

ex3-Experiment-class

June 1, 2021

1 Example 3: The mm2SANS Experiment class

Calculate and plot the neutron scattering cross sections. Uses the settings specified in the Sample and Probe objects.

```
[1]: import mm2SANS
import numpy as np

[2]: """ create the Sample object (using settings from Example 1) """
sample = mm2SANS.Sample(
    positions=[[0, 0, 0]],
    moments=[[0, 0, 1]],
    scattering_length_density=(8.024-0.001j),
    saturation_magnetisation=800e3,
    voxel_volumes= 4/3 * np.pi * 10e-9**3 ,
    periodicity=(50e-9, 50e-9, 50e-9),
    print_diagnostics=True,
)

""" create a Detector object (using Settings from Example 2) """
print()
probe = mm2SANS.Probe(
    sans_instrument='test'
    , neutron_wavelength=6e-10 # in m
    , detector_distance=15 # in m
    , neutron_polarisation=(0,0,1)
    , qmap_disorder=0.35 # to avoid Fourier transform artefacts
)
probe.Beamline.print_beamline_settings()

""" create an Experiment object and calculate the scattering patterns """
experiment = mm2SANS.Experiment(sample, probe, print_diagnostics=False)
experiment.calc_scattering_pattern(uc_repetitions=(1,1,1),
    ↪ print_diagnostics=False)
print('\nscattering patterns calculated!')
```

Data bounding box size: (0.0, 0.0, 0.0) nm.

REMARK: Voxel volumes were not corrected.

1 positions with an average sphere diameter of 20.00 nm, and an average moment of $1.2 \times 10^5 \mu_B$.

Neutron wavelength = 6.0 Angstrom, detector distance = 15 m
 Neutron polarisation set to [0. 0. 1.] in sample environment coordinate system (u, v, w),

scattering patterns calculated!

```
[3]: """ The calculated patterns are stored in a pandas Dataframe """
experiment.data.head()
```

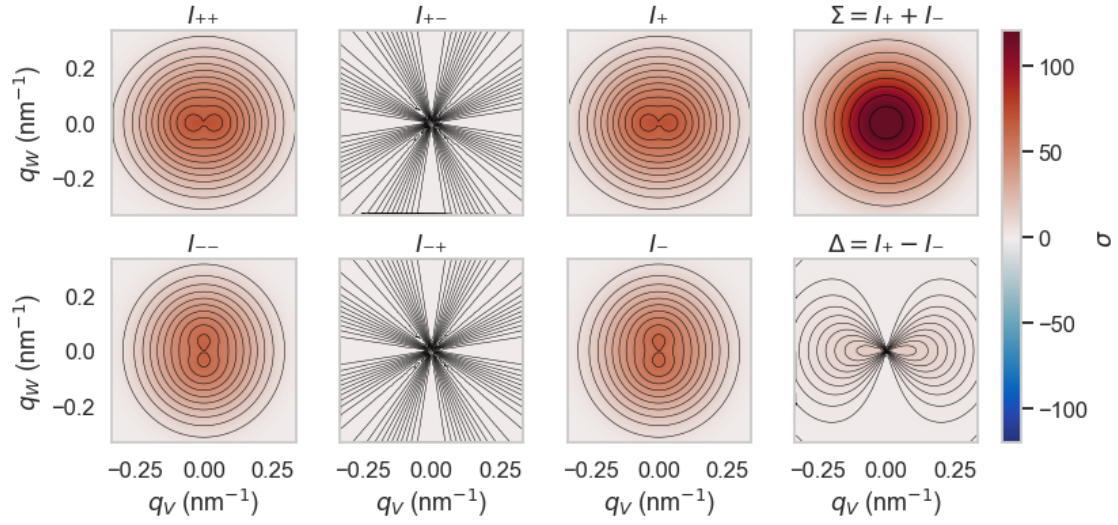
```
[3]:   q_U          q_V          q_W          q_phi          q_abs \
0  0.0 -3.279993e+08 -3.273456e+08  45.057146  4.633991e+08
1  0.0 -3.275223e+08 -3.172074e+08  45.916588  4.559511e+08
2  0.0 -3.290999e+08 -3.052907e+08  47.149357  4.488977e+08
3  0.0 -3.294786e+08 -2.970386e+08  47.964033  4.436081e+08
4  0.0 -3.271980e+08 -2.879599e+08  48.649685  4.358663e+08

                                sld_struct  sld_mag_U \
0      (-0.153369317888801+1.9113823266301225e-05j)      0j
1      (-0.07466244638001275+9.304891124129207e-06j)      0j
2      (0.0051683584350431504-6.441124669794554e-07j)      0j
3      (0.0684185966973143-8.526744354101983e-06j)      0j
4      (0.166205601108031-2.071355946012351e-05j)      0j

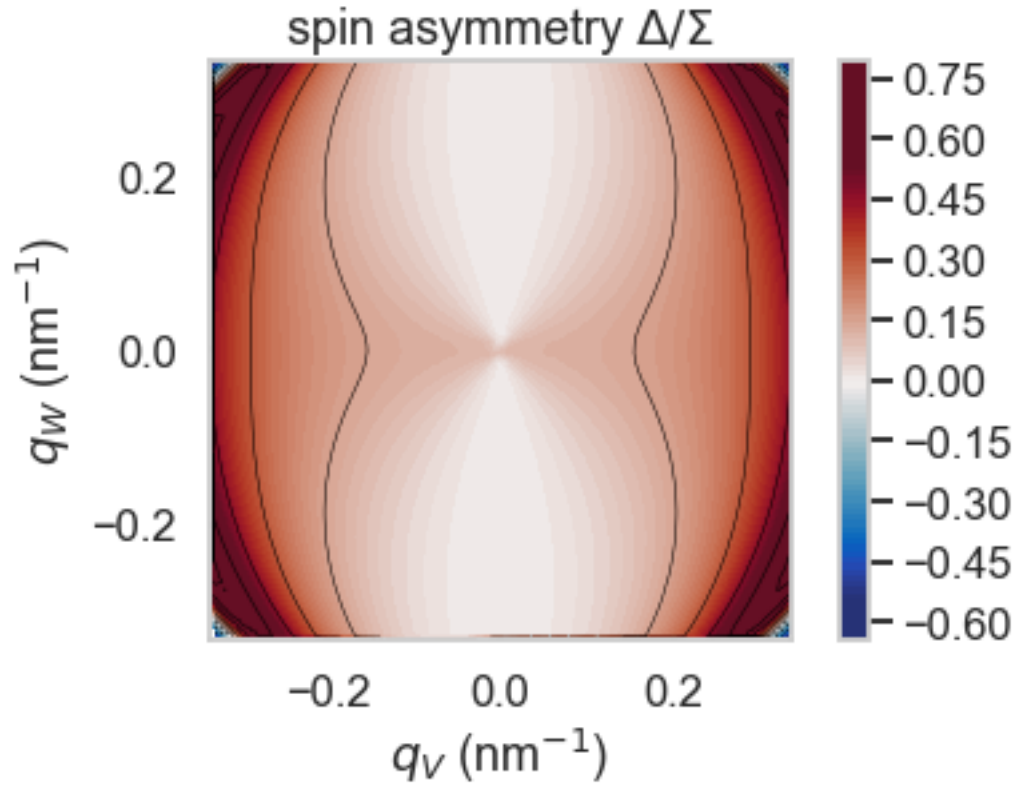
                                sld_mag_V          sld_mag_W          I_pp          I_pm \
0      (-0.237170201378092+0j)  (0.23764377446720789+0j)  0.007102  0.056250
1      (-0.23704929044476666+0j)  (0.24475764537451447+0j)  0.028932  0.056192
2      (-0.2365034685819089+0j)  (0.2549481194942424+0j)  0.067661  0.055934
3      (-0.23590236659548114+0j)  (0.2616656049869285+0j)  0.108956  0.055650
4      (-0.23524860363826552+0j)  (0.2673040887934099+0j)  0.187931  0.055342

          I_mp          I_mm          I_m          I_p          I_sum          I_dif          asym
0  0.056250  0.152891  0.209141  0.063352  0.272493 -0.145789 -0.535020
1  0.056192  0.102029  0.158222  0.085125  0.243346 -0.073097 -0.300382
2  0.055934  0.062390  0.118324  0.123594  0.241918  0.005271  0.021787
3  0.055650  0.037344  0.092994  0.164606  0.257600  0.071611  0.277994
4  0.055342  0.010221  0.065563  0.243273  0.308835  0.177710  0.575419
```

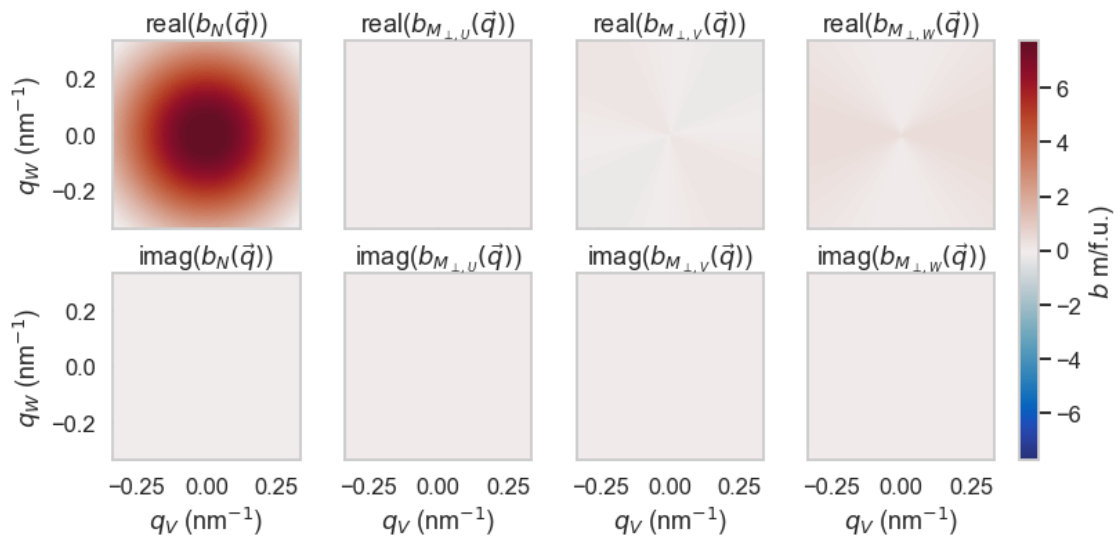
```
[3]: """ plot all scattering cross sections """
experiment.plot_scattering_patterns()
```



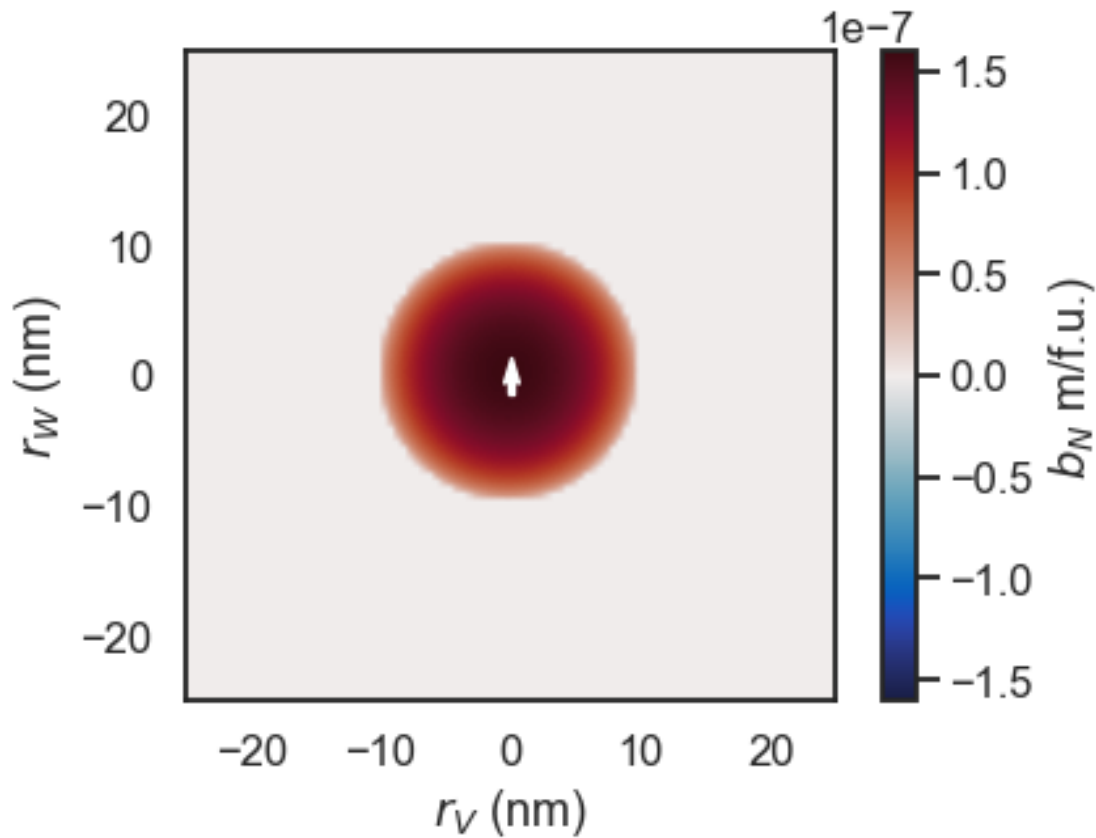
```
[5]: """
Plot a specific property from the data output only, e.g. I_pp, I_pm, I_mp,
→ I_mm, I_m, I_p, I_sum, I_dif, asym
This function can be used to plot onto specific axes of a custom display layout
→ (ax and title keywords).
"""
experiment.plot_property('asym', plot_imag=False, contours=True)
```



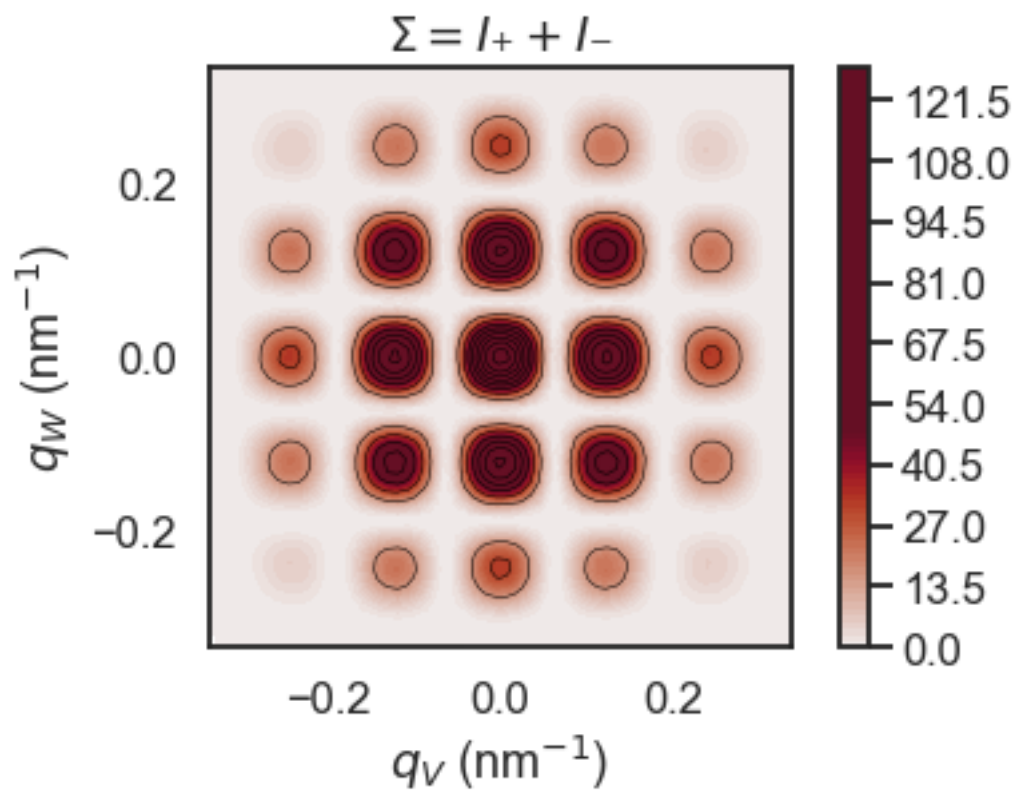
[6]: `""" plot structural and magnetic scattering length components in reciprocal_`
`→space """`
`experiment.plot_scattering_lengths()`



```
[7]: """ plot real value of the scattering length of sample transformed into the
      ↪ beamline coordinate system U, V, W """
experiment.Sample.plot_scattering_length(plane='VW', step_size=0.5e-9,
      ↪ show_magnetic=True)
```



```
[8]: """ (brute-force) calculation scattering pattern for a periodic repetition
      ↪ (usually only a few are needed) """
# use with caution, result is very dependent on number of repetitions!
experiment.calc_scattering_pattern(uc_repetitions=(2,2,2),
      ↪ print_diagnostics=False)
experiment.plot_property('I_sum')
```



[: