Spectrum

I’m getting really annoyed by the spectrum data variable shenanigans. It seems like these issues exist because spectrum contains a copy of all the datasets attributes. This is obviously wrong imo. The whole package is built on packaging data into a DataSet so you should be able to provide that dataset to any function. It’s super clunky to sometimes be able to give a dataset and other times functions need the spectrum DataArray.

I think the reason things are this way is because you can have multiple spectra in a single dataset.

I think all functions should work like this:

1. take in full DataSet
2. have optional argument to specify which spectrum should be used. Otherwise default to the .spectrum attribute which consistently refers to the most preferable spectrum
3. get necessary attributes from the DataSet and get the raw data from spectrum

This should avoid all situations where a function expects a spectrum but got a DataSet.

Here’s an example of the issues this situation has caused me. I was trying to convert a dataset to k-space with offsets to center the fermi surface. I was applying the offsets to the dataset so they weren’t getting transferred over to the spectrum. Then when doing the k-space conversion, all of the offsets were missing and nothing was changing. Using the ktool worked fine because you have to supply it the spectrum which it applies offsets to, but I couldn’t figure out why doing the same thing to the dataset had no effect. After probably half an hour I figured out that I needed to apply the offsets to the spectrum.

The only issue with making these changes is it will require a ton of work to fix code broken by the change.

Notes while refactoring

- for k-space conversion, I’m getting the offsets from the ds instead of spectrum. This could cause an issue if different spectra in a single ds have different offsets. I’m struggling to see why someone would want multiple spectra in a single ds