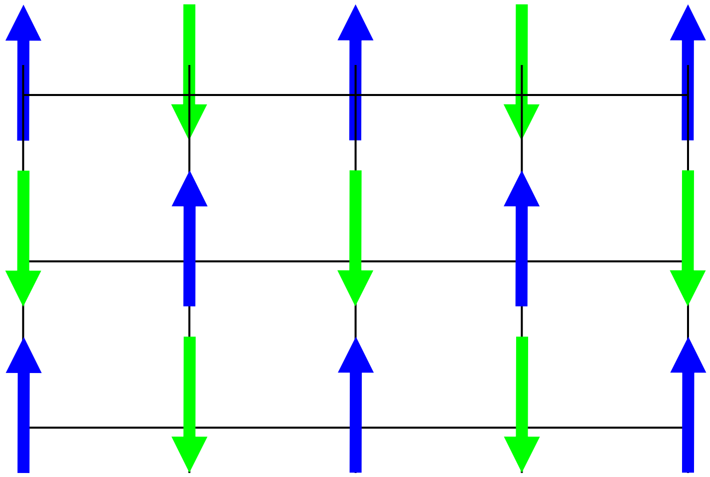




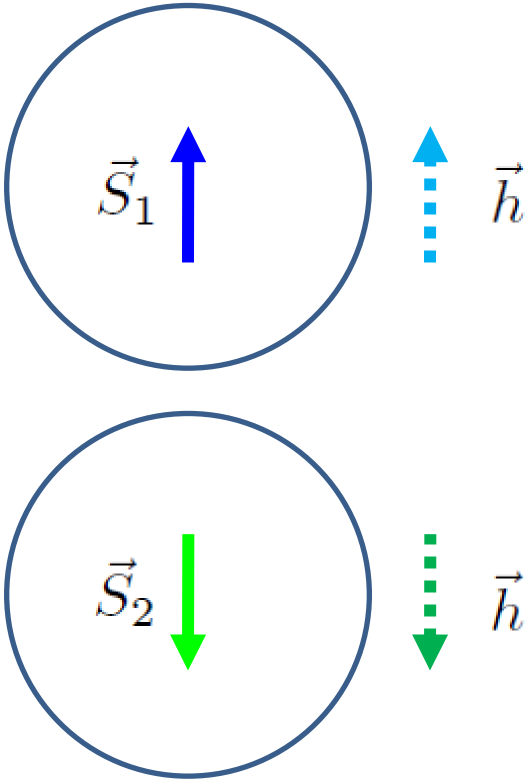
A spin experiences a **molecular field** due to the interactions with its neighbours.
This leads to long range ordering

Mean field

Depending on the nature of the interactions, this molecular field can induce a new periodicity

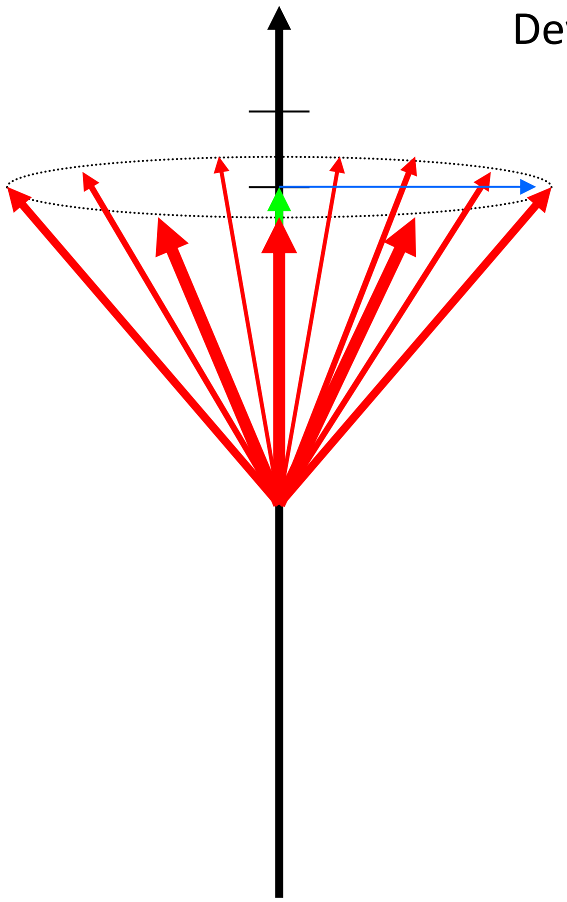


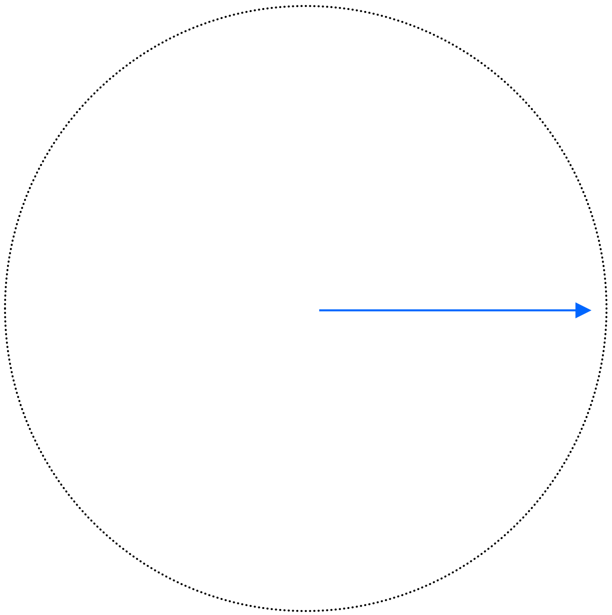
Example : AF ordering



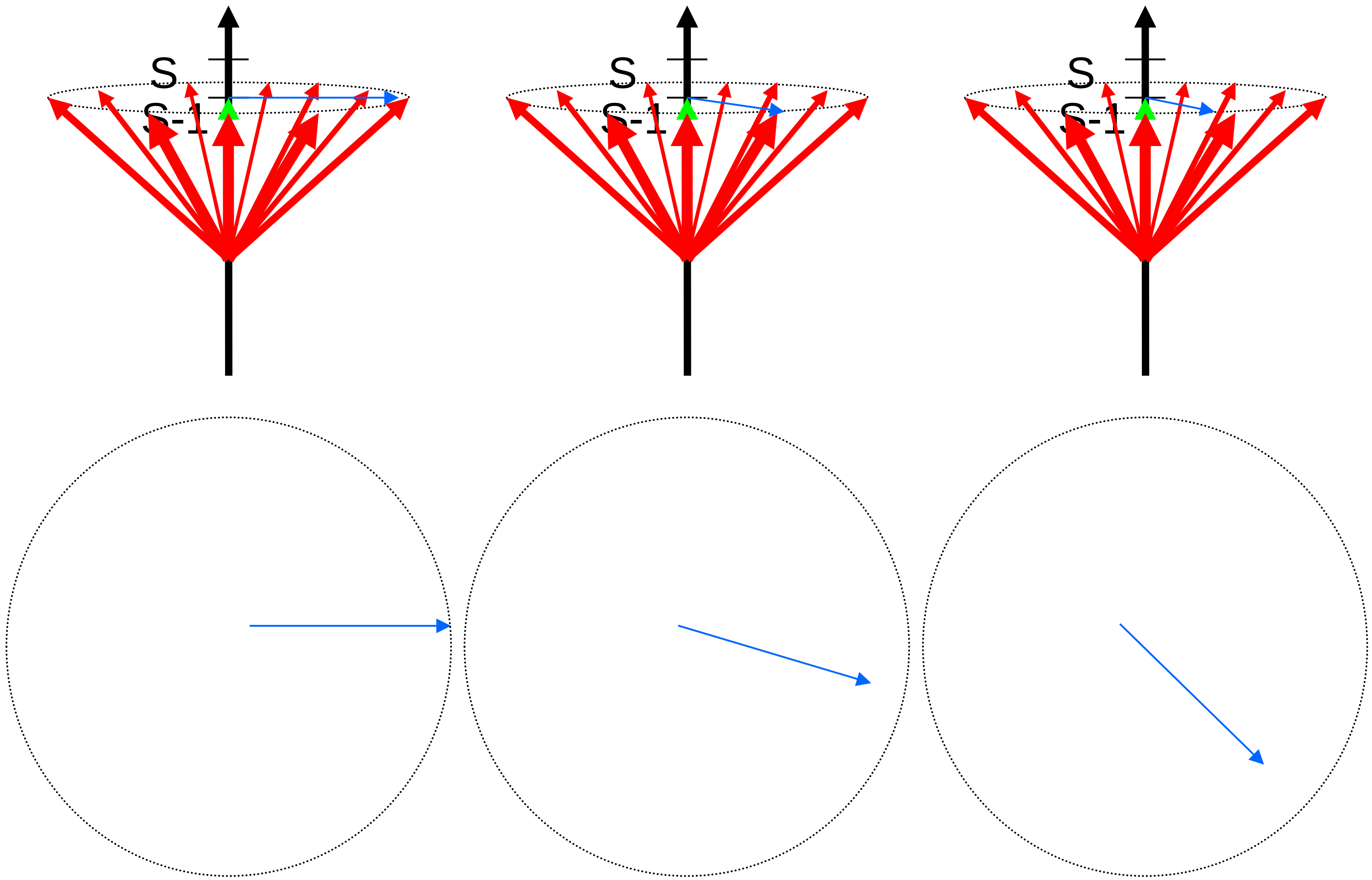
Precession

Precession of a spin in a the molecular field
Deviation away from local equilibrium magnetization





Precession



How to describe the « deviation » ?

Polar coordinates:

$$
\begin{aligned}
S_x &= S\cos\theta\sin\phi \\
S_y &= S\sin\theta\sin\phi \\
S_z &= S\cos\phi
\end{aligned}
$$

$$
\begin{aligned}
S^+ &= S\sin\phi\; e^{+i\theta} \\
S^- &= S\sin\phi\; e^{-i\theta}
\end{aligned}
$$

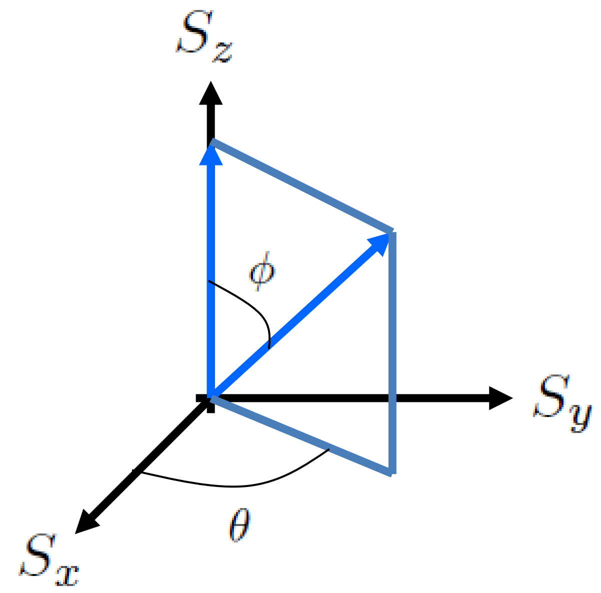
Deviation away from saturation:

$$S_z = S - D$$

$$\cos\phi = 1 - \frac{D}{S}$$

Spin components written in terms of the deviation:

$$
\boxed{
\begin{aligned}
S^+ &= \sqrt{2S}\sqrt{1-\frac{D}{2S}}\,\sqrt{D}\; e^{+i\theta} \\
S^- &= \sqrt{2S}\sqrt{1-\frac{D}{2S}}\,\sqrt{D}\; e^{-i\theta} \\
S_z &= S - D
\end{aligned}
}
$$



How to describe the « deviation » ?

The deviation is expressed using a boson operator:

$$[b, b^+] = 1$$

$$n_b = b^+ b = 0, 1, 2, \dots, \infty$$

$$\begin{aligned} S^+ &= \sqrt{2S}\sqrt{1-\frac{D}{2S}}\,\sqrt{D}\; e^{+i\theta} \\ S^- &= \sqrt{2S}\sqrt{1-\frac{D}{2S}}\,\sqrt{D}\; e^{-i\theta} \\ S_z &= S - D \end{aligned}$$

$$\begin{aligned} S^+ &= \sqrt{2S}\sqrt{1-\frac{n_b}{2S}}\; b \\ S^- &= \sqrt{2S}\; b^+ \sqrt{1-\frac{n_b}{2S}} \\ S_z &= S - n_b \end{aligned}$$

« Holstein – Primakov »

$$\begin{aligned} S^+ &\approx \sqrt{2S}\; b \\ S^- &\approx \sqrt{2S}\; b^+ \\ S^z &= S - n_b \end{aligned}$$

How to describe the « deviation » ?

The deviation is expressed using a boson operator:

$$[b, b^+] = 1$$

$$n_b = b^+ b = 0, 1, 2, ..., \infty$$

May become unphysical

$$\begin{aligned} S^+ &= \sqrt{2S}\sqrt{1 - \frac{n_b}{2S}}\; b \\ S^- &= \sqrt{2S}\; b^+ \sqrt{1 - \frac{n_b}{2S}} \\ S_z &= S - n_b \end{aligned}$$

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« Holstein – Primakov »

$$\begin{aligned} S^+ &\approx \sqrt{2S}\; b \\ S^- &\approx \sqrt{2S}\; b^+ \\ S^z &= S - n_b \end{aligned}$$

Ferromagnet

Heisenberg Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_{m,n} \mathbf{S}_m J_{m,n} \, \mathbf{S}_n$$

Holstein-Primakov

$$\begin{aligned} S_m^x &\approx \frac{\sqrt{2S}}{2} \left(b_m + b_m^+\right) \\ S_m^y &\approx \frac{\sqrt{2S}}{2i} \left(b_m - b_m^+\right) \\ S_m^z &\approx S - b_m^+ \, b_m \end{aligned}$$

Keep 2nd order terms (small deviations)

$$\mathcal{H} \approx \frac{1}{2} \sum_{m,n} \frac{S}{2}(b_m + b_m^+) \, J_{m,n} \, (b_n + b_n^+) - \frac{S}{2}(b_m - b_m^+) \, J_{m,n} \, (b_n - b_n^+) + (S - b_m^+ b_m) \, J_{m,n} \, (S - b_n^+ b_n)$$

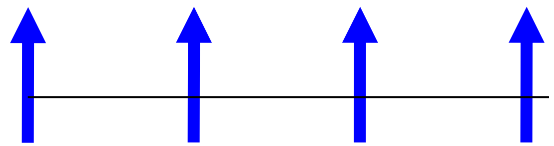
$$\mathcal{H} \approx \frac{1}{2} \sum_{m,n} S \, J_{m,n} \, (b_m \, b_n^+ + b_m^+ \, b_n) - S \, J_{m,n} \, b_n^+ b_n - b_m^+ b_m \, J_{m,n} \, S$$

Fourier Transform : dispersion of the spin waves

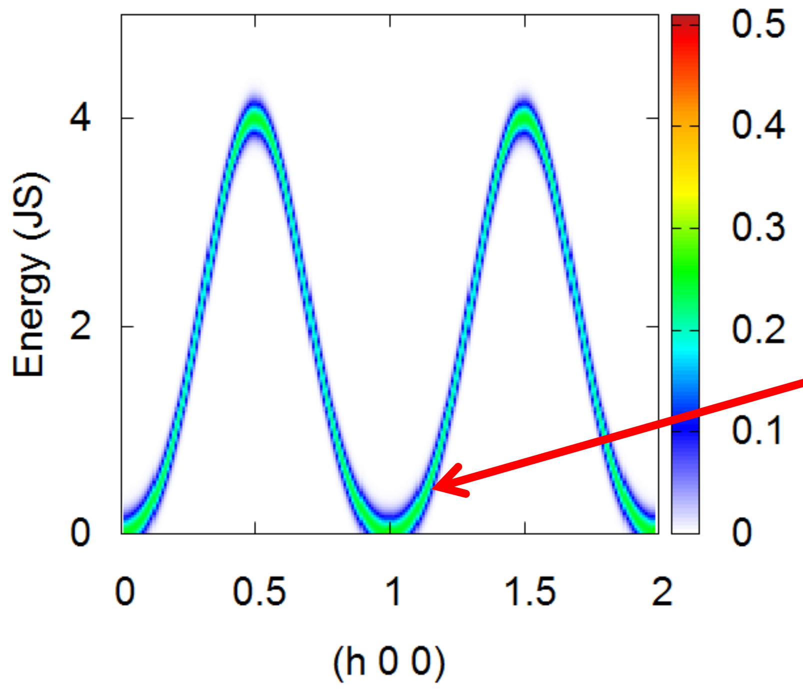
$$\mathcal{H} \approx \sum_k J_k \, S \, b_k^+ \, b_k - \left(\sum_\Delta J_{m,m+\Delta} \right) b_k^+ b_k$$

$$\omega_k = (J_k - zJ) \, S = z|J| \, S \, (1 - \gamma_k) \qquad \gamma_k = \frac{1}{z} \sum_\Delta e^{ik\Delta}$$

Ferromagnet



$$\omega_k = (J_k - zJ)\,S = z|J|\;S\;\;(1-\gamma_k) \qquad \gamma_k = \frac{1}{z}\sum_{\Delta} e^{ik\Delta}$$



Parabolic dispersion
at small k

$$\omega_k \approx |J|\;S\;\;\left((k_x\;a_x)^2 + (k_y\;a_y)^2 + (k_z\;a_z)^2\right)$$

Ferromagnet

Checking consistency of the approximation

$$\begin{aligned}\langle S^z \rangle &\approx S - \sum_k \langle b_k^+ \, b_k \rangle \\ &\approx S - \sum_k n_B(\omega_k)\end{aligned}$$

$$\sum_k \longrightarrow \int dk^d = \int dk \, \frac{k^{d-1}}{(2\pi)^d}$$

$$n_B(E) \longrightarrow \frac{k_B T}{E}$$

$$\sum_k n_B(\omega_k) \longrightarrow \int dk \, \frac{k^{d-1}}{(2\pi)^d} \, \frac{T}{k^2}$$

The thermal fluctuations prevent long range ordering for $d \leq 2$

The breakdown of the spin wave theory is consistent with the « Mermin and Wagner » theorem

To calculate the cross section from spin waves, we calculate the spin in terms of the spin wave bosons:

$$\sum_m e^{i\mathbf{k}\mathbf{R}_m}\,\mathbf{S}_m(t) = \mathbf{S}_k(t) = \begin{pmatrix} \frac{\sqrt{2S}}{2}(b_k e^{+i\omega_k t} + b_k^+ e^{-i\omega_k t}) \\ \frac{\sqrt{2S}}{2i}(b_k e^{+i\omega_k t} - b_k^+ e^{-i\omega_k t}) \\ S - \sum_k b_k^+ b_k \end{pmatrix}$$

The time dependency is known and directly reflects the spin wave energies:

$$\begin{aligned} \langle b_k b_k^+(t)\rangle &= (1 + n_B(\omega_k))e^{-i\omega_k t} \\ \langle b_k^+ b_k(t)\rangle &= n_B(\omega_k)e^{+i\omega_k t} \end{aligned}$$

Cross section (inelastic + elastic)

$$\begin{aligned} \mathcal{S}(Q,\omega) &= S\left(1 + \frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\sum_\tau \\ &\times \sum_k \{n_B(\omega_k)\delta(\omega+\omega_k)\;\delta(Q+k-\tau)\; + \;(1+n_B(\omega_k))\delta(\omega-\omega_k)\;\delta(Q-k-\tau)\} \\ &+ \left(1 - \frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\,\langle S\rangle^2 \sum_\tau \delta(\omega)\;\delta(Q-\tau) \end{aligned}$$

Ferromagnet

$$
\begin{aligned}
\mathcal{S}(Q,\omega) &= S\left(1+\frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\sum_\tau \\
&\times\sum_k\{n_B(\omega_k)\delta(\omega+\omega_k)\;\delta(Q+k-\tau)\;+\;(1+n_B(\omega_k))\delta(\omega-\omega_k)\;\delta(Q-k-\tau)\} \\
&+\left(1-\frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\langle S\rangle^2\sum_\tau\delta(\omega)\;\delta(Q-\tau)
\end{aligned}
$$

Elastic term : Bragg peaks with structure factor
Note the geometric factor (is zero if Q is along z)

Ferromagnet

Inelastic term :

$$\mathcal{S}(Q,\omega) = S\left(1+\frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\sum_\tau$$
$$\times\sum_k\{n_B(\omega_k)\delta(\omega+\omega_k)\;\delta(Q+k-\tau)\;+\;(1+n_B(\omega_k))\delta(\omega-\omega_k)\;\delta(Q-k-\tau)\}$$
$$+\left(1-\frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\langle S\rangle^2\sum_\tau\delta(\omega)\;\delta(Q-\tau)$$

Elastic term : Bragg peaks with structure factor
Note the geometric factor (is zero if Q is along z)

Ferromagnet

Periodic (reciprocal lattice)

Inelastic term :

$$
\begin{aligned}
\mathcal{S}(Q,\omega) \;=\; & S \left(1 + \frac{Q^z\, Q^z}{Q^2}\right) \frac{(2\pi)^3}{v_o} \sum_{\tau} \\
& \times \sum_{k} \{ n_B(\omega_k)\delta(\omega+\omega_k)\; \delta(Q+k-\tau) \;+\; (1+n_B(\omega_k))\delta(\omega-\omega_k)\; \delta(Q-k-\tau)\} \\
& + \left(1 - \frac{Q^z\, Q^z}{Q^2}\right) \frac{(2\pi)^3}{v_o} \langle S \rangle^2 \sum_{\tau} \delta(\omega)\; \delta(Q-\tau)
\end{aligned}
$$

Elastic term : Bragg peaks with structure factor
Note the geometric factor (is zero if Q is along z)

Ferromagnet

Periodic (reciprocal lattice)

Creation and annihilation & Detailed Balance

Inelastic term :

$$\begin{aligned}\mathcal{S}(Q,\omega) \;&=\; S\left(1+\frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\sum_{\tau} \\ &\times\sum_k \{n_B(\omega_k)\delta(\omega+\omega_k)\;\delta(Q+k-\tau)\;+\;(1+n_B(\omega_k))\delta(\omega-\omega_k)\;\delta(Q-k-\tau)\} \\ &+\left(1-\frac{Q^z\,Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\langle S\rangle^2\sum_{\tau}\delta(\omega)\;\delta(Q-\tau)\end{aligned}$$

Elastic term : Bragg peaks with structure factor

Note the geometric factor (is zero if Q is along z)

Ferromagnet

Inelastic term :

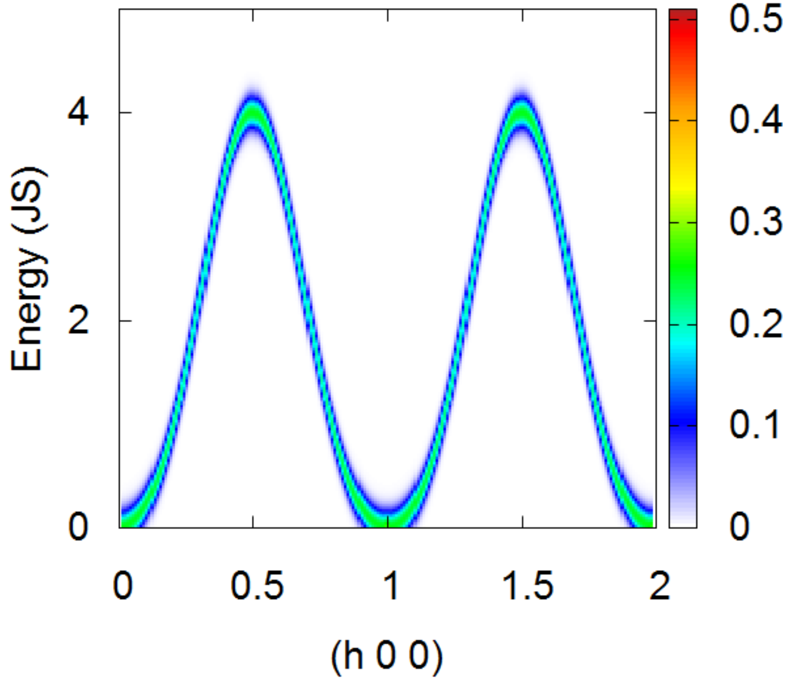
Periodic (reciprocal lattice)
Creation and annihilation & Detailed Balance
Geometric factor (maximum when Q is along z)

$$
\begin{aligned}
\mathcal{S}(Q,\omega) \quad = \quad & S\left(1+\frac{Q^z\,Q^z}{Q^2}\right)\,\frac{(2\pi)^3}{v_o}\,\sum_{\tau} \\
& \times \sum_k \{n_B(\omega_k)\delta(\omega+\omega_k)\ \delta(Q+k-\tau)\ +\ (1+n_B(\omega_k))\delta(\omega-\omega_k)\ \delta(Q-k-\tau)\} \\
& +\left(1-\frac{Q^z\,Q^z}{Q^2}\right)\,\frac{(2\pi)^3}{v_o}\,\langle S\rangle^2\,\sum_{\tau}\,\delta(\omega)\ \delta(Q-\tau)
\end{aligned}
$$

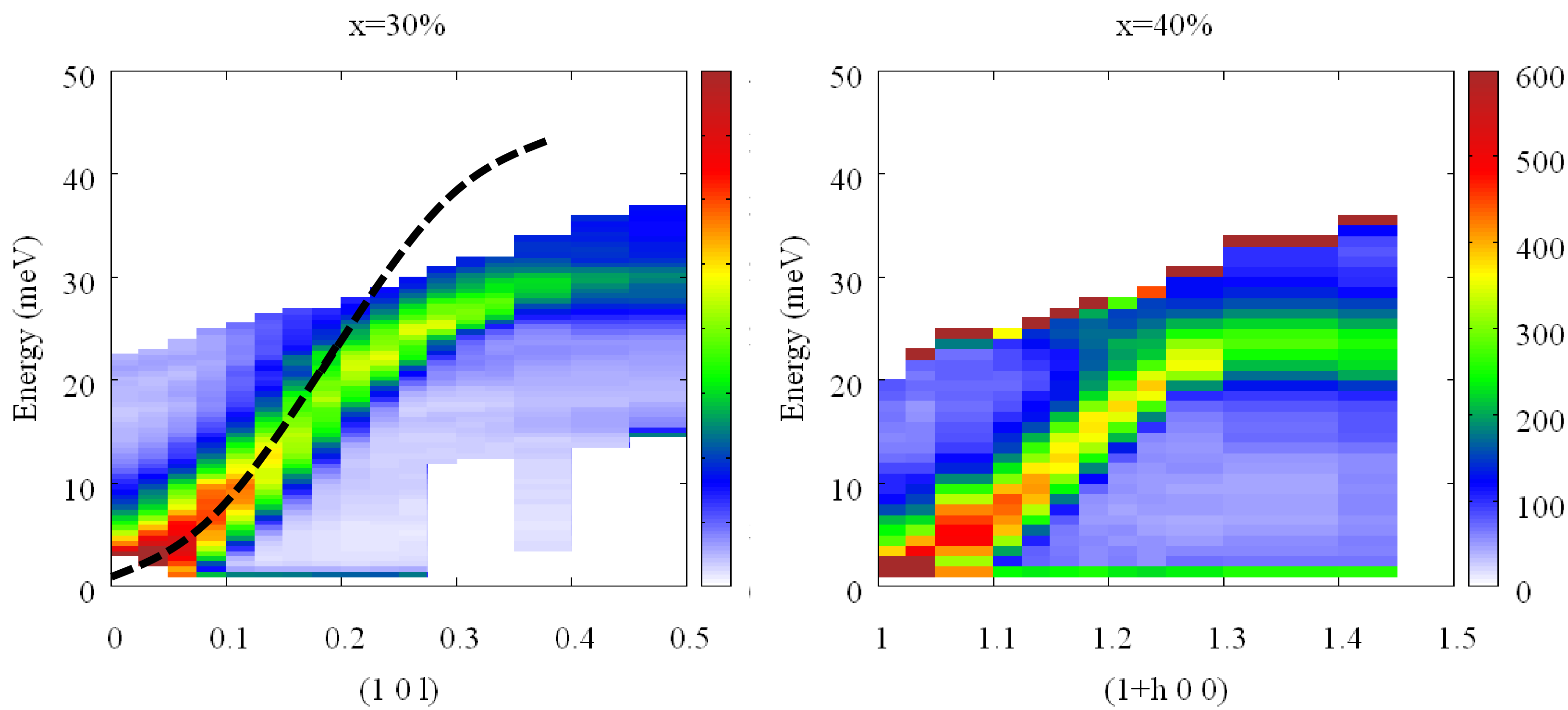
Elastic term : Bragg peaks with structure factor
Note the geometric factor (is zero if Q is along z)

Ferromagnet

$$
\begin{aligned}
\mathcal{S}(Q,\omega) &= S\left(1+\frac{Q^z\ Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\sum_\tau \\
&\times\sum_k\{n_B(\omega_k)\delta(\omega+\omega_k)\ \delta(Q+k-\tau)\ +\ (1+n_B(\omega_k))\delta(\omega-\omega_k)\ \delta(Q-k-\tau)\} \\
&+\left(1-\frac{Q^z\ Q^z}{Q^2}\right)\frac{(2\pi)^3}{v_o}\langle S\rangle^2\sum_\tau\delta(\omega)\ \delta(Q-\tau)
\end{aligned}
$$

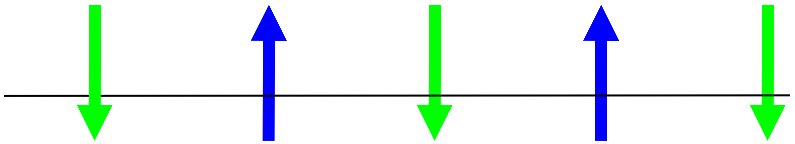


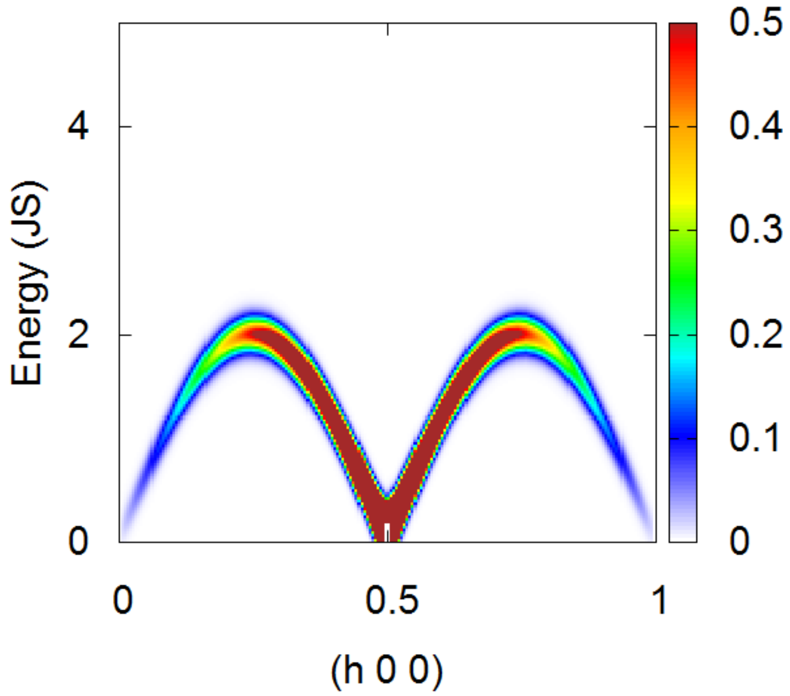
Spin waves also in the metallic state of (doped) manganites



Antiferromagnet

$$
\begin{aligned}
\mathcal{S}(Q,\omega) &= I_{\mathrm{Bragg}}\;\delta(\omega) \\
&+ S\,\frac{(2\pi)^3}{v_o}\sum_s\sum_{\tau,k} \\
&\quad |A_{k,s}|^2\; n_B(E_{k,s})\delta(\omega+E_{k,s})\;\delta(Q+k-\tau)\;+ \\
&\quad |A_{k,s}|^2(1+n_B(E_{k,s}))\delta(\omega-E_{k,s})\;\delta(Q-k-\tau)
\end{aligned}
$$

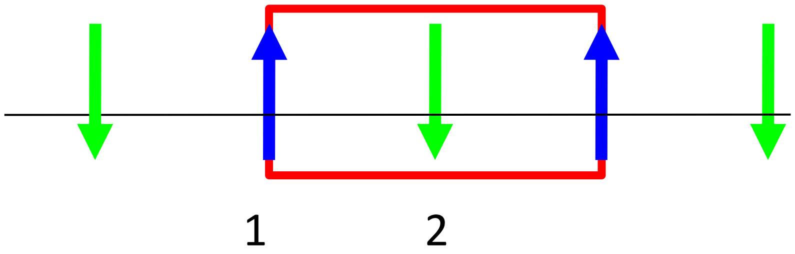




Antiferromagnet

AF Heisenberg Hamiltonian : distinguish up and down spins

$$\mathcal{H} = \frac{1}{2} \sum_{m,n} \mathbf{S}_{m,1} J\, \mathbf{S}_{n,2} \;+\; \mathbf{S}_{m,2} J\, \mathbf{S}_{n,1}$$



« Holstein-Primakov » representation for the two sites (two quantification axes)

$$\begin{aligned} S^x_{m,1} &\approx \frac{\sqrt{2S}}{2}\,(b_{m,1} + b^+_{m,1}) \\ S^y_{m,1} &\approx \frac{\sqrt{2S}}{2i}\,(b_{m,1} - b^+_{m,1}) \\ S^z_{m,1} &\approx S - b^+_{m,1}\, b_{m,1} \end{aligned}$$

$$\begin{aligned} S^x_{m,2} &\approx +\frac{\sqrt{2S}}{2}\,(b_{m,2} + b^+_{m,2}) \\ S^y_{m,2} &\approx -\frac{\sqrt{2S}}{2i}\,(b_{m,2} - b^+_{m,2}) \\ S^z_{m,2} &\approx -\left(S - b^+_{m,2}\, b_{m,2}\right) \end{aligned}$$

Antiferromagnet

Keep 2nd order terms (small deviations)

$$
\begin{aligned}
\mathcal{H} &\approx \frac{1}{2}\sum_{m,n}\frac{S}{2}(b_{m,1} + b^+_{m,1})\ J\ (b_{n,2} + b^+_{n,2}) + \frac{S}{2}(b_{m,1} - b^+_{m,1})\ J\ (b_{n,2} - b^+_{n,2}) \\
&- \left(S - b^+_{m,1}b_{m,1}\right)\ J\ \left(S - b^+_{n,2}b_{n,2}\right) \\
&+ 1 \leftrightarrow 2
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{H} &\approx \frac{1}{2}\sum_{m,n} JS(b_{m,1}\ b_{n,2} + b^+_{m,1}\ b^+_{n,2}) + J\ S\ \left(b^+_{m,1}b_{m,1} + b^+_{n,2}b_{n,2}\right) \\
&+ 1 \leftrightarrow 2
\end{aligned}
$$

Fourier Transform :

$$
\begin{aligned}
\mathcal{H} &\approx \frac{1}{2}\sum_{k} J\ S\ (\gamma_{-k}\ b_{k,1}\ b_{-k,2} + \gamma_k\ b^+_{-k,1}\ b^+_{k,2}) + J\ S\ \left(b^+_{k,1}b_{k,1} + b^+_{k,2}b_{k,2}\right) \\
&+ J\ S\ (\gamma_{-k}\ b_{k,2}\ b_{-k,1} + \gamma_k\ b^+_{-k,2}\ b^+_{k,1}) + J\ S\ \left(b^+_{k,2}b_{k,2} + b^+_{k,1}b_{k,1}\right)
\end{aligned}
$$

$$
\mathcal{H} \approx \frac{1}{2}\sum_{k} \left(b^+_{k,1}\ b^+_{k,2}\ b_{-k,1}\ b_{-k,2}\right) \begin{pmatrix} z\ J\ S & 0 & 0 & z\ J\ S\ \gamma_{-k} \\ 0 & z\ J\ S & z\ J\ S\ \gamma_{-k} & 0 \\ 0 & z\ J\ S\ \gamma_k & z\ J\ S & 0 \\ z\ J\ S\ \gamma_k & 0 & 0 & z\ J\ S \end{pmatrix} \begin{pmatrix} b_{k,1} \\ b_{k,2} \\ b^+_{-k,1} \\ b^+_{-k,2} \end{pmatrix}
$$

Antiferromagnet: Bogolubov transform

We need a final transform to get a free bosons Hamiltonian.

$$\begin{pmatrix} b_{k,1} \\ b_{k,2} \\ b^+_{-k,1} \\ b^+_{-k,2} \end{pmatrix} = P \begin{pmatrix} y_{k,1} \\ y_{k,2} \\ y^+_{-k,1} \\ y^+_{-k,2} \end{pmatrix}$$

$$\mathcal{H} = \sum_k E_{k,1}\ y^+_{k,1} y_{k,1} \ + \ E_{k,2}\ y^+_{k,2} y_{k,2}$$

This transformation (due to Bogolubov) is a « rotation » defined as:

$$B \ = \ P\,Y \qquad\qquad P^{-1} = P^+$$

We impose that the Hamiltonian describes free independent bosons:

$$B^+\ h\ B = Y^+\ E\ Y \qquad\qquad P^+\ h\ P = E$$

Since the Y are bosons :

$$[B, B^+] = g$$

$$[Y, Y^+] = g$$

$$g = \begin{pmatrix} 1 & & & & & \\ & .. & & & & \\ & & 1 & & & \\ & & & -1 & & \\ & & & & .. & \\ & & & & & -1 \end{pmatrix}$$

$$g = P\ g\ P^+$$

Antiferromagnet: Bogolubov transform

$$P^{-1} = P^{+}$$
$$P^{+}\ h\ P = E$$
$$g = P\ g\ P^{+}$$

$$(g\ h)\ P \ = \ (P\ g\ P^{+})\ h\ P = P\ (g\ E)$$

1. The spin wave energies are eigenvalues of the (g h) matrix (and not of the h matrix)
2. Because of the Bogolubov transform, the number of deviations at low T is **not** zero !

$$g\ h = \frac{z\ J\ S}{2} \begin{pmatrix} 1 & 0 & 0 & \gamma_{-k} \\ 0 & 1 & \gamma_{-k} & 0 \\ 0 & -\gamma_k & -1 & 0 \\ -\gamma_k & 0 & 0 & -1 \end{pmatrix}$$

$$E_k = \pm \frac{zJS}{2} \sqrt{1 - |\gamma_k|^2}$$

Antiferromagnet: Bogolubov transform

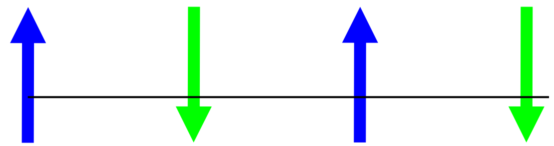
$$P = \begin{pmatrix} u & & & v^* \\ & u & v^* & \\ & v & u^* & \\ v & & & u^* \end{pmatrix}$$

$$u_k^2 - v_k^2 = 1$$

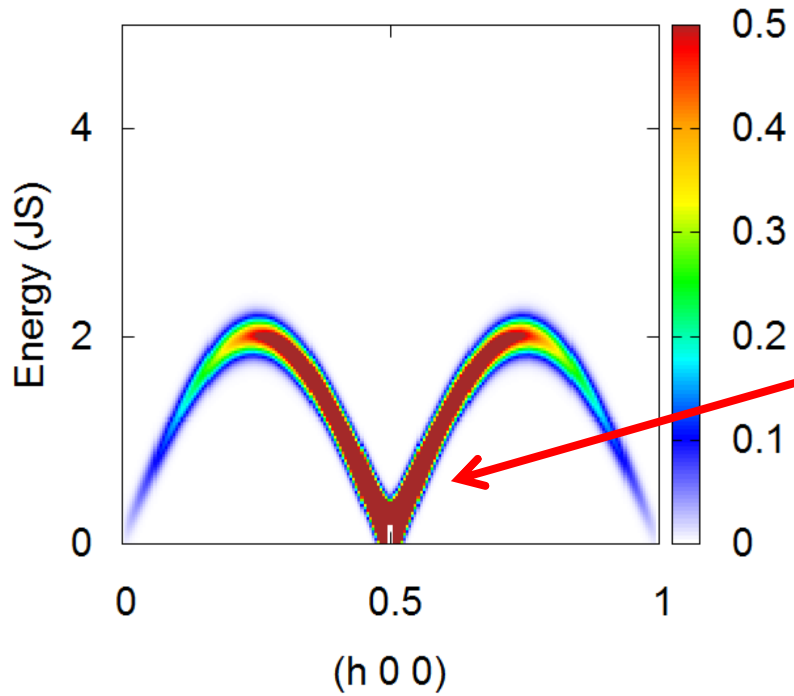
$$\begin{aligned} u_k^2 &= \frac{1}{2}\left(+1 + \frac{z\ J\ S}{E_k}\right) \\ v_k^2 &= \frac{1}{2}\left(-1 + \frac{z\ J\ S}{E_k}\right) \\ u_k\ v_k &= \frac{z\ J\ S\ \gamma_k}{2\ E_k} \end{aligned}$$

Antiferromagnet

1. Spin wave energies



$$E_k = \pm \frac{zJS}{2}\sqrt{1-|\gamma_k|^2} \qquad \gamma_k = \frac{1}{z}\sum_{\Delta} e^{ik\Delta}$$



Linear dispersion at small k

$$E_k \sim |k|$$

Antiferromagnet

2. Average deviation away from equilibrium direction (at low T): reduction of the average moment

Bogolubov transform

$$b_{k,1} = u\ y_{k,1}\ +\ v\ y^{+}_{-k,2}$$

Average deviation

$$\langle b^{+}_{k,1} b_{k,1} \rangle = u^2\ \langle y^{+}_{k,1} y_{k,1} \rangle\ +\ v^2\ \langle y_{-k,2} y^{+}_{-k,2} \rangle$$

Quantum effect

$$\langle b^{+}_{k,1} b_{k,1} \rangle = u^2\ n_B(E_{k,1})\ +\ v^2\ [1\ +\ n_B(E_{k,2})]$$

Antiferromagnet

2. Average deviation away from equilibrium direction (at low T): reduction of the average moment

$$\langle S^z \rangle \approx S - \sum_k \langle b_k^+ \; b_k \rangle$$

$$\langle S \rangle \approx S - \sum_k v_k^2 + (u_k^2 + v_k^2)\; n_B(E_k)$$

$$\langle S \rangle \approx S + \frac{1}{2} - \sum_k \frac{z\; J\; S}{E_k} \left(n_B(E_k) + \frac{1}{2} \right)$$

Thermal fluctuations

Quantum fluctuations

The vacuum of the Bogolubov bosons is not « the vaccum of deviations »

Antiferromagnet

$$\sum_k \frac{z\ J\ S}{E_k}\left(n_B(E_k)+\frac{1}{2}\right) \longrightarrow \int dk\ \frac{k^{d-1}}{(2\pi)^d}\frac{1}{k}\left(\frac{T}{k}+\frac{1}{2}\right)$$

The thermal fluctuations prevent long range ordering for $d \leq 2$

The Quantum fluctuations already destroy LRO in $d \leq 1$

Breakdown of the spin wave theory is consistent with Mermin and Wagner theorem

Antiferromagnet

To calculate the cross section from spin waves, we calculte the spin in terms of the Bogolubov bosons:

$$\sum_m e^{i\mathbf{k}\mathbf{R}_m}\,\mathbf{S}_{m,1}(t) = \mathbf{S}_{k,1} \quad = \quad \begin{pmatrix} \frac{\sqrt{2S}}{2}(b_{k,1} + b^+_{-k,1}) \\ \frac{\sqrt{2S}}{2i}(b_{k,1} - b^+_{-k,1}) \\ S - \sum_k b^+_{k,1} b_{k,1} \end{pmatrix}$$

$$\sum_m e^{i\mathbf{k}\mathbf{R}_m}\,\mathbf{S}_{m,2}(t) = \mathbf{S}_{k,2} \quad = \quad \begin{pmatrix} + \frac{\sqrt{2S}}{2}(b_{k,2} + b^+_{-k,2}) \\ - \frac{\sqrt{2S}}{2i}(b_{k,2} - b^+_{-k,2}) \\ - \left(S - \sum_k b^+_{k,2} b_{k,2}\right) \end{pmatrix}$$

The time dependency is known and directly reflects the spin wave energies:

$$\begin{aligned} \langle y_k y_k^+(t)\rangle &= (1 + n_B(E_k))e^{-iE_k t} \\ \langle y_k^+ y_k(t)\rangle &= n_B(E_k)e^{+iE_k t} \end{aligned}$$

Cross section

$$\begin{aligned} \mathcal{S}(Q,\omega) &= I_{\text{Bragg}}\ \delta(\omega) \\ &+ S\,\frac{(2\pi)^3}{v_o}\sum_s \sum_{\tau,k} \\ &\quad |A_{k,s}|^2\ n_B(E_{k,s})\delta(\omega + E_{k,s})\ \delta(Q + k - \tau)\ + \\ &\quad |A_{k,s}|^2(1 + n_B(E_{k,s}))\delta(\omega - E_{k,s})\ \delta(Q - k - \tau) \end{aligned}$$

Antiferromagnet

Elastic term : Bragg peaks with structure factor
Geometric factor (is zero if Q is along z)

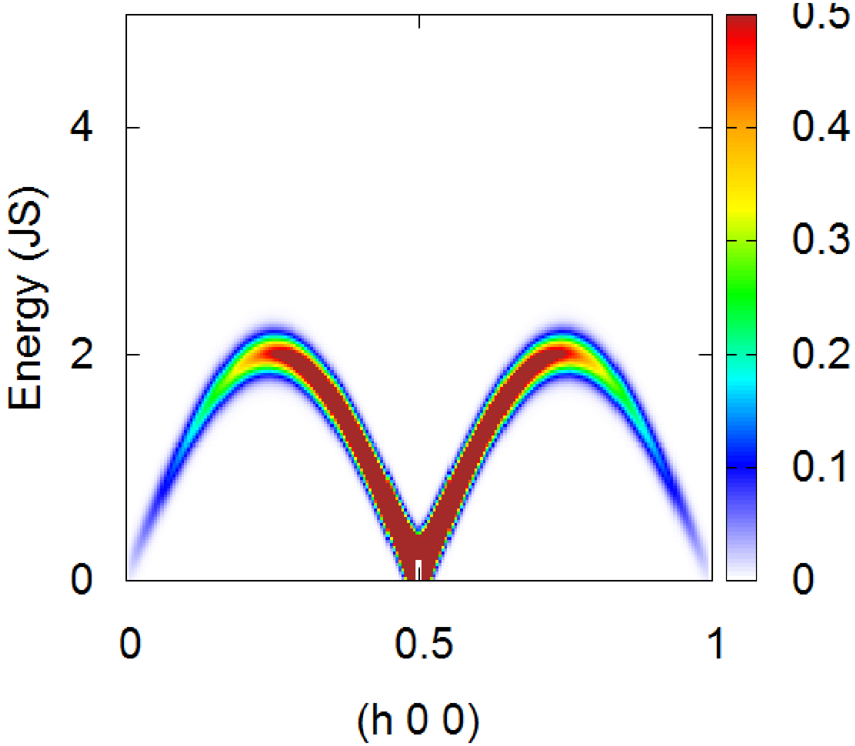
$$
\begin{aligned}
\mathcal{S}(Q,\omega) &= I_{\text{Bragg}}\ \delta(\omega) \\
&+ S\ \frac{(2\pi)^3}{v_o} \sum_s \sum_{\tau,k} \\
&\quad |A_{k,s}|^2\ n_B(E_{k,s})\delta(\omega + E_{k,s})\ \delta(Q + k - \tau)\ + \\
&\quad |A_{k,s}|^2(1 + n_B(E_{k,s}))\delta(\omega - E_{k,s})\ \delta(Q - k - \tau)
\end{aligned}
$$

Inelastic term :

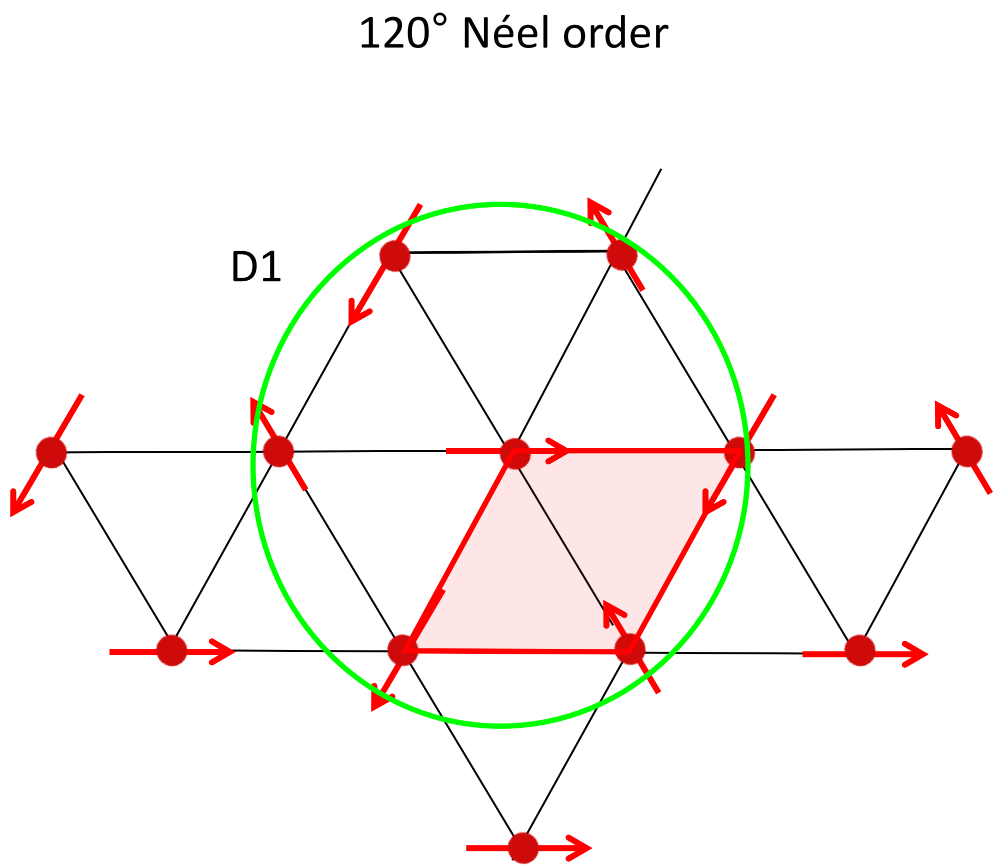
Periodic (reciprocal lattice)
Creation, annihilation & Detailed Balance
Geometric factor (maximum when Q is along z)

Antiferromagnet

$$
\begin{aligned}
\mathcal{S}(Q,\omega) &= I_{\text{Bragg}}\ \delta(\omega) \\
&+ S\,\frac{(2\pi)^3}{v_o}\sum_s\sum_{\tau,k} \\
&\quad |A_{k,s}|^2\ n_B(E_{k,s})\delta(\omega+E_{k,s})\ \delta(Q+k-\tau)\ + \\
&\quad |A_{k,s}|^2(1+n_B(E_{k,s}))\delta(\omega-E_{k,s})\ \delta(Q-k-\tau)
\end{aligned}
$$

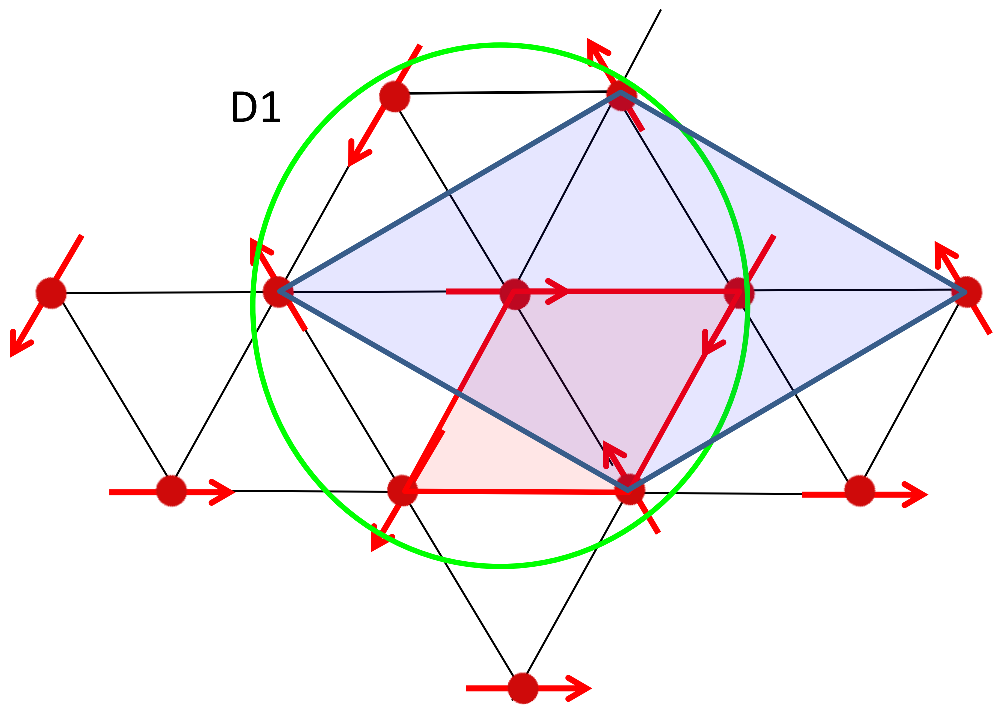


Triangular lattice



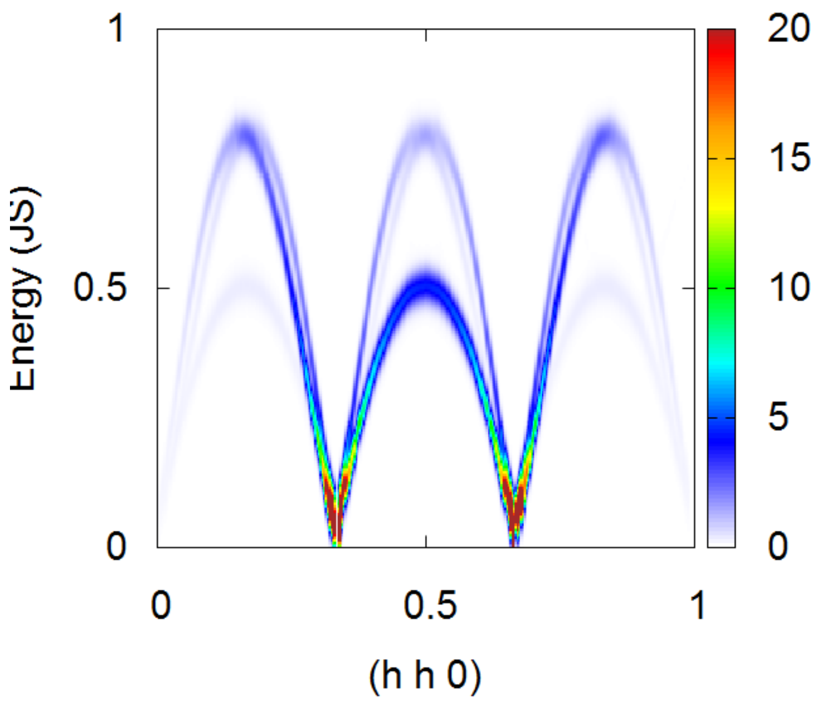
Triangular lattice

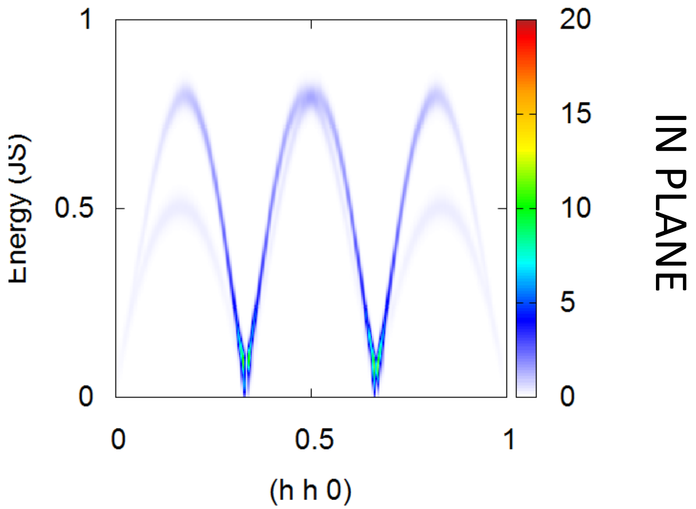
The magnetic unit cell contains 3 spins

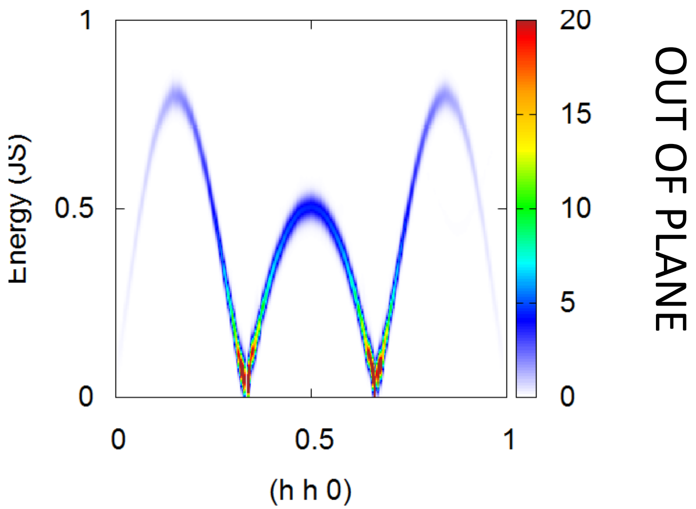


Triangular lattice

3 spins per unit cell : 3 branches

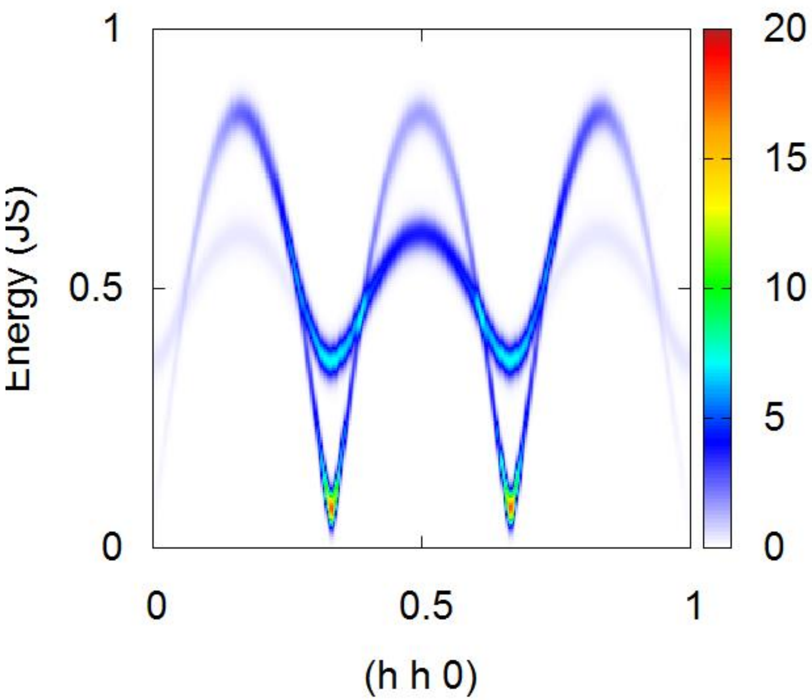


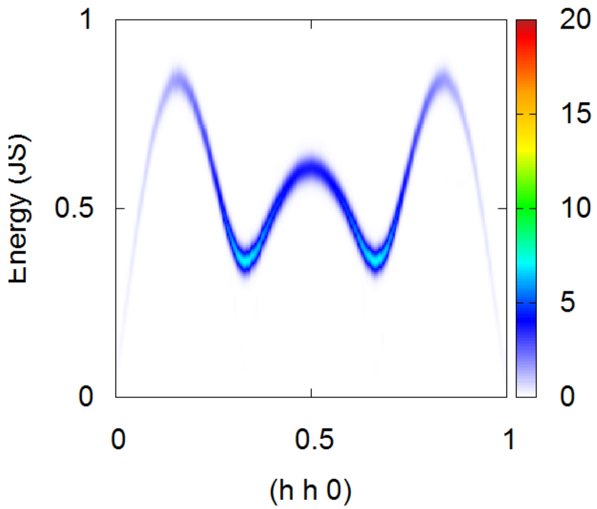




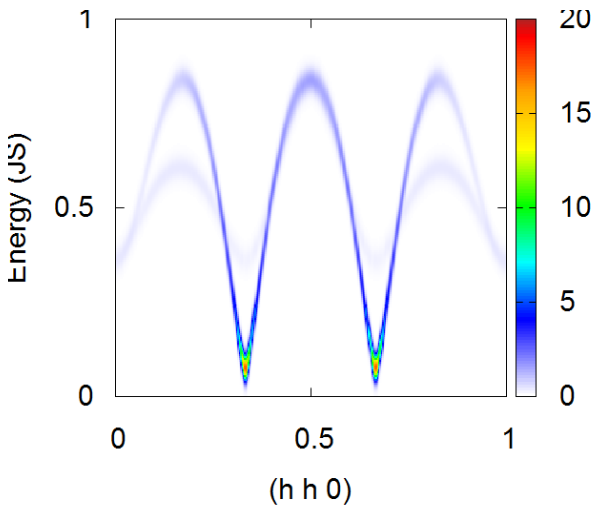
Triangular lattice

Planar anisotropy gap





IN PLANE



OUT OF PLANE

General case

Cross section

$$\boxed{\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \sum_s A_s \left[(1+n(\omega_{Q,s}))\ \delta(\omega-\omega_{Q,s}) + n(\omega_{Q,s})\ \delta(\omega+\omega_{Q,s})\right]}$$

Dynamical Structure factor **Creation** **Annihilation**

$$n(\omega_{Q,s}) = \frac{1}{e^{\frac{\hbar\omega_{Q,s}}{k_B T}} - 1}$$

- Conventional magnets (molecular field)
- S=1 bosonic excitations
- L spins in the magnetic unit cell : L branches

- The theory is wrong at high T
- The theory is badly false for d=1,2
- Notice the « detailed balance »

General case

SW

$$A_s \sim \sum_\ell P_{\ell,s}\ e^{\,i\mathbf{Q}\mathbf{r}_\ell}$$

Cross section of the sth mode
=
Interference effect between
« partial » spin fluctuations of
the spin ℓ in mode s

Phonon

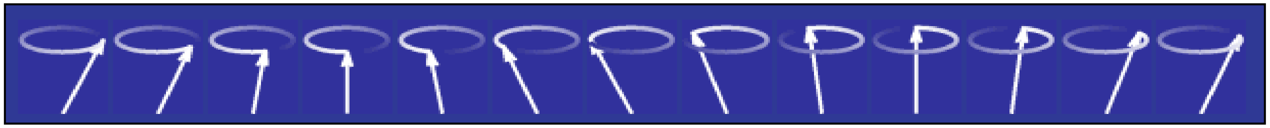
$$F_s \sim \sum_\ell b_\ell \frac{\hbar}{\sqrt{M_\ell \omega_{k,s}}} \left(\mathbf{Q}\cdot\mathbf{e}_{k,\ell,s}\right)\ e^{\,i\mathbf{Q}\mathbf{r}_\ell}$$

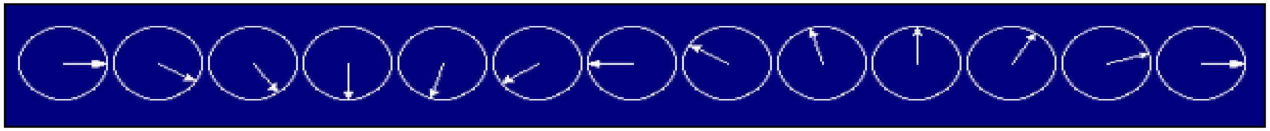
Cross section of the sth mode
=
Interference effect between
« partial » atomic motion of
the atom ℓ in mode s

Part 4 : practical

Summary

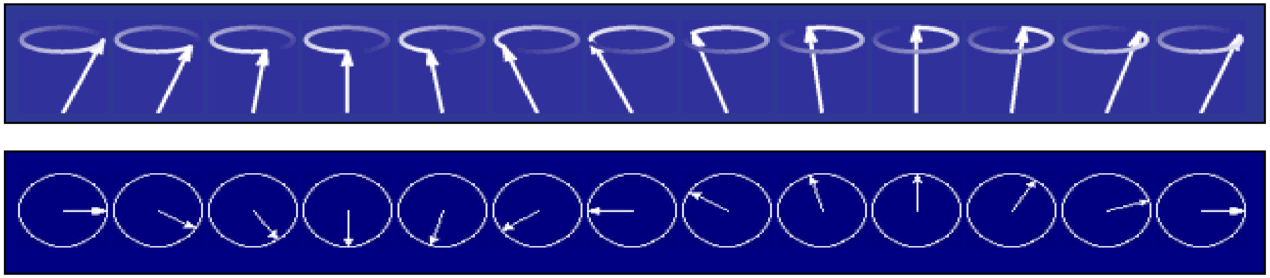
1. Spin waves are conventional excitations of the assembly of spins in magnets (precession of the spins)





2. INS allows to measure the dispersion of those modes

Summary

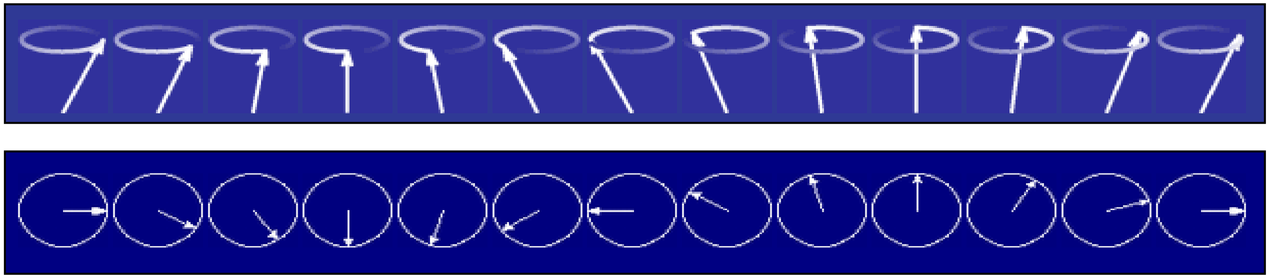


1. With the help of numerical simulations, it becomes possible to determine exchange couplings, anisotropies

$$\mathcal{H} = \frac{1}{2} \sum_{m,i,n,j} \mathbf{S}_{m,i} \mathcal{J}_{m,i,n,j} \mathbf{S}_{n,j} + \sum_{n,m} B_{n,m} O_{n,m}$$

Summary

Cross section



$$\frac{\partial^2\sigma}{\partial\Omega\partial E'} = \sum_s A_s \left[(1+n(\omega_{Q,s}))\ \delta(\omega-\omega_{Q,s}) + n(\omega_{Q,s})\ \delta(\omega+\omega_{Q,s})\right]$$

Dynamical Structure factor

Creation

Annihilation

- On your Virtual Machine, create a directory « TP-spinwave »
- Copy the exemples files sent by e-mail
- Other important features in the directory -already installed
- /usr/share/opt/spinwave/

The « spinwave » software

tenerife >
tenerife >
tenerife > spinwave < inputfile.txt   > listing.txt

SW-chaineF.txt
SW-chaineAF.txt
SW-triangular.txt
SW-LaMnO3.txt
…

The « spinwave » software

tenerife >

tenerife >

tenerife > gnuplot/bin/wgnuplot.exe

Copy and paste lines from plot.txt

The « spinwave » software

```
# ------------------------------------------
# definition of the lattice
#
AX  = 6.28
AY  = 20.
AZ  = 20.
ALFA= 90.0
BETA= 90.0
GAMA= 90.0
#
```

Unit cell definition

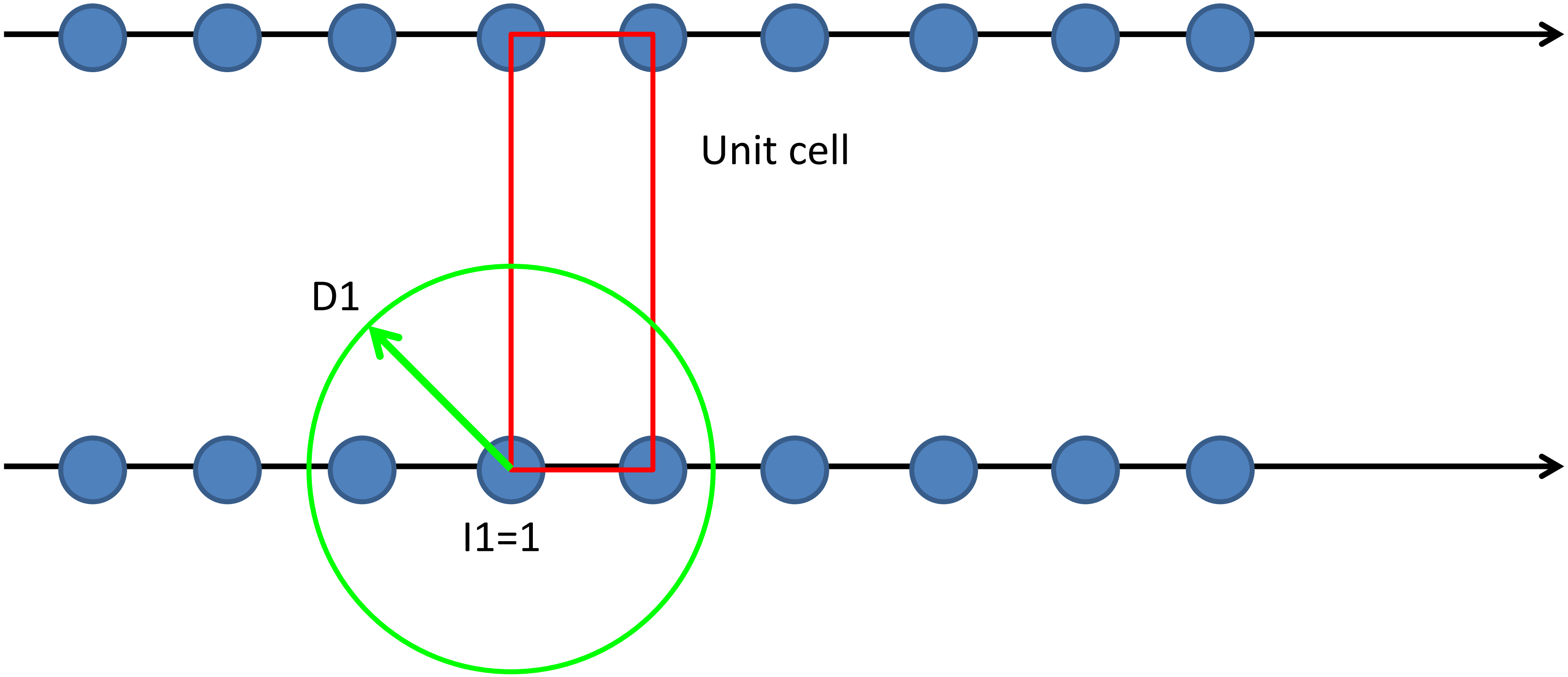
```
# ------------------------------------------
# Spin positions (SD2 is S=1/2) along the chain
# here, on the nodes of the underlying lattice
#
I= 1,NOM=SD2, X= 0.00, Y= 0.00, Z=0.00, SX=0, SY=0, SZ=1, CX=0, CY=0, CZ=1, B20=0.0
I= 2,NOM=SD2, X= 0.50 ,Y= 0.00, Z=0.00, SX=0, SY=0, SZ=1, CX=0, CY=0, CZ=1, B20=0.0
#
```

Spin positions

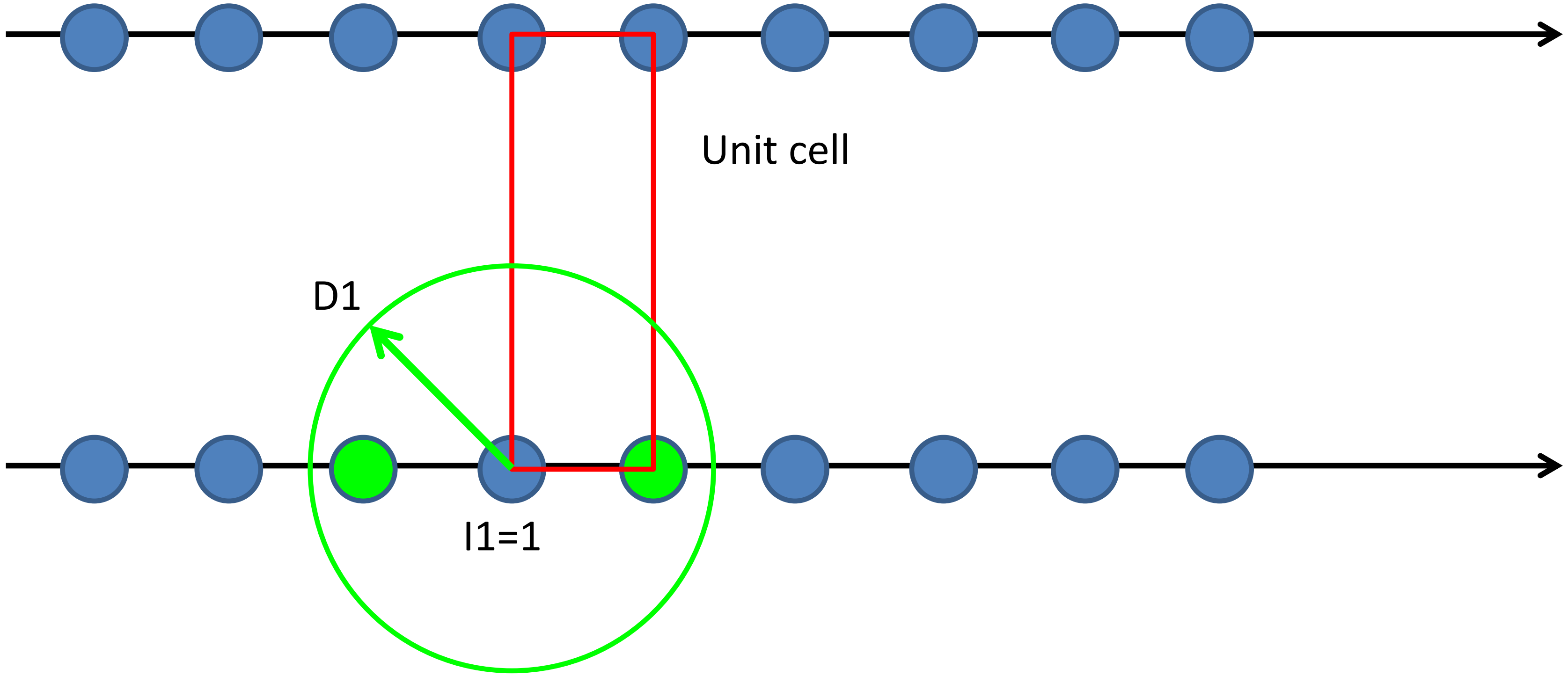
```
# ------------------------------------------
#
# First-neighbour coupling J1
#
I1= 1,I2= 2,J1= 4,D1= 7,J2=0.0,D2=14
#
```

couplings

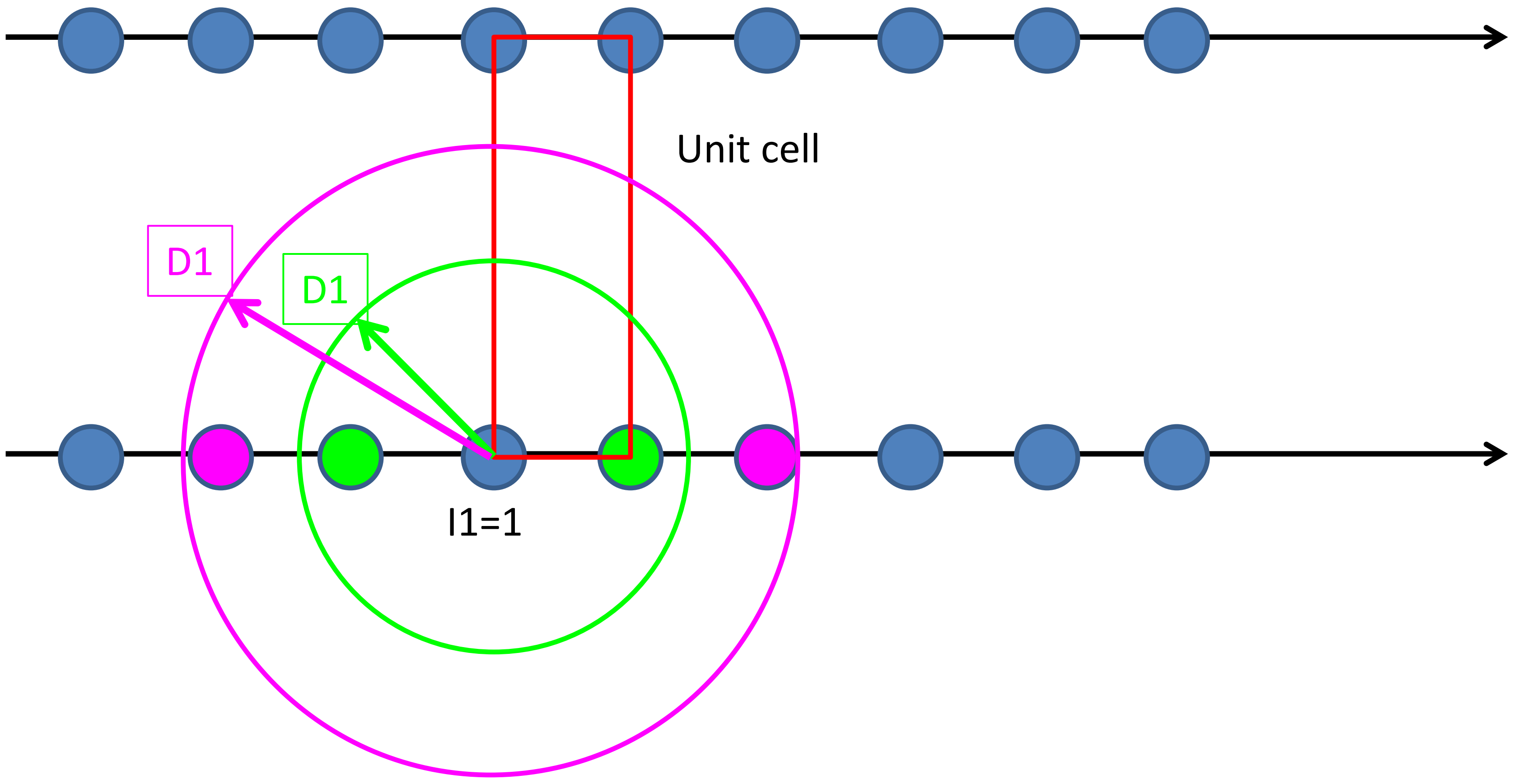
Couplings



Couplings



Couplings



The « spinwave » software

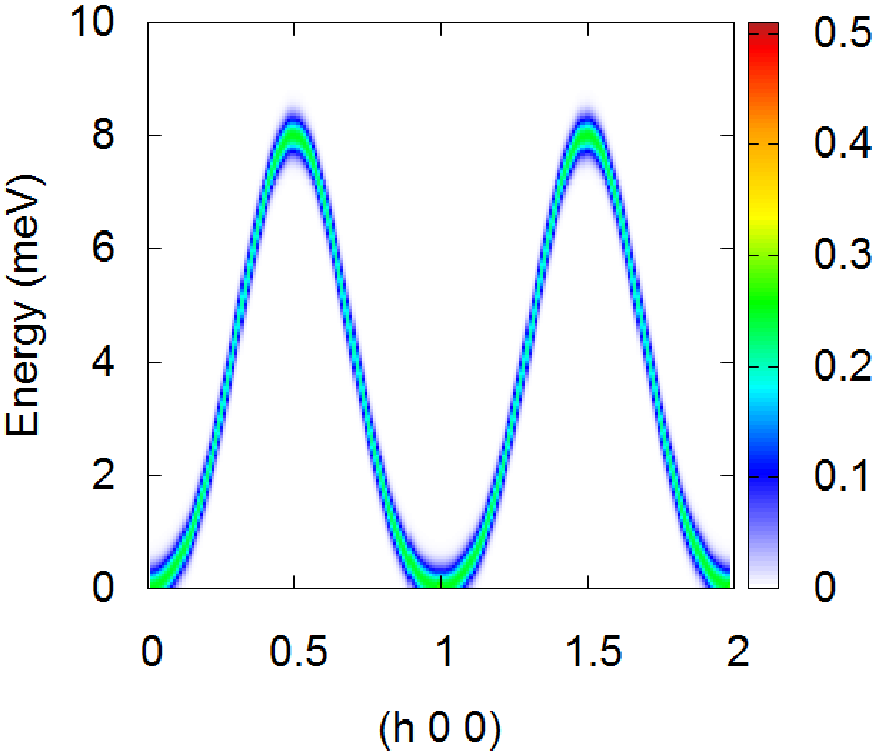
```
-------------------------------------------
# Scan definition
#
Q0X=0.0,Q0Y=0.0,Q0Z=0.0
DQX=0.01,DQY=0.00,DQZ=0.00
NP=200
#
# outputfile
FICH=res-chaine-af-h00.txt
#
# -------------------------------------------
# mean field
#
MF,NITER=50
CALC=2,REG1=0.01,REG2=0.01,REG3=0.01
#
# options (energy width, number of points in energy)
WMAX=35,NW=150,SIG=1
#
#
```

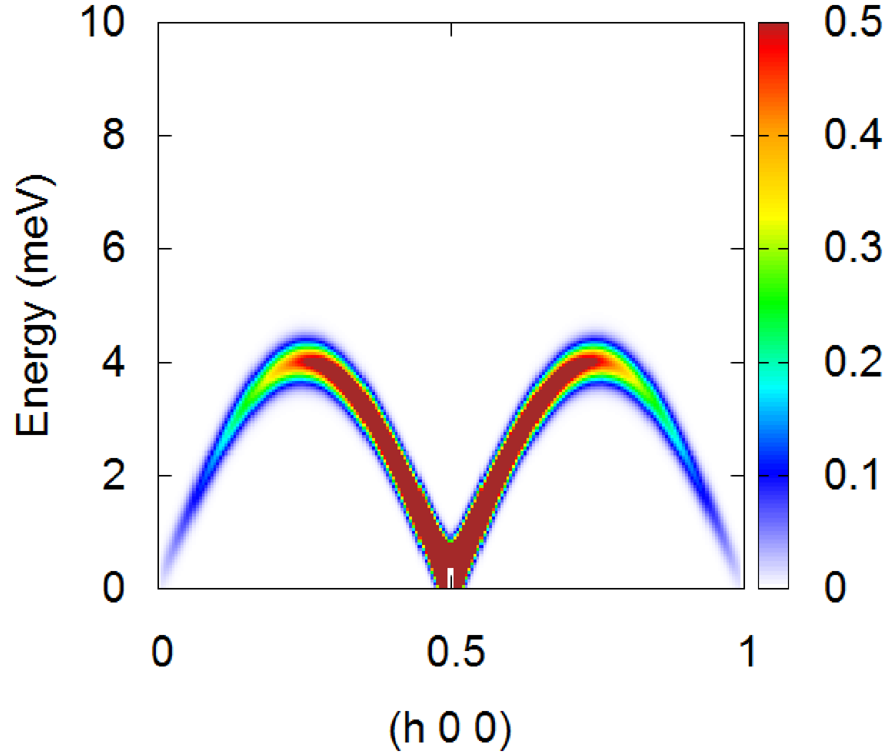
Scan defintion in reciprocal space
Q = QO + DQ,
NP #points

Mean field step
MF = mean field step
NITER = # iterations
CALC= 2 , REG1,REG2,REG3 = regularization

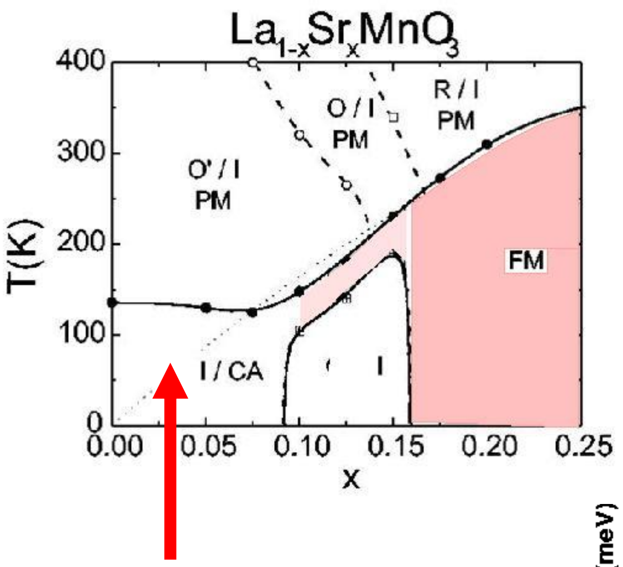
Output file (to vizualize with Gnuplot)
WMAX = max energy
NW = nb points in energy

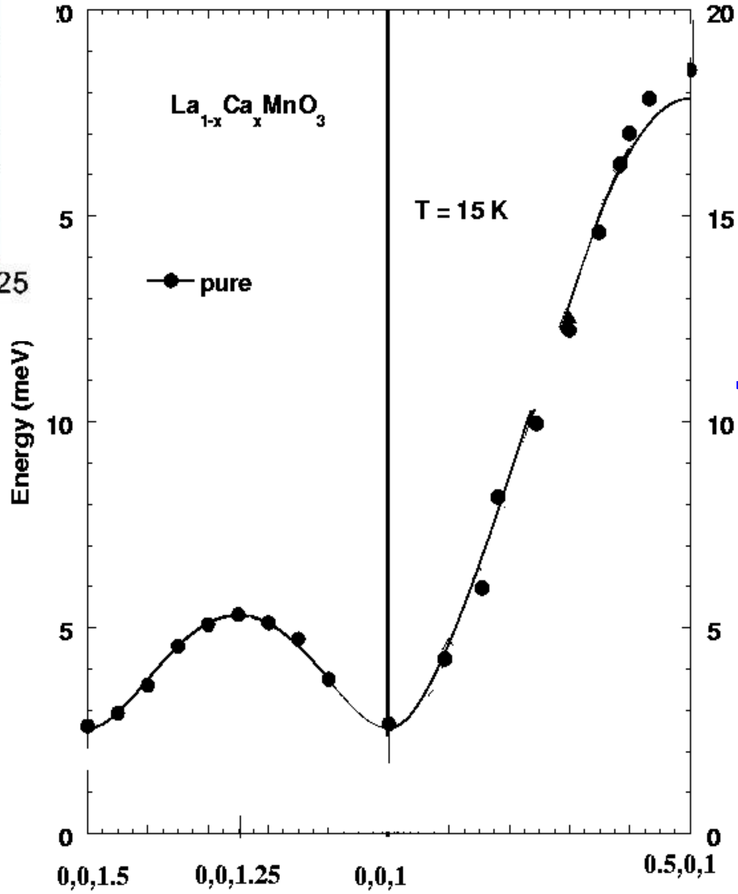
1D chains

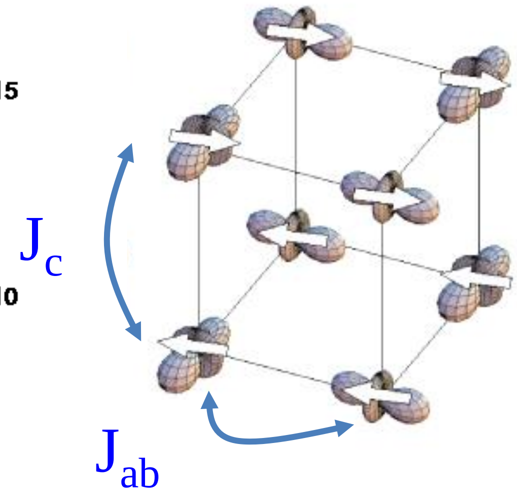

Energy (meV)
(h 0 0)
10
8
6
4
2
0
0.5
1
1.5
2
0.4
0.3
0.2
0.1


Energy (meV)
(h 0 0)
10
8
6
4
2
0
0.5
1
0.4
0.3
0.2
0.1

LaMnO$_3$

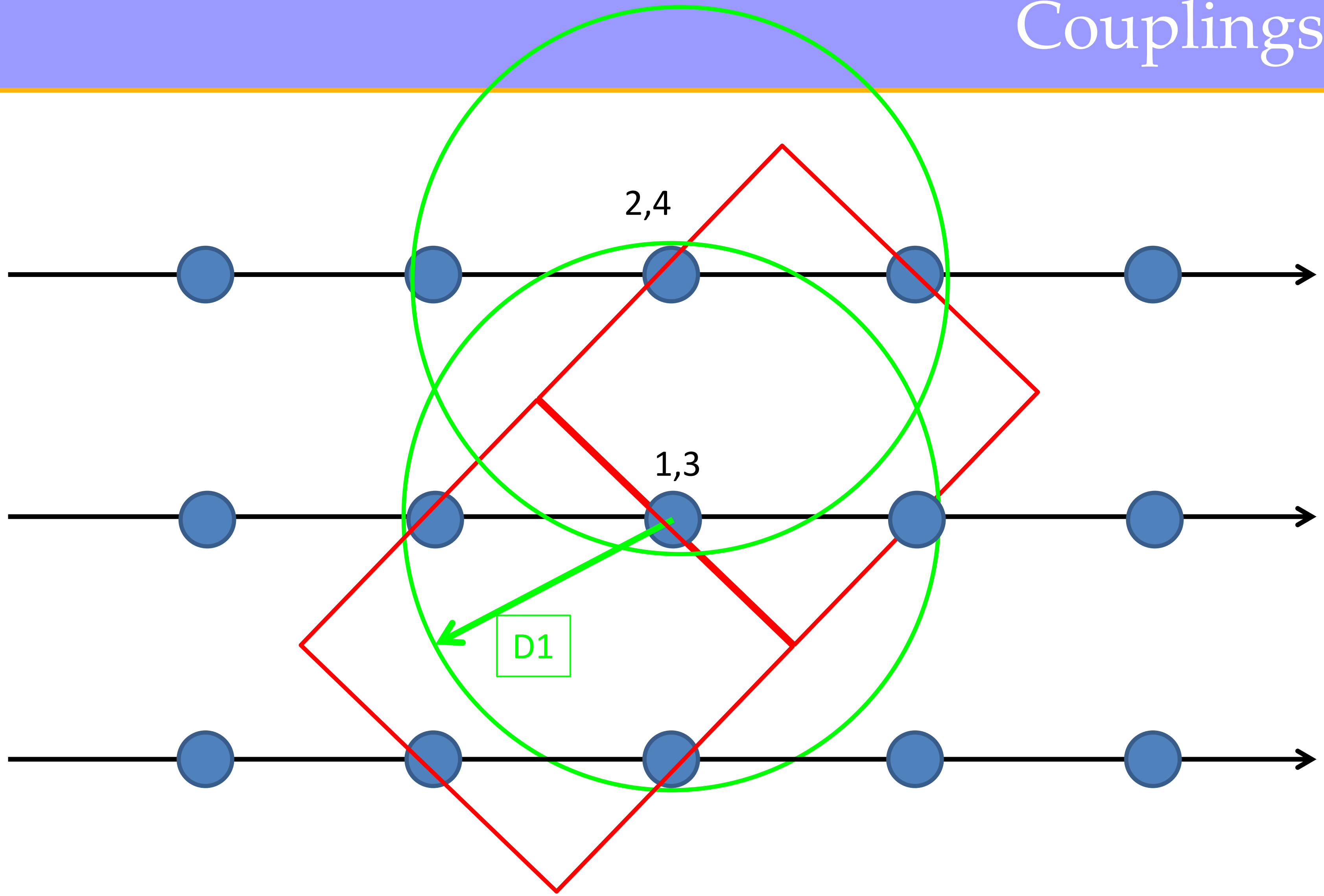






J_c ~ 1.0 meV
J_{ab} ~ -1.7 meV

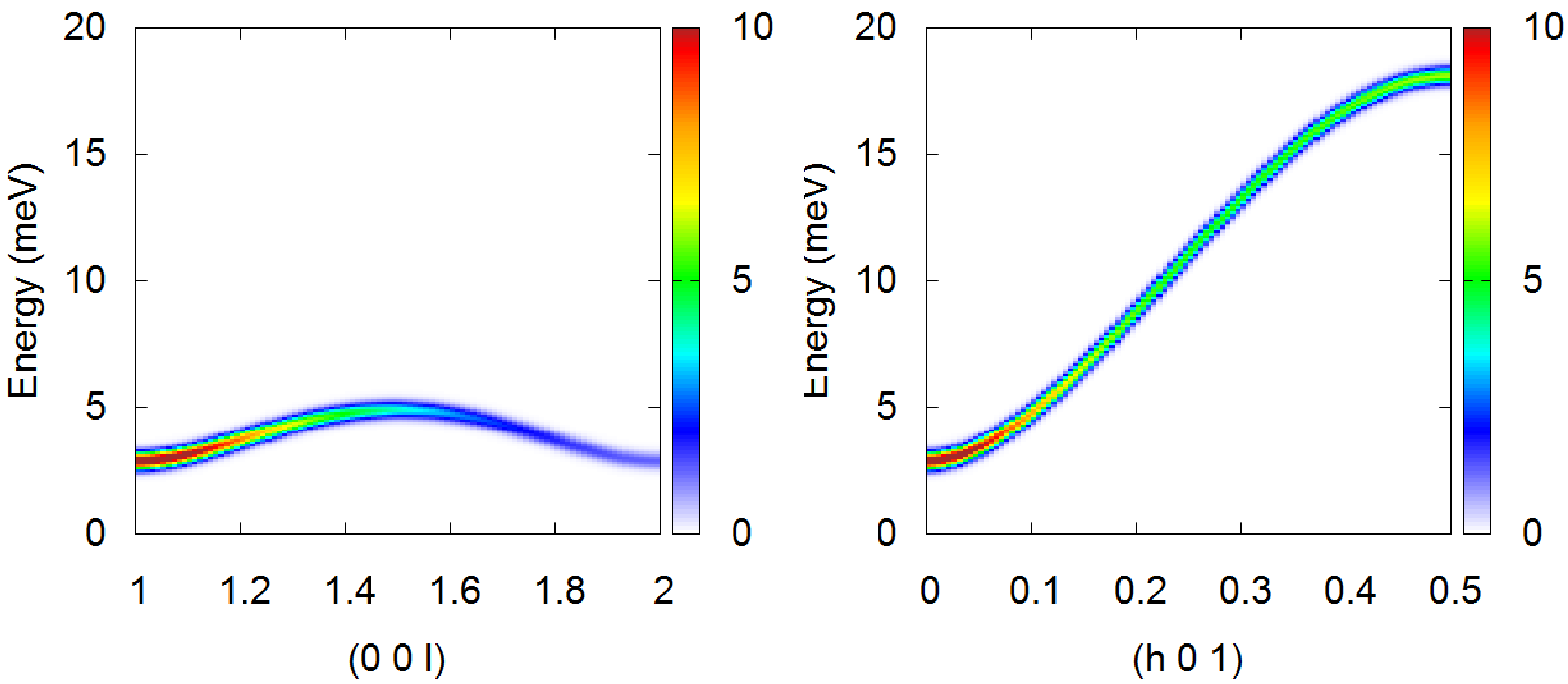
Couplings



I1= 1,I2= 2,J1=-1.7,D1= 4.1
I1= 3,I2= 4,J1=-1.7,D1= 4.1

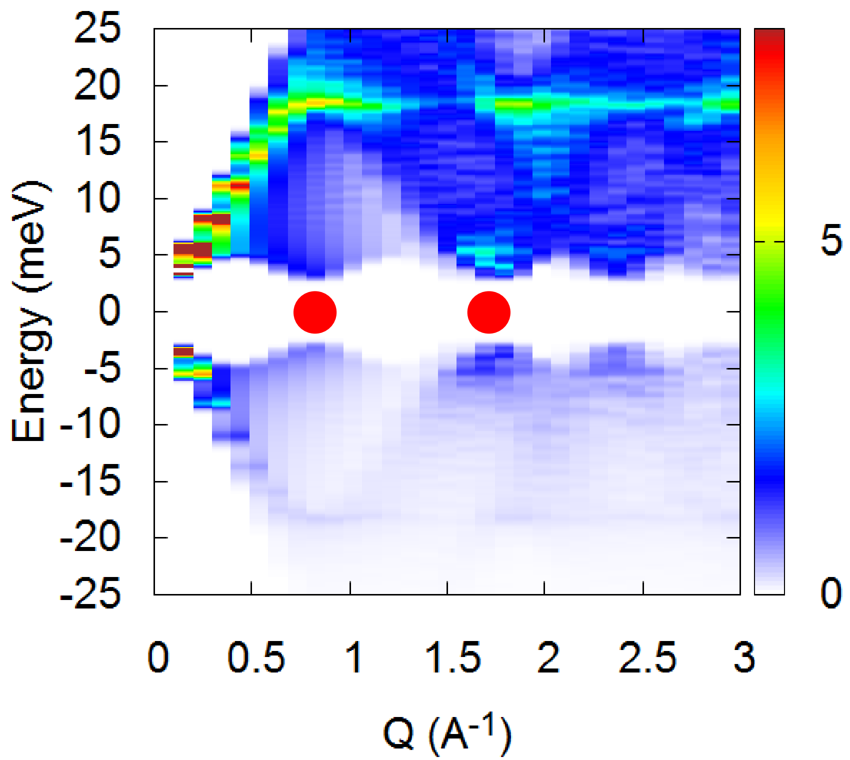
$LaMnO_3$

Play with anisotropy and parameters to reproduce the spectrum

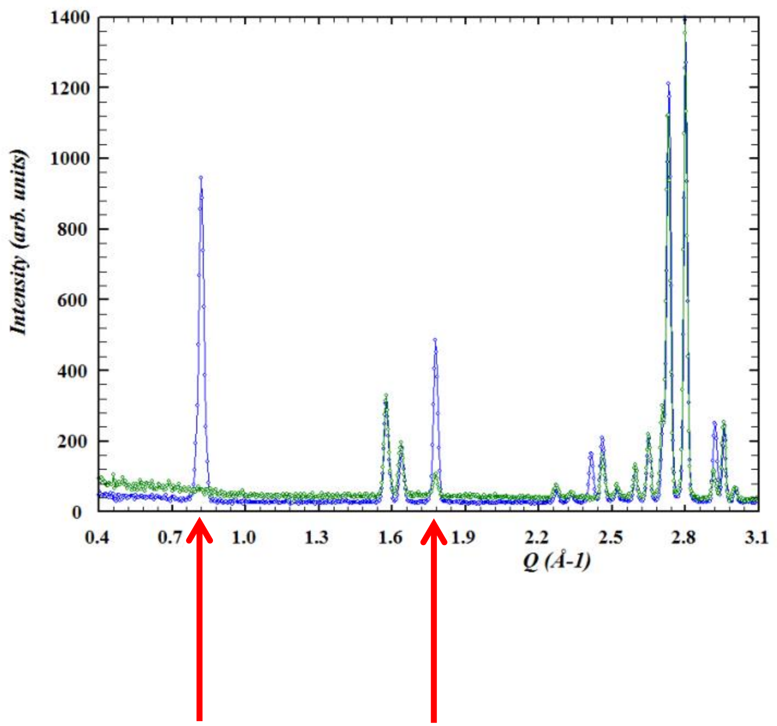


$LaMnO_3$

Powder averaged spectrum



Diffraction



Magnetic Bragg peaks

Local frames

The long range ordering defines local frames (attached to the direction of the local magnetization)

$$S^{a=x,y,z} = \mathcal{R}\ S^{a=\xi,\zeta,\eta}$$

$$\mathcal{R} = \begin{pmatrix} R_{11} & R_{12} & R_{13} \\ R_{21} & R_{22} & R_{23} \\ R_{31} & R_{32} & R_{33} \end{pmatrix} \qquad \mathbf{z} = \begin{pmatrix} R_{11} + iR_{12} \\ R_{21} + iR_{22} \\ R_{31} + iR_{32} \end{pmatrix} \quad \eta = \begin{pmatrix} R_{13} \\ R_{22} \\ R_{32} \end{pmatrix}$$

$$S_\ell^{a=x,y,z} = \frac{\sqrt{2S}}{2}\bar{z}_\ell^a\ b_\ell\ +\ \frac{\sqrt{2S}}{2}\ z_\ell^a b_\ell^+\ +\ \eta_\ell^a\ \left(S - b_\ell^+ b_\ell\right)$$

A spin in a field

Spin operator $\mathbf{S} = (S_x, S_y, S_z)$

Hamiltonian $\mathcal{H} = -\mathbf{S} \cdot \mathbf{h} = -h\ S_z$

Energies $E_n = h\ n \qquad n = -S, ..., S$

Manetization $S_z|n\rangle = n\ |n\rangle$

Raising and lowering operators

$$\begin{aligned} S^+|n\rangle &= \sqrt{S(S+1) - n(n+1)}\ |n+1\rangle \\ S^-|n\rangle &= \sqrt{S(S+1) - n(n-1)}\ |n-1\rangle \end{aligned}$$