# SpinW

SW SpinW

# A crash course on SpinW

SpinW (spin-double-u) is a MATLAB library that can optimize magnetic structures using mean field theory and calculate spin wave dispersion and spin-spin correlation function for complex crystal and magnetic structures.

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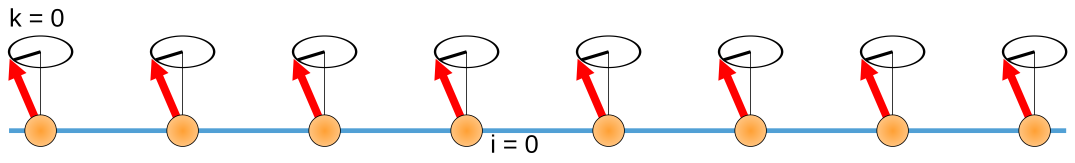
# Linear Spin Wave Theory Review

15 minute introduction on LSWT

## Spin waves

Spin waves (magnons) are propagating disturbances of an ordered magnetic lattice



The magnetic ordering arises due to the exchange interactions $J_{ij}$ between electrons on atomic sites $i$ and $j$.

The dispersion relation $\omega(\mathbf{q})$ of spin waves can be measured by inelastic neutron scattering, and directly depends on the exchange interactions

Spin waves are deviations from an ordered state, so in principle can only be seen in the ordered state

## Linear Spin Wave Theory

We'll now derive the spin wave dispersion for a ferromagnet in linear spin wave theory

The steps involved in the derivation are:

1. Beginning with a spin Hamiltonian, express the spin operator vector $\mathbf{S}_i = (\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z)$ as the ladder operators $(\hat{S}_i^+, \hat{S}_i^-, \hat{S}_i^z)$

2. Map the raising (lowering) operators to bosonic anihilation (creation) operators $a^\dagger$ $(a)$ via the Holstein-Primakoff transformation.

3. The transformed Hamiltonian is a series expansion in powers of $a^\dagger, a$, but in linear spin wave theory we take only the terms which are linear in $a^\dagger a$.

4. Fourier transform the Hamiltonian.

5. Diagonalise the Hamiltonian, ensuring that the commutation relation of the bosonic operators are respected (for two-sublattice system such as antiferromagnetic, the Bogoliubov transformation can be used for this purpose).

## Heisenberg Hamiltonian:

The Hamiltonian of an ordered magnet can be expressed in terms of the spin operators for site $i$, $\mathbf{S}_i$.

For example, the Heisenberg Hamiltonian is:

$$\mathcal{H} = \sum_{mi,nj} J_{mi,nj} \mathbf{S}_i \cdot \mathbf{S}_j$$

where $J_{mi,nj}$ is the exchange interaction with the indices $i$ and $j$ running over magnetic atoms within a single magnetic unit cell, and $m$ and $n$ label different unit cells.

$\mathbf{S}_i = (\hat{S}_i^x, \hat{S}_i^y, \hat{S}_i^z)$ is the spin operator for site $i$, which can be re-expressed in terms of the ladder operators $\hat{S}_i^+, \hat{S}_i^-, \hat{S}_i^z$:

$$\begin{aligned}\mathcal{H} &= \sum_{mi,nj} J_{mi,nj} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \hat{S}_i^z \hat{S}_j^z) \\ &= \sum_{mi,nj} J_{mi,nj} ((\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+)/4 + \hat{S}_i^z \hat{S}_j^z)\end{aligned}$$

since $\hat{S}^{\pm} = \hat{J}^x \pm i\hat{S}^y$ so $\hat{S}^{x,y} = \frac{\sqrt{\pm 1}}{2}(\hat{S}^+ \pm \hat{S}^-)$

## Holstein-Primakoff transformation

To determine the magnons (magnetic normal modes), we map the excitations to a simple harmonic operator

The ordered ground state is the state with the maximum azimuthal quantum number $|m=S\rangle$, and the action of the ladder operator is:

$$\hat{S}^{\pm}|m\rangle = \sqrt{(S\mp m)(S+1\pm m)}|m\pm 1\rangle$$

We now map the ladder operators to boson creation and anihilation operators $a^{\dagger}$ and $a$:

$$a|n\rangle\sqrt{n}|n-1\rangle \qquad a^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle$$

mapping also the ordered state $|m=S\rangle$ to the vacuum state $|n=0\rangle$, such that the action of $a^{\dagger}|n\rangle$ is analogous to $\hat{S}^{-}|S\rangle$

So, substituting $m=S-n$ and re-arranging the ladder operator terms:

$$\hat{S}^{+}|n\rangle = \sqrt{(2Sn)(1-{\color{red}\frac{n-1}{2S}})}|n-1\rangle$$
$$\hat{S}^{-}|n\rangle = \sqrt{2S(n+1)(1-{\color{red}\frac{n-1}{2S}})}|n+1\rangle$$

In linear spin wave theory we ignore the terms in red

Using the identities $n = aa^\dagger$ and $S^z|m\rangle = m|m\rangle$ we have the following mappings

$$\begin{aligned}\hat{S}_i^+ &= a_i\sqrt{2S_i}\\ \hat{S}_i^- &= a_i^\dagger\sqrt{2S_i}\\ \hat{S}_i^z &= S_i - aa^\dagger\end{aligned}$$

So the Heisenberg Hamiltonian (ignoring terms which are not linear in $aa^\dagger$) is now:

$$\mathcal{H} = \sum_{mi,nj} J_{mi,nj}\left[\frac{\sqrt{S_iS_j}}{2}\left(a_ia_j^\dagger + a_i^\dagger a_j\right) - S_ia_ia_i^\dagger - S_ja_ja_j^\dagger\right]$$

## Fourier transformation

In the expression for the spin Hamiltonian we have a sum over all magnetic sites. This can be simplified to just sites $i$ and $j$ within the magnetic unit cell by Fourier transforming the Hamiltonian. The Fourier transform of the Holstein-Primakoff operator is:

$$a^{(\dagger)} = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \exp(-i\mathbf{q}\cdot\mathbf{r}) b_{\mathbf{q}}^{(\dagger)}$$

Let us take one term from the Hamiltonian, $\sum_{mi,nj} J_{mi,nj} a_i a_j^\dagger$; its Fourier transform is:

$$\mathrm{FT}\left[\sum_{mi,nj} J_{mi,nj} a_i a_j^\dagger\right] = \frac{1}{N} \sum_{mi,nj} \sum_{\mathbf{q},\mathbf{q}'} J_{mi,nj} \exp(-i\mathbf{q}\cdot\mathbf{r}_m) \exp(-i\mathbf{q}'\cdot\mathbf{r}_n) b_{i,\mathbf{q}} b_{j,\mathbf{q}'}^\dagger$$

The periodicity of the crystal implies that the exchange interaction is translationally invariant such that $J_{mi,nj} = J_{ij}(\mathbf{d})$ where $\mathbf{d} = \mathbf{r}_m - \mathbf{r}_n$ so the Fourier transform becomes:

$$\frac{1}{N} \sum_{\mathbf{q},\mathbf{q}'} \left[\sum_{ij} J_{ij}(\mathbf{d}) \exp(-i\mathbf{q}'\cdot\mathbf{d})\right] \exp(-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}_m) b_{i,\mathbf{q}} b_{j,\mathbf{q}'}^\dagger$$

where the terms in the square brackets is the Fourier transform of the exchange interactions $J_{ij}(\mathbf{q})$ where the indices $ij$ label only sites within the magnetic unit cell. We now use the identity $(1/N)\sum_{\mathbf{q},\mathbf{q}'} \exp(-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}) = \delta_{\mathbf{q}\mathbf{q}'}$ to obtain:

$$\mathrm{FT}\left[\sum_{mi,nj} J_{mi,nj} a_i a_j^\dagger\right] = \sum_{ij} J_{ij}(\mathbf{q}) b_{i,\mathbf{q}} b_{j,\mathbf{q}}^\dagger$$

So the Fourier transformed Hamiltonian becomes:

$$\mathcal{H}_{\mathbf{q}} = \sum_{ij} J_{ij}(\mathbf{q}) \left[ \frac{\sqrt{S_i S_j}}{2} \left( b_{i,\mathbf{q}} b^\dagger_{j,\mathbf{q}} + b^\dagger_{i,\mathbf{q}} b_{j,\mathbf{q}} \right) - S_i b_{i,\mathbf{q}} b^\dagger_{i,\mathbf{q}} - S_j b^\dagger_{j,\mathbf{q}} b_{j,\mathbf{q}} \right]$$

Which can be expressed as a matrix equation:

$$\mathcal{H}_{\mathbf{q}} = \begin{pmatrix} b_1^\dagger & \dots & b_N^\dagger & b_1 & \dots & b_N \end{pmatrix} \begin{pmatrix} \left[ \frac{\sqrt{S_i S_j}}{2} J_{ij}(\mathbf{q}) - \delta_{ij} S_i J_{ij}(\mathbf{q}=0) \right] & 0 \\ 0 & \left[ \frac{\sqrt{S_i S_j}}{2} J_{ij}(\mathbf{q}) - \delta_{ij} S_i J_{ij}(\mathbf{q}=0) \right] \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_N \\ b_1^\dagger \\ \vdots \\ b_N^\dagger \end{pmatrix}$$

where the square brackets denote a block matrix and we have omitted the $\mathbf{q}$ indices on the bosonic operators.

The off-diagonal blocks are only zero in this case because we are using the Heisenberg Hamiltonian. For anisotropic Hamiltonians (e.g. $XXZ$ or Dzyaloshinskii-Moriya interactions), these blocks will not be zero

Setting:

$$\mathbf{b} = \begin{pmatrix} b_1 \\ \vdots \\ b_N \\ b_1^\dagger \\ \vdots \\ b_N^\dagger \end{pmatrix}$$

The Hamiltonian is:

$$\mathcal{H}_\mathbf{q} = \mathbf{b}^\top h_\mathbf{q} \mathbf{b}$$

With the matrix $h_\mathbf{q}$ as shown previously and $\top$ indicates a complex conjugate transpose.

At each $\mathbf{q}$ the eigenvalues of the matrix $h_\mathbf{q}$ will be the magnon energies $\omega(\mathbf{q})$ and the eigenvalues can be used to calculate the spin-spin correlation function and hence the neutron scattering cross-section.

## Heisenberg Ferromagnet

For a ferromagnet, there is only one magnetic atom in the unit cell, so the Hamiltonian is diagonal already:

$$\mathcal{H}_{\mathbf{q}} = \begin{pmatrix} b^\dagger & b \end{pmatrix} \begin{pmatrix} \frac{S}{2}J(\mathbf{q}) - SJ & 0 \\ 0 & \frac{S}{2}J(\mathbf{q}) - SJ \end{pmatrix} \begin{pmatrix} b \\ b^\dagger \end{pmatrix}$$

The Fourier transform is just:

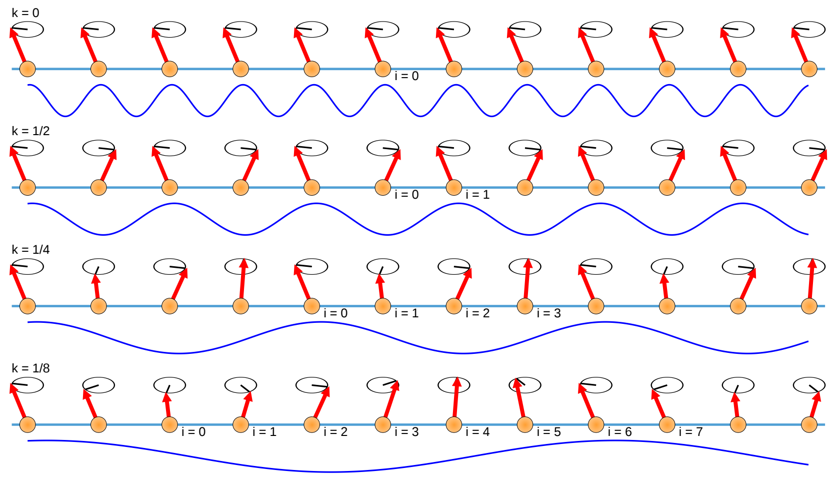
$$\begin{aligned} J(\mathbf{q}) &= J\left(\exp(-i\mathbf{q}\cdot\mathbf{d}) + \exp(i\mathbf{q}\cdot\mathbf{d})\right) \\ &= 2J\cos(\mathbf{q}\cdot\mathbf{d}) \end{aligned}$$

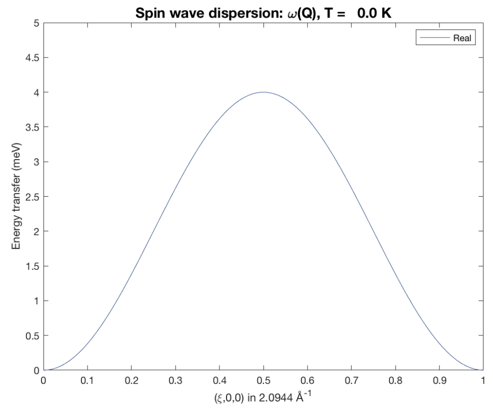
So we obtain $\omega(\mathbf{q}) = JS\left(\cos(\mathbf{q}\cdot\mathbf{d}) - 1\right)$

In general, however, the Hamiltonian is not diagonal and so must be diagonalised.

This can be done using the Bogoliubov transformation for an antiferromagnet

SpinW uses a more general method due to Colpa, as explained in the SpinW paper





Now we have $\omega_{\mathbf{q}}$ and half the story. Remember for neutron scattering:

$$\frac{d^2\sigma}{d\Omega dE} \propto F^2(\mathbf{Q}) \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \hat{q}_\alpha \hat{q}_\beta) S^{\alpha\beta}(\mathbf{q},\omega)$$

With the correlation function:

$$S^{\alpha\beta}(\mathbf{k},\omega) = \frac{1}{2\pi\hbar} \int dt e^{-i\omega t} \langle S^\alpha(\mathbf{q},0) S^\beta(-\mathbf{q},t)\rangle$$

$\langle S^\alpha(\mathbf{q},t)\rangle$ is related to the Fourier transform of the eigenvectors of the Hamiltonian at $\mathbf{q}$.

## Summary

Linear spin wave theory calculations requires:

- The exchange interactions
- The magnetic structure

It expands the spin ladder operators as a power series in bosonic creation/anihilation operators, keeping only linear terms

For each momentum transfer $\mathbf{q}$ a Hamiltonian matrix has to be diagonalised to obtain the magnon energies and spin-spin correlation functions

The size of the matrix is proportional to the number of magnetic atoms in the unit cell

So, larger (or more complex) magnetic structures require more memory; and more $\mathbf{q}$-points require longer processing time

## References

S. Toth and B. Lake, J. Phys.: Condens. Matter **27** 166002 (2015) arxiv:1402.6069

S. Petit Collection SFN **12** 105-121 (2011) 10.1051/sfn/201112006

## Crash course in MATLAB

SpinW runs in MATLAB and Python, but today we will be focusing on MATLAB.

The concepts.... Arrays, Indexing, Objects

They are created using square brackets – comma or space separation for columns in a row, semi-colon separation for new rows, higher dimensions using indexing / repmat command

## 1D arrays

```
w_1row = [1,2,3];
w_1col = [1;2;3];
w_1col_to_1row = [1;2;3]’;
```

## 2D arrays

```
w_rowcol = [1,2,3;4,5,6];
```

## 3D arrays

```
w3d = repmat(w_rowcol,[1,1,3])
w3d(:,:,1) = w_rowcol;  w3d(:,:,2) = w_rowcol+2;
```

## Creating Strings

```
my_string = ‘hello world’;
```

Strings arrays are concatenated similar to numeric arrays....

```
my_string2 = [my_string, ’ hello everyone’];
```

## ARRAYS - STRUCTURED

Structure arrays provide a way of storing more general information, referenced by *fields*.

```
w = struct();
w.tom = [1,2,3];
w.dick = ‘hello world’;
w.harry = [4,5,6,7;8,9,10,11];
```

Cell arrays are another generic data storage mechanism, with a matrix-like structure.

```
cell1 = {[1,2,3], ’hello_world’, [4,5,6;7,8,9]};
cell2 = {[1,23], ’hello_world’; [4,5,6;7,8,9], cell1};
```

Note that the cell array is described by a curly bracket, not a square bracket!

Arrays can be indexed. Note that the ordering is the reverse to Python and indexes start from 1!.

```
w1 = [1,3,5,7]
```

So `w1(3) = 5` etc.

```
wcell = {‘hello’,’world’,[1,2,3]}
```

So `wcell{3} = [1,2,3]` etc.

In 2D:

```
w2 = [1,2,3; 4,5,6]
```

So `w2(2,3) = 6`

```
w2(:,[1:2]) = [1,2;4,5]
w2(:,[1,3]) = [1,3;4,6]
```

Objects are data structures with defined properties, and internal self-consistency checks.

- Cell arrays, structure arrays etc. are examples of Matlab's built-in objects.
- You can define your own, which is what we have done with SpinW

You create a SpinW object with:

```
s = spinw();
```

Methods are the functions that work on defined objects.

SpinW has many methods. e.g.

```
s.plot()
```

## Getting help for objects and methods

To find all the methods working on an object, use the `methods` function which the name of the object class.

```
methods(spinw)
```

Get help if you already know the name of a particular method for an object class *e.g.* *`addatom`*:

```
help spinw/addatom
doc spinw/addatom
```

## Function help

For any function that starts with `sw_*` use:
`help sw_*`

## SpinW class methods

for spinw class methods use:
`help spinw.function_name`.
For help on plotting commands, use:
`help swplot`.

## Online Documentation

All help can be found on http://www.spinw.org or https://spinw.github.io/spinwdoc

## The cheatsheet

Many of you might not have extensive experience in MATLAB, so a cheatsheet of common and useful commands might be helpful

>

I've found that the one on the MATLAB file Exchange to be quite useful.

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# Introduction to SpinW

So, how does SpinW work?

## SpinW

- Solves the general spin Hamiltonian
- Calculates spin-spin correlation function
- Numerical and symbolical
- Can apply crystal symmetry operators on the Hamiltonian - Solving single-q magnetic structures
- Solves multi-q magnetic structures on a magnetic supercell
- Open source, runs on MATLAB and now python
- More information: http://www.spinw.org
- Download from: https://www.github.com/spinw/spinw

## The General Spin Hamiltonian

SpinW solves the general spin hamiltonian:

$$H = \sum_{mi,nj} \mathbf{S}_{mi}^T \cdot J_{mi} \cdot \mathbf{S}_{nj} + \sum_{mi} \mathbf{S}_{mi}^T \cdot A_i \cdot \mathbf{S}_{mi} + \mu_B \mathbf{H}^T \sum_{mi} g_i \mathbf{S}_{mi}$$

Where:

- Term 1: Bi-linear interactions between site $i$ and site $j$
- Term 2: Single ion terms acting on site $i$
- Term 2: Effect of applied magnetic field on site $i$

## Exchange/Interaction Matrices

There are a few matrices of note (that you will use later):

- Anisotropic and antisymmetric (Dzyaloshinskii-Moriya) exchange interactions:

$$J_S = \begin{bmatrix} J_x & 0 & 0 \\ 0 & J_y & 0 \\ 0 & 0 & J_z \end{bmatrix}; J_A = \begin{bmatrix} 0 & D_z & -D_y \\ -D_z & 0 & D_x \\ D_y & -D_x & 0 \end{bmatrix}$$

- Easy-plane and easy-axis anisotropy:

$$A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \pm A_0 \end{bmatrix}$$

## Creating a SpinW object.

Assuming that everything is properly installed*, you can create an empty `spinw` object with the following:

```
s = spinw();
```

You can also create populated `spinw` objects from cif files.

```
s = spinw('./my_crystal.cif');
```

∗ More on this later.....

## The General Spin Hamiltonian

Necessary input information:

$$H = \sum_{mi,nj} \mathbf{S}_{mi}^T \cdot J_{mi} \cdot \mathbf{S}_{nj} + \sum_{mi} \mathbf{S}_{mi}^T \cdot A_i \cdot \mathbf{S}_{mi} + \mu_B \mathbf{H}^T \sum_{mi} g_i \mathbf{S}_{mi}$$

In order to solve the above Hamiltonian in SpinW you need the following components:

- **Crystal structure**: Cell lengths/angles, Symmetry.
- **Exchange structure**: Atomic sites, Interaction matrices, Single ion matrices.
- **Magnetic Structure**: Spin vectors in the unit cell.*

$*$This is often the hardest part

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## Crystal structure

The crystal structure is usually the easiest to determine, commonly by x-rays or powder neutron diffraction.

- **Lengths**: $a$, $b$, $c$, given in Angstroms
- **Angles**: $\alpha$, $\beta$, \gamma$, given in degrees or radians with an additional flag.
- **Symmetry**:Given as a symbol/number from the international table of crystallography or a string of symmetry operations.

This information is added to the object via:

```
s.genlattice('lat_const',[3 3 4],'angled',[90 90 120],'spgr','P 6')
s.genlattice('lat_const',[3 3 4],'angled',[90 90 120],'spgr',168)
s.genlattice('lat_const',[3 3 4],'angled',[90 90 120],'spgr','-y,x-y,z; -x,-y,z','label','R -3 m')
```

## Adding Atoms

Object now needs some atoms which may have/not have spin. To add a magnetic atom with $S = 1$ at position $r = (0, 0, 0)$ and a non-magnetic one at $r = (1/2, 0, 0)$ with red and blue color respectively use the following command:

```
s.addatom('r',[0 1/2; 0 0; 0 0],'S',[1 0],'color',{'red' 'blue'}, 'label', {'Co', 'H'})
```

## Adding Matrices

Before you can say how atoms are linked or their properties, you need to add matrices to define the property. For example, an exchange matrix $(J_1)$ and an easy axis matrix $(K_0)$.

```
s.addmatrix('value', 1, 'label', 'J1');
s.addmatrix('value', [0, 0, -0.1], 'label', 'K0');
```

## Assigning Matrices

Now you have all the atoms in the unit cell, you have to calculate all the possible exchanges. Luckily, symmetry is used in this calculation. Possible couplings are generated and can be viewed with:

```
s.gencoupling()
s.table('bond',1:3)
```

If you want to add our exchange $J_1$ as defined earlier to bond 2 in the list:

```
s.addcoupling('mat','J1','bond',2)
```

And single ion anisotropy defined by $A_0$

```
s.addaniso('A0')
```

## Defining the magnetic structures

As alluded to earlier, defining the magnetic structure is one of the hardest aspects of `spinw` and could easily take a 2-hour lecture.

**DON'T PANIC!**

We will introduce a few concepts in the examples and there is a presentation here which goes into more detail. Some important points to remember are:

- Magnetic structures can be extracted from powder diffraction measurements.
- In real life the obtained magnetic structure will probably need tweaking.
- SpinW has spin-energy minimization codes to help you.

## Generating a magnetic structure

Rather than inputting the magnetic structure directly, it is recommended to use the `spinw.genmagstr()` function to generate the magnetic structure.

This function checks your input for errors and also provides short-cuts for common use-cases, using various `modes`:

| | |
|---|---|
| `helical` | single-$k$ helix |
| `fourier` | single-$k$ helix or modulated structure |
| `rotate` | uniform rotation of all moments |
| `direct` | direct input of structure using all fields `k`, `F`, `nExt` |
| `tile` | tile a magnetic supercell |
| `func` | using a function to generate `k`, `F`, `nExt` |
| `random` | random moments |

`genmagstr()` always respects `nExt`, so a combination of an input `nExt` and `k` will generate a magnetic supercell which is extended first by `nExt` and then by `k`

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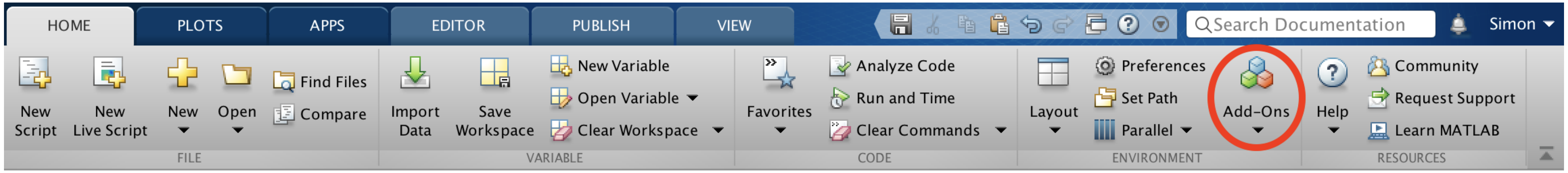
## Does anyone have any questions?

## Using the MATLAB package - The easy way

SpinW is now a MATALB add-on and can be downloaded directly from Mathworks.



Then search for SpinW and hit install.

Verify with `s = spinw;`

## Updating:

Add-Ons → Check for updates → Update

## NOTE

This version may not correspond to the `sw_update` version!

## Get the code - The manual way:

SpinW is available at:
https://www.github.com/spinw/spinw/releases/latest

## Steps:

- Unzip the archive into your preferred directory
- Open MATLAB and run `install_spinw` from inside this directory
- Verify with `s = spinw;`

## Updating:

I am trying to make releases 2-3 times a year. It's always nice to be on the latest code!
There is a self update function `sw_update`
This retrieves and installs the package from the link above.

## Developing:

If you want to help develop a feature and contribute, please git clone https://www.github.com/spinw/spinw.git and create a pull request (to development branch)

## Function help

For any function that starts with `sw_*` use:
`help sw_*`

## SpinW class methods

for spinw class methods use:
`help spinw.function_name`.
For help on plotting commands, use:
`help swplot`.

## Online Documentation

All help can be found on http://www.spinw.org or https://spinw.github.io/spinwdoc

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An introductory live notebook can be found here and in pdf form.

SW

For the things we have to learn before we can do them, we learn by doing them.

Aristotle

# Tutorials 1

Getting started in SpinW

## Excitations on a triangular lattice

Download the script here: `sw_tutorial_01.m`

## $\boldsymbol{k} = [1\,1\,0]/3$ magnetic structure

Let's try this with a $k = [1\,1\,0]/3$ magnetic structure

## Creating the lattice

```
tri = spinw;
tri.genlattice('lat_const',[3 3 4],'angled',[90 90 120])
plot(tri)
```

We have:

- Created a SpinW object
- Generated a lattice of $a = 3\text{Å}$, $b = 3\text{Å}$, $c = 4\text{Å}$ and $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$

In the plot window, you can zoom with the mouse wheel, pan by pressing the Ctrl button while dragging. Change the plot range and view direction by pressing the corresponding button on the top.

### Questions:

*What is the default symmetry and what does it mean?*

## Adding atoms

```
tri.addatom('r',[0 0 0],'S',3/2,'label','MCr3')
plot(tri)
```

We have added an magnetic Cr$^{3+}$ at position $[0, 0, 0]$ with spin $S = 3/2$

## Creating the Spin-Hamiltonian

We create an antiferromagnetic first neighbor Hamiltonian plus easy plane single ion anisotropy

```
A0 = -0.1;
tri.addmatrix('label','J1','value',1)
tri.addmatrix('label','A','value',[0 0 0;0 0 0;0 0 A0])

tri.gencoupling

tri.addcoupling('mat','J1','bond',1)
tri.addaniso('A')

plot(tri,'range',[3 3 1/2],'cellMode','inside')
```

Red ellipsoids represent the single ion anisotropy on the plot (equienergetic surface)

### Questions:

*What have we done in each code part?*
*Examine the plot and test different values of `A0` with different signs*

## Creating the magnetic structure:

We have seen the ground state magnetic structure of the above Hamltonian is a spiral, with propagation vector of $(1/3, 1/3, 0)$. We define the plane of the spiral as the $ab$ plane

```
tri.genmagstr('mode', 'helical', 'S', [1;0;0], 'k',[1/3 1/3 0], 'n', [0 0 1], 'nExt', [1 1 1])
plot(tri, 'range', [3 3 1/2], 'cellMode', 'inside', 'magColor', 'red')
```

Careful: the given spin vector is column vector!

### Questions:

*What are the angles between nearest neighbor moments?*

## Calculating the spin wave dispersion

We calculate the spin wave dispersion along the $(H,H,0)$ high symmetry direction

```
spec = tri.spinwave({[0 0 0] [1 1 0] 500}, 'hermit', false);
figure
sw_plotspec(spec, 'mode', 'disp', 'imag', true, 'colormap', [0 0 0], 'colorbar', false)
axis([0 1 0 5])
```

### Questions:

*How many modes are there and why?*
*What does the red line mean?*
*Did you get any warning?*

## Calculating the spin-spin correlations

The spin-spin correlations are already calculated, however it contains 9 numbers per Q-point per mode. It is not possible to show this on a single plot. But:

1. we can calculate the neutron scattering cross section
2. we can select one of the components $S^{\alpha\beta}(\mathbf{Q},\omega)$
3. we can sum up the diagonal $S^{\alpha\alpha}(\mathbf{Q},\omega)$

```
spec = sw_egrid(spec, 'component', {'Sxx+Syy' 'Szz'}, 'Evect', 0:0.01:5);
% Try other components!
figure
sw_plotspec(spec,'mode','color','dE',0.2,'imag',false)
axis([0 1 0 5.5])
caxis([0 3])
```

### Questions:

*How is it related to the magnetic propagation vector?*
*Why are some modes gapped? Which correlations are gapped?*
*Why do we have Szz ?*

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# $\boldsymbol{k} = 0$ magnetic structure

Let's try this with a $k = 0$ magnetic structure

## $k = 0$ magnetic structure

Duplicate the original object using the `.copy()` command,
*Why are we using the `.copy()` command?*

```
triNew = copy(tri);
triNew.genmagstr('mode','rotate','n',[0 0 1])
phi1 = atan2(triNew.magstr.S(2,1),triNew.magstr.S(1,1));
triNew.genmagstr('mode','rotate','n',[0 0 1],'phi',-phi1)
plot(triNew,'range',[3 3 1])
```

Compare the energy per spin of the old magnetic structure and the new magnetic structure using the `spinw.energy()` function.

### Questions:

*How does the magnetic structures compare?*
*Are they the same?*
*Why?*

## Calculating the spin wave dispersion

We calculate the spin wave dispersion along the $(H, H, 0)$ high symmetry direction

```
spec = triNew.spinwave({[0 0 0] [1 1 0] 500}, 'hermit', false);
figure
subplot(2, 1, 1)
sw_plotspec(spec, 'mode', 'disp', 'imag', true, 'colormap', [0 0 0], 'colorbar', false)
axis([0 1 0 5])
spec = sw_egrid(spec, 'component', 'Sperp', 'Evect', 0:0.01:5.5);
subplot(2, 1, 2)
sw_plotspec(spec, 'mode', 'color', 'dE', 0.2, 'imag', false)
axis([0 1 0 5.5])
caxis([0 3])
```

### Questions:

*How many number of modes are there and why?*
*Is there more than before?*
*Why are there vertical lines in the dispersion?*
*Which structure is the correct one?*

SW SpinW

# Tutorial 2

The FM kagome lattice, a user worked example.

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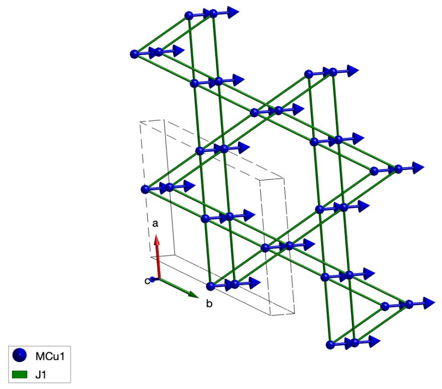
## The FM kagome lattice

Download the script here: `sw_tutorial_02.m`



Expected magnetic structure of our Kagome lattice

## Tutorial 2: The FM Kagome Lattice

This tutorial puts the emphasis on you, it is mostly fill in the blanks using the previous tutorial as a template.

It is useful to remember the SpinW stages:

- Define the crystal/atomic structure.
- Add magnetic interactions.
- Define a magnetic structure.
- Perform a calculation.

This tutorial is a little tricky, all details are in the text and the SpinW help is useful for syntax.

I will also be walking around to help.

SW SpinW

## Thank you!

Well done if you're still awake!

SW

SpinW