ex3-Experiment-class

June 2, 2021

1 Example 3: The mm2SANS Experiment class

Calculate and plot the neutron scattering cross sections. The following example uses the settings specified in the previous Sample and Probe examples.

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

[2]:
```
""" create the Sample object (using settings from Example 1)"""
sample = mm2SANS.Sample(
    sample_name = 'test',
    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!')
```

```
REMARK: Voxel volumes were not corrected.
1 positions with an average sphere diameter of 20.00 nm, and an average moment
of 1.2e+05 mu_Bohr.

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!
```

1.1 Data table for the calculated scattering patterns

The calculated values are stored in `Experiment.data`, which is a `pandas` DataFrame table with the following columns:

- `q_U`, `q_V`, `q_W`, `q_abs`, `q_phi` Scattering vector components q_U, q_V, q_W (in m^{-1}). In addition, the lengths $|q_{VW}|$ of the scattering vectors and their angle $\phi_{q_{VW}}$ in the detector plane are stored.
- `sld_struct`, `sld_mag_U`, `sld_mag_V`, `sld_mag_W`: Complex-valued scattering length for the nuclear component $b_N(\vec{Q})$ and the magnetic components $\vec{b}_{\vec{M}_\perp}(\vec{Q})$. These values (in m) already take into account the pre-factors from the material scattering length densities and saturation magnetisation, respectively.
- `T1` to `T5`: Real-valued individual components to the scattering cross sections (in m^2), which are:
  - `T1` = $|b_N|^2$
  - `T2` = $\vec{P} \cdot (b_N \vec{b}^*_{\vec{M}_\perp} + b^*_N b_{\vec{M}_\perp})$
  - `T3` = $|\vec{P} \cdot \vec{b}_{\vec{M}_\perp}|^2$
  - `T4` = $|\vec{b}_{\vec{M}_\perp}|^2$
  - `T5` = $\vec{P} \cdot (\vec{b}_{\vec{M}_\perp} \times \vec{b}^*_{\vec{M}_\perp})$. This one is a purely imaginary component.
- `I_?`: Scattering cross sections (in m^2), which include:
  - `I_pp`, `I_mm`, `I_pm`, `I_mp`: Non-spin-flip and spin-flip cross sections accessible in a SANS experiment with polariser and analyser.
  - `I_p`, `I_m`, `I_dif`: Half-polarised cross sections for flipper on/off, and difference signal $\Delta(\vec{Q}) = I_+ - I_-$.
  - `I_sum`: Total scattering cross section $\Sigma(\vec{Q}) = I_+ + I_-$.
- `asym`: Spin asymmetry Δ/Σ (value between -1 and +1).

At the moment (2021-06-02) the scattering cross sections are calcualted using a perfect spin flipping ratio.

The table is a `pandas` DataFrame object, and all available package operations to filter, sort, or otherwise process data can be used, see e.g. https://pandas.pydata.org/ for further information. The data can be stored in a comma-separated file using the command `experiment.save_data(filename)`.

[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 -3.271433e+08 -3.263092e+08  45.073128  4.620611e+08
1  0.0 -3.292570e+08 -3.170050e+08  46.086098  4.570583e+08
2  0.0 -3.273659e+08 -3.066340e+08  46.872919  4.485453e+08
3  0.0 -3.265922e+08 -2.963847e+08  47.776034  4.410287e+08
4  0.0 -3.295693e+08 -2.868069e+08  48.968658  4.368914e+08

                                       sld_struct  sld_mag_U  \
0  (-0.13965257236825002+1.7404358470619397e-05j)         0j
1  (-0.08672643672130101+1.0808379451807207e-05j)         0j
2  (0.009292418715754033-1.1580781051537929e-06j)         0j
3    (0.10031097185087347-1.250136737922152e-05j)         0j
4   (0.15290192458086532-1.9055573851055002e-05j)         0j

                   sld_mag_V                  sld_mag_W        T1  ...   T5  \
0  (-0.23716990054796877+0j)  (0.23777608265786998+0j)  0.019503  ...  0.0
1  (-0.23700024886152948+0j)   (0.2461601274013195+0j)  0.007521  ...  0.0
2  (-0.23666399888524986+0j)  (0.25266518446900105+0j)  0.000086  ...  0.0
3  (-0.23605803162433248+0j)  (0.26011700088239487+0j)  0.010062  ...  0.0
4   (-0.2348985157264203+0j)   (0.2699214832484282+0j)  0.023379  ...  0.0

       I_pp      I_pm      I_mp      I_mm       I_m       I_p     I_sum  \
0  0.009628  0.056250  0.056250  0.142452  0.198702  0.065878  0.264580
1  0.025419  0.056169  0.056169  0.110813  0.166983  0.081588  0.248571
2  0.068622  0.056010  0.056010  0.059230  0.115240  0.124632  0.239872
3  0.129908  0.055723  0.055723  0.025538  0.081261  0.185632  0.266893
4  0.178780  0.055177  0.055177  0.013694  0.068871  0.233957  0.302828

      I_dif      asym
0 -0.132824 -0.502019
1 -0.085394 -0.343541
2  0.009391  0.039152
3  0.104370  0.391057
4  0.165086  0.545148

[5 rows x 23 columns]
```

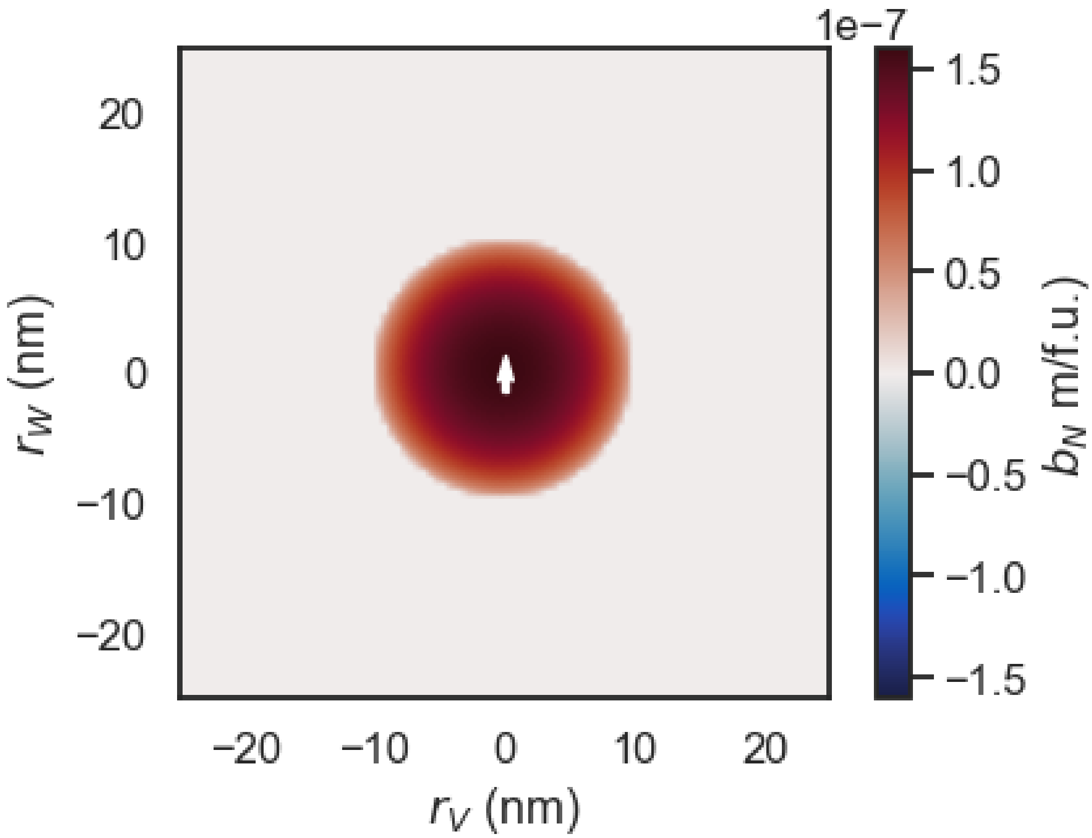
[4]:

```
""" Save calculated scattering data in a comma-separated file. """
# if no filename is given, an automatic one will be generated
experiment.save_data()
```

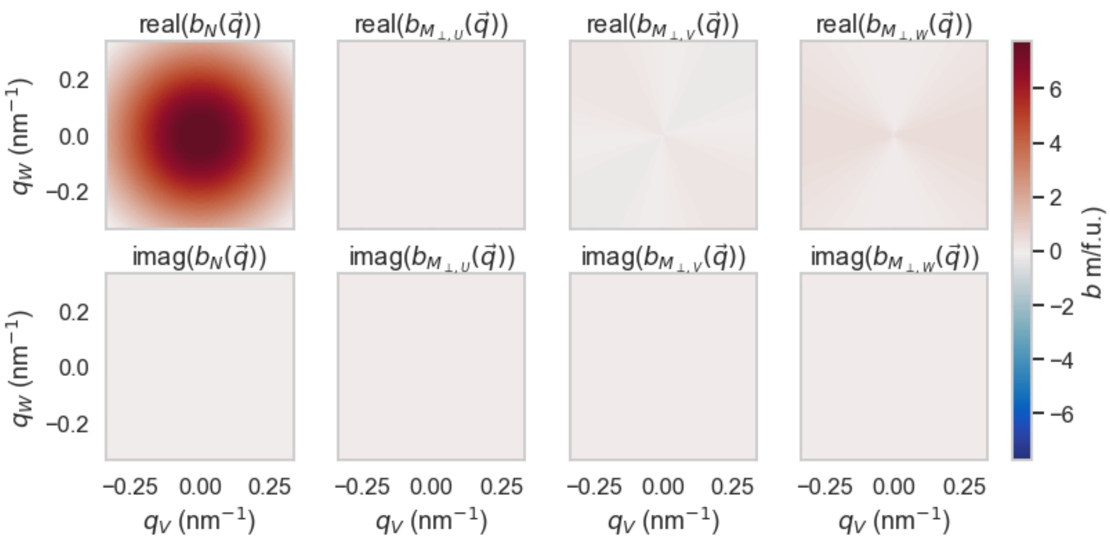
```
Data saved to mm2SANS_lamda0.6nm_det15m.dat
```

1.2 Plotting scattering lengths in real and reciprocal space

[5]:
```
"""
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)
```

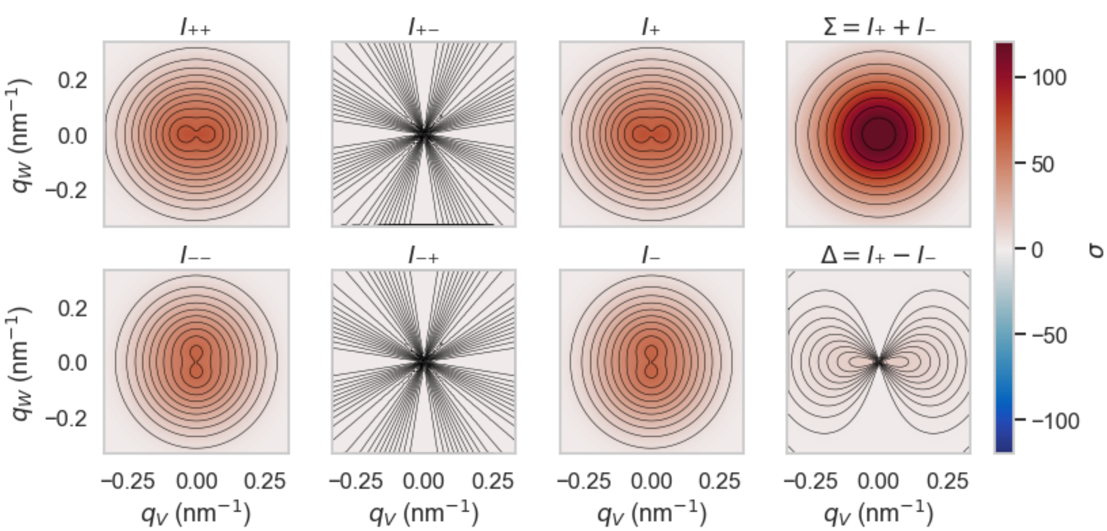


[6]:
```
""" plot structural and magnetic scattering length components in reciprocal␣
 ↪space """
experiment.plot_scattering_lengths()
```



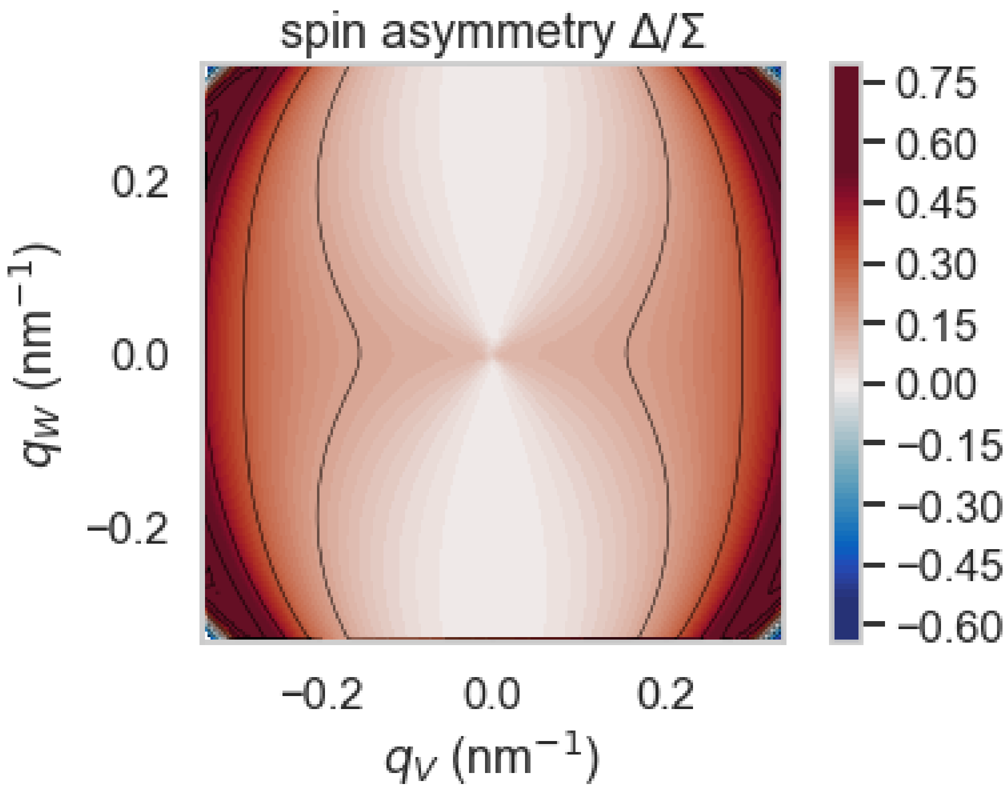
1.3 Plotting (polarisation-dependent) scattering cross sections

[7]:
```
""" plot all scattering cross sections """
# if halfpol=True only the right four plots are shown
experiment.plot_scattering_patterns(halfpol=False)
```



[8]:
```
"""
Plot a specific property from the data output only (see data columns given␣
↪above).

All terms to the scattering cross section are real-valued.
```

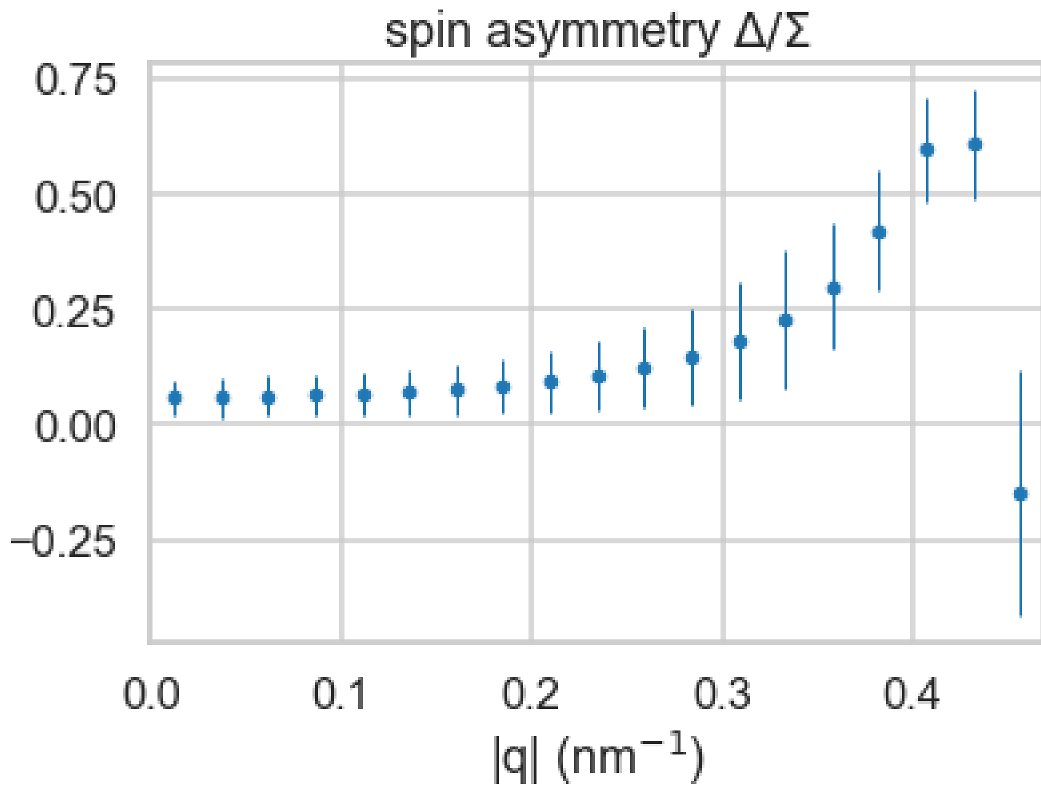
```
Imaginary terms of the scattering

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)
```



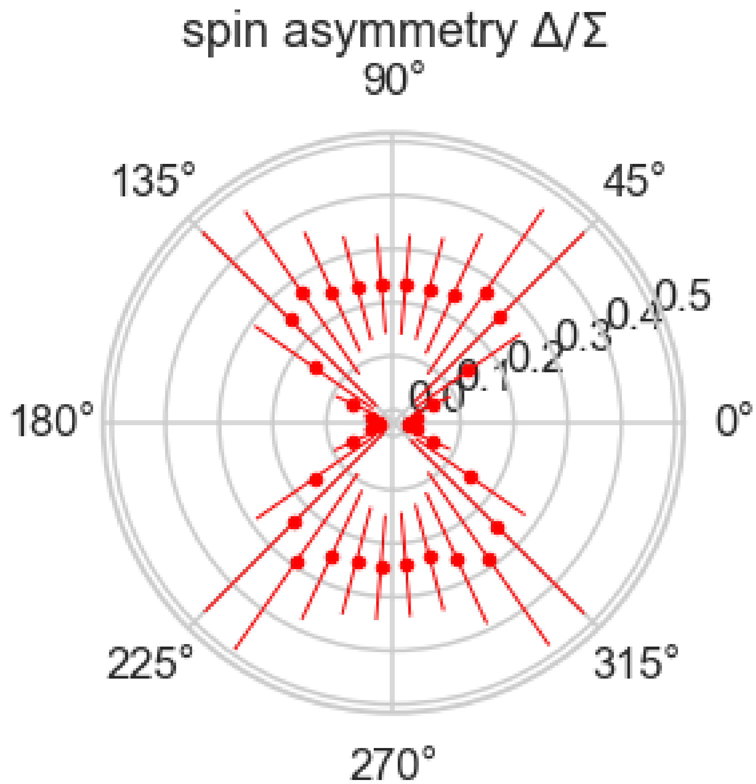
1.4 Plotting radial and angular averages

Functions are work in progress. Further options can be viewed using `experiment.command?`.

[9]:
```
experiment.plot_radial_average(column_name='asym')
```

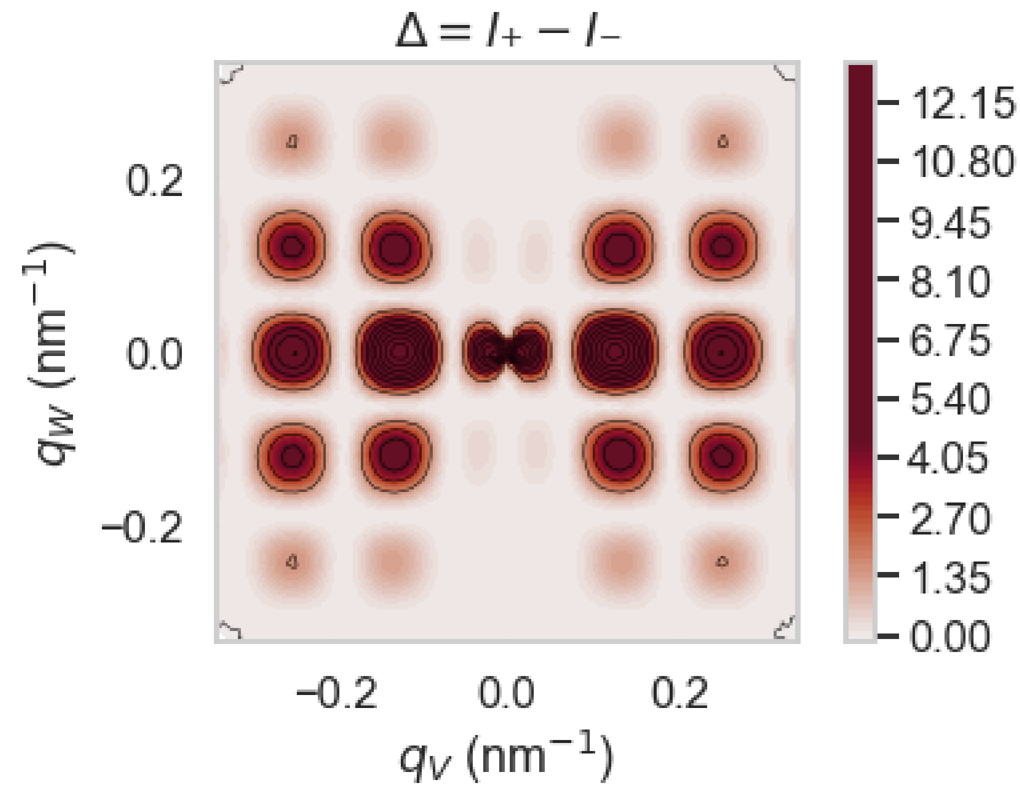


[10]:
```
experiment.plot_angular_average(column_name='asym')
```



1.5 Brute-force calculation of periodic repetitions

[11]:
```
""" (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_dif')
```



$\Delta = I_+ - I_-$
0.2
0.0
−0.2
q_W (nm^{-1})
−0.2
0.0
0.2
q_V (nm^{-1})
12.15
10.80
9.45
8.10
6.75
5.40
4.05
2.70
1.35
0.00

[ ]: