Overview of use cases (DAS-33)

[DAS-34] For spectroscopy (magnetism) Created: 2019-Mar-26 Updated: 2019-Apr-03 Resolved: 2019-Apr-03

Status:	Done
Project:	Diffraction Analysis Software
Component/s:	None
Affects Version/s:	None
Fix Version/s:	None

Type:	Sub-task	**Priority:**	Normal
Reporter:	Thomas Holm Rod	**Assignee:**	Piotr Rozyczko
Resolution:	Done	**Votes:**	0
Labels:	VISPY		
Remaining Estimate:	Not Specified		
Time Spent:	Not Specified		
Original Estimate:	Not Specified		

Attachments:	tutorial10_03.png tutorial12_03.png tutorial21_01.png tutorial3_05.png tutorial4_04.png tutorial5_01.png tutorial5_02.png tutorial5_03.png tutorial7_04.png tutorial8_07.png			
Issue Links:	**Dependency**			
	is depended on by	DAS-42	Structure viewer/editor	To Do
	Hierarchy			
	is part of	~~DAS-44~~	For spectroscopy (chemical)	Done

Comments

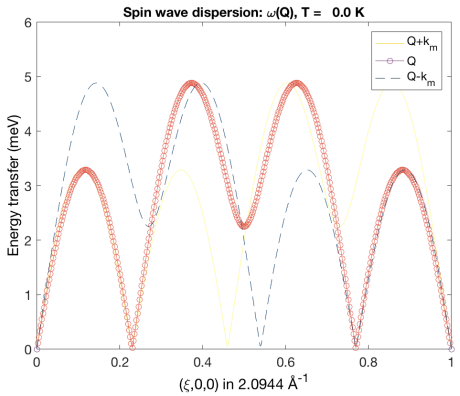
Comment by Simon Ward [2019-Apr-01]

Data Presentation

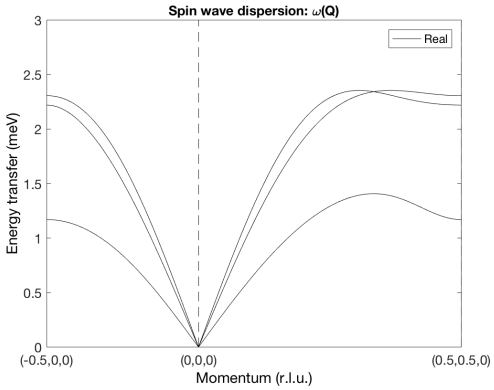
1D Plots

Line plots

These plots are an arbitrary XY plot used to show data. There may be stacking of multiple lines. Lines must be able to be represented as data points. Legend entries must also be available. e.g:

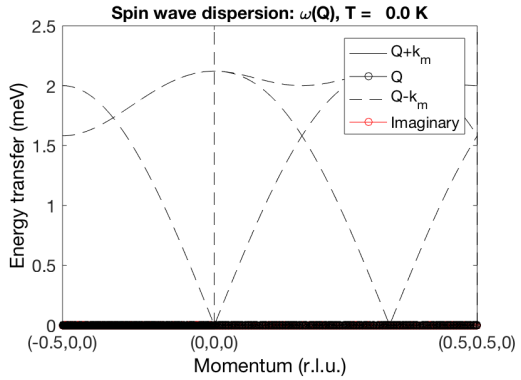


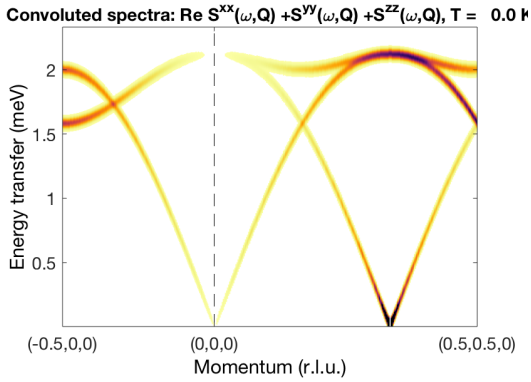
The plots must also be able to have non-standard axes. i.e going from [2, 0, 0]~~>[0, 0, 0]~~>[0, 2, 0]



Multiple plots

We must be able to have multiple plots on a graph

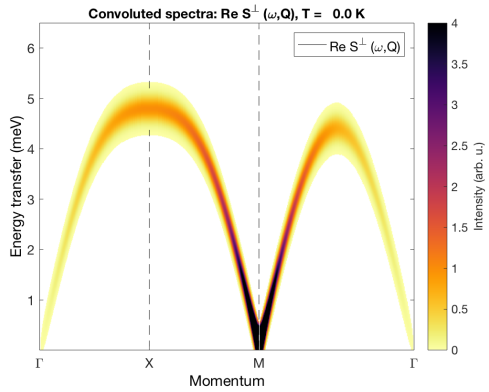




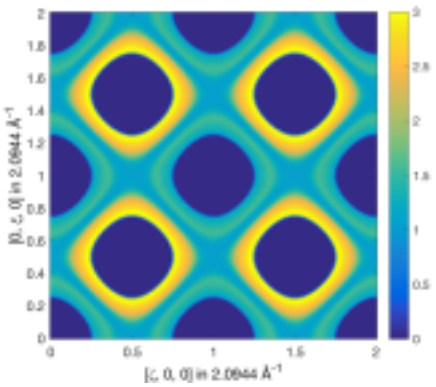
2D plots

As seen above 2D plots are needed to visualise intensities.

These are line plots which also contain intensity which is mapped to a colour bar e.g.



Also 2D maps can be shown



Note:

We will want to overlay plot types. E.g add a line plot to a colour map

Comment by Simon Ward [2019-Apr-01]

Atom plots

General information

Plots of atoms must have:

- Atoms which are generated by symmetry operations
- The visual properties of the atom must be editable (size, color, specularity etc...)
- The unit cell must be visible
- There must also be a way of showing bonds between atoms
- Each atom has a spin-moment. This has to be depicted by an arrow.
- 2D surfaces for anisotropies, chemical environment etc must also be plotable.
- Plotting in lattice units or cartesian units.
- Visualisation of x,y,z which rotates with the unit cell

Interactivity:

- The plot must be 3D and rotatable
- Clicking on an item must display information on the item
- Clicking on an atom shows other symmetry equivalent atoms.
- The extent can be changed i.e more than 1 unit cell
- The view can be reset or set to an axis

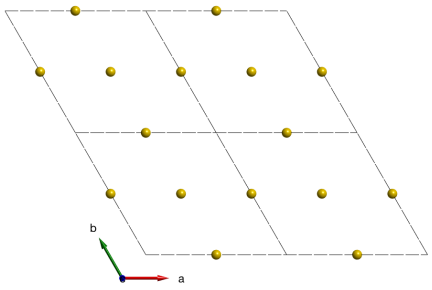
Interfaces

The plot must be usable in the following:

- Ipython notebooks
- python scripting. i.e complete control of the plot from the command line.
- QT widget so it can be embedded in other applications

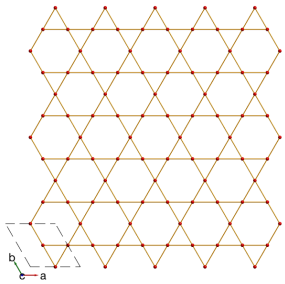
Examples

Atoms

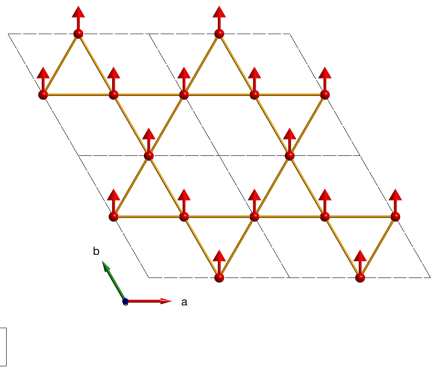


Atoms + Bonds

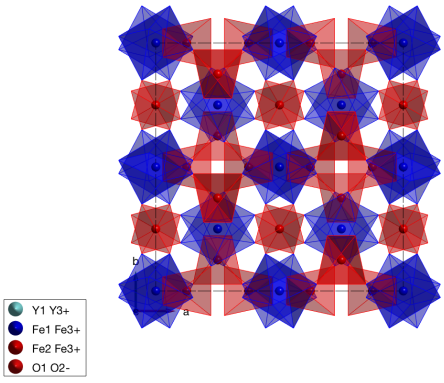
Note the increase in number of unit cells along the *a* and *b* direction.



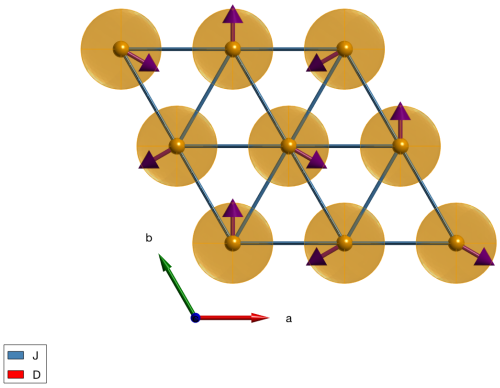
Atoms + Bonds + Spins



Chemical Environment



Anisotropies



Comment by Simon Ward [2019-Apr-01]

Symmetries

We want to be able to:

- Generate atomic equivalent positions based on crystal symmetry
- From a position, give other symmetry equivalent positions.
- If 2 atoms are selected, we have a bond. What are the symmetry equivalent bonds in the unit cell.
- If you select a bond, using the space group determine what off-diagonal exchange components are allowed to form an exchange matrix.
- Apply symmetry elements to an exchange matrix for equivalent bonds in the unit cell.

Why?

- We need all atomic positions
- We need to select all equivalent positions (also for visualisation)
- Equal bond length is not a determining factor for equal exchanges. It is symmetry environment+bond length
- Exchange matrix symmetry allows for physically correct setups and no easy mistakes.
- We want to plot the bond for all elements in the unit cell.

Comment by Piotr Rozyczko [2019-Apr-03]

Minor comments:

for **atom plots** we need a bit more functionality, I think.

- arrows on atoms should be used to represent any vector atomic quantity, not just spin (velocity, force etc)
- cell view should be extendable for supercells so we can easily see bonds between atoms in different cells
- we probably need to make visual distinction between multiple bonds (single, double, hydrogen etc)
- lattice specific visualization needs to be implemented for Miller planes, bandstructure path etc.

Interactivity should include zooming and possibly z-clipping (important when you have many atoms in the cell)

For **symmetry**:

- generate primitive cell
- generate conventional cell
- given a structure find symmetry within a specific tolerance

Maybe we need extra functionality for **surfaces** in reflectometry like:

- cleave surface
- build surface
- create vacuum slab

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