ex2-Probe-class

June 2, 2021

1 Example 2: The `mm2SANS` `Probe` class

The `Probe` class describes all settings specific to a particular SANS experiment.

Most importantly, it combines the properties of `Detector` (specifying size and layout of the SANS detector) and `Beamline` (setting neutron wavelegth, neutron polarisation, and orientation of coordinate systems) objects to calculate the q-map, as well as the neutron polarisation $\vec{P}$ within the beamline coordinate system U, V, W.

To specify the rotations of the sample and the sample environment the the fields `Probe.Beamline.sample_rotations` and `probe.Beamline.sample_environment_rotations`, respectively, are used. As this is a headache on its own, find details and explanations in the corresponding example notebook.

1.1 Things you can do with a `Probe` object

- Modify the $\vec{Q}$ map, e.g. select a region of interest or thin out the values to evaluate in order to execute the code faster.
- You can also set up a log-scale $\vec{Q}$ map using the `Detector.calc_log_qmap` function (see example below). Note that it does not make sense to go to q ranges that correspond to distances lower than the mean distance in your real-space mesh, though.
- Vary the sample or sample environment orientation, and re-calculate the transformation matrices. This allows to e.g. simulate rocking curves.

[1]:
```
import mm2SANS
import matplotlib.pyplot as plt
```

[2]:
```
probe = mm2SANS.Probe(
                  sans_instrument='test'
                , neutron_wavelength=6e-10 # in m
                , detector_distance=15 # in m
                , neutron_polarisation=(1,0,0) # U || along beam, V & W in␣
 ↪detector plane
                , qmap_disorder=0.35 # to avoid Fourier transform artefacts
               )
```

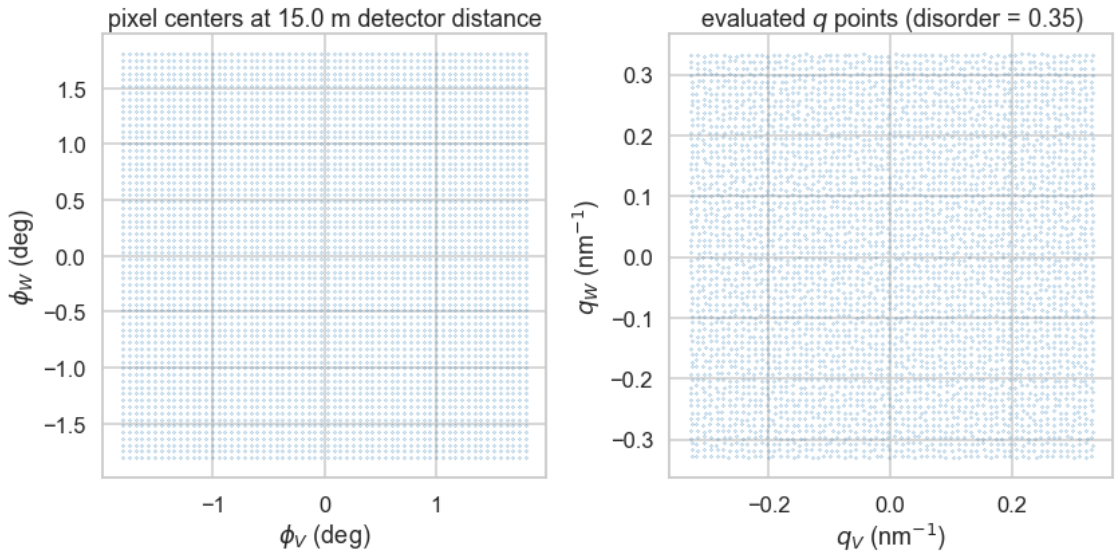
[3]:
```
# print detector properties
probe.Detector.print_detector_info()
```

```
test detector has 64.0 x 64.0 pixels with a size of 15.00 mm x 15.00 mm.
```

[4]:
```
# print beamline settings
probe.Beamline.print_beamline_settings()
```

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

[5]:
```
# plot detector map
probe.plot_qmap()
```



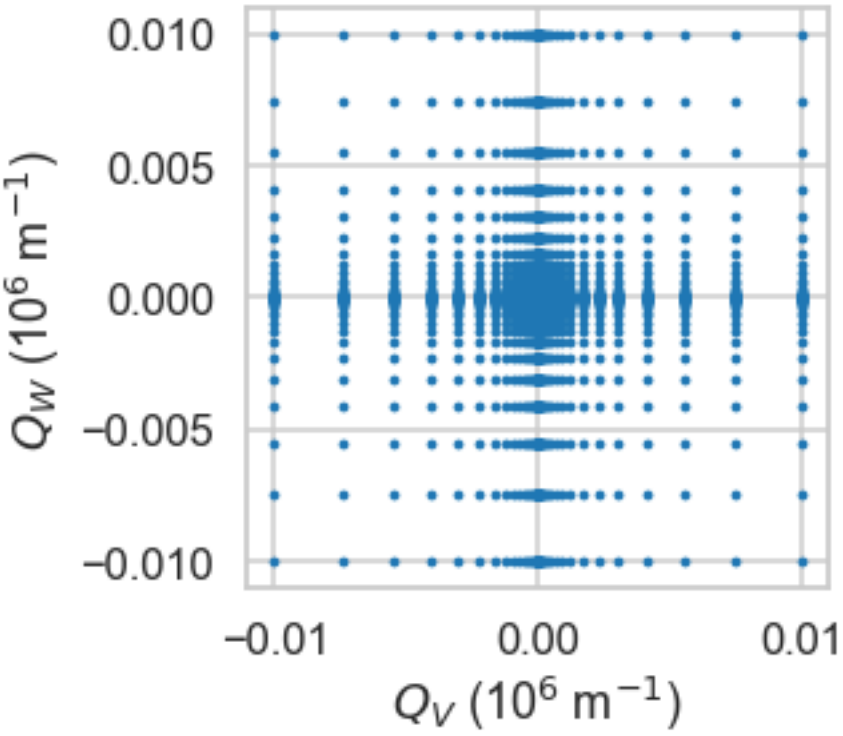
1.2 Function to generate logarithmic $\vec{Q}$-maps

This could be e.g. used to calculate radially-averaged form factors of magnetic particles extending to large q values (correspoding to small distances). Note that it does not make sense to go to q ranges that correspond to distances lower than the mean distance in your real-space mesh, though.

[6]:
```
probe.Q_veclist = probe.calc_log_qmap()

fig = plt.figure()
ax = plt.subplot(aspect='equal')
ax.set_xlabel('$Q_V$ (10$^6$ m$^{-1}$)')
ax.set_ylabel('$Q_W$ (10$^6$ m$^{-1}$)')
ax.scatter(
      probe.Q_veclist[:,1] / 1e6
    , probe.Q_veclist[:,2] / 1e6
    , s = 5
    )
```

[6]:
```
<matplotlib.collections.PathCollection at 0x20f5b701f28>
```


0.010
0.005
0.000
−0.005
−0.010
Q_W (10^6 m^{-1})
−0.01
0.00
0.01
Q_V (10^6 m^{-1})

[ ]: