Physics with Neutrons I

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Exercise sheet 2 https://wiki.mlz-garching.de/n-lecture06:index

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Solutions

1. Useful Links

- neutron scattering lengths and cross sections for elements and isotopes:
  https://www.ncnr.nist.gov/resources/n-lengths/
- neutron activation, scattering and transmission calculator:
  https://www.ncnr.nist.gov/resources/activation/

2. Chopper

Time-of-flight instruments, such as TOFTOF at the FRM II and most instruments at spallation sources, often use ^{10}B-coated (neutron absorbing) chopper disks with small notches (transparent for neutrons), rotating very fast (comparable to aircraft engines). In pairs of two these choppers can be used to select a certain velocity (or energy or wavelength) from a white beam of neutrons. The first chopper cuts small bunches out of a continuous beam. This bunch spreads out due to the velocity distribution, until it reaches the second chopper where a small part with a fairly distinct speed is cut out.
What are possible problems and limitations with such devices? How could they be improved?

Solution

Let us first consider an exemplary chopper system consisting of two discs. Typical dimensions are a diameter $d \approx 0.5$m and a distance between discs of $l \approx 1$m. The windows are at the outer edges of the choppers and have an angular offset of $\phi \approx 90°$. If we want to select neutrons with a wavelength of $\lambda = 6$Åthis corresponds to a velocity of $v_n \approx 660$m/s. (see sheet 1 exercise 1). This results in a time of flight of these neutrons in the chopper system of:

$$t = l/v_n \approx 1.5\text{ms}$$

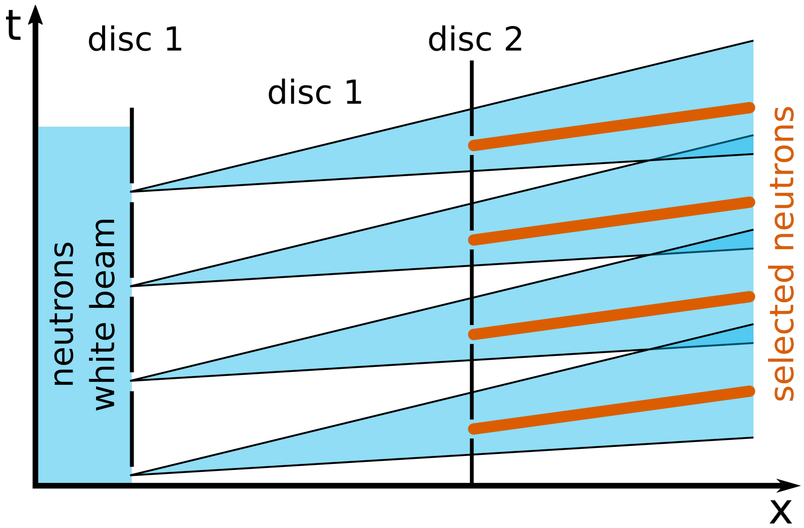
In this time the chopper hat to perform a 90°rotation which gives the frequency f:

$$f = \frac{\phi}{360° \cdot t} \approx 170\text{Hz} \approx 10000\text{rpm}$$

The diameter d has no influence on the chopper frequency f but has two main influences on the overall performance:

1. For larger disks, the neutron windows can be chosen larger while maintaining the same angular width. This is important, because the window size should be larger than the neutron beam so you can actually see the whole beam. if the window is smaller, the beam gets cropped and you will have a smaller beam (with fewer neutrons) wandering over your field of view.
2. The drawback of a large disc is the required structural durability. The choppers have to endure high centrifugal forces which limit in praxis the maximal diameter to $d \approx 1$m.

over the distance l between choppers, the pulses of neutrons will spread out due to their distribution of velocities. This means, that a specific wavelength can be selected more precisely if the l is large. However, at some point, spread out bunches from different pulses will start to overlap which has to be avoided. The image below shows a graphical representation of neutrons in a chopper system.



A further point which has to be considered with choppers is their neutron absorbing coating. As the absorption cross section is proportional to the neutron wavelength, a background of high energetic neutrons might pass through the choppers. This can be avoided or reduced by some measures (using a cold source, bent waveguides, neutron filters, etc.) but generally has to be accounted for in measurements.

An improved version of a chopper system are so called velocity selectors. Shown below is an example where between the front and end 'chopper discs' helical walls have been installed which are neutron absorbing. This means, that neutrons of the right velocity see a tunnel in the selector they can pass through, while slower or faster neutrons crash into the walls and are absorbed. The main advantage is, that the overlap of various neuron pulses from different windows do not have to be considered anymore and the windows can be placed very close to each other. In this way around 75% of the desired neutrons can pass the velocity selector.

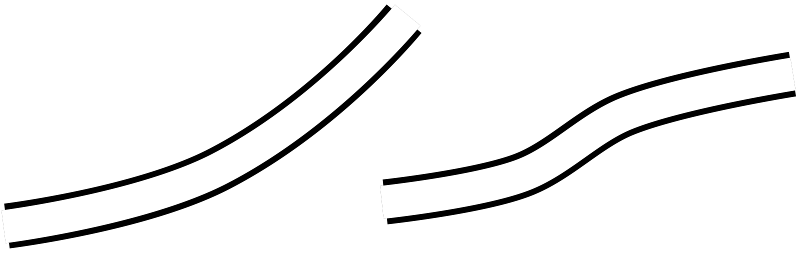
3. Neutron Optics

- Optical elements for neutrons are very limited, because the refractive index n for neutrons is typically very close to 1. Nickel is one of the elements with the largest $n - 1 = -1.58 \cdot 10^{-5}$ at a wavelength $\lambda = 4\text{Å}$. How should a thin focusing lens made of nickel with a focal length $f = 5\text{m}$ look like?

- Neutron guides are one of the few prevalent optical devices used with neutrons. In principle, they act like glass fibers for light, making use of total reflection at an interface. The most common type consists of rectangular glass tubes, which are evacuated and coated with a layer of nickel on the inside. What is the maximum angle under which neutrons with $\lambda = 4\text{Å}$ can pass such a guide?

- The refractive index depends on the neutron wavelength like $1 - n^2 \propto \lambda^2$. Which neutrons are best suited for the use of guides?

- Neutron guides are often curved in a c-shape or even s-shape. What is the advantage of using guides with a curvature? Is one of these shapes superior?



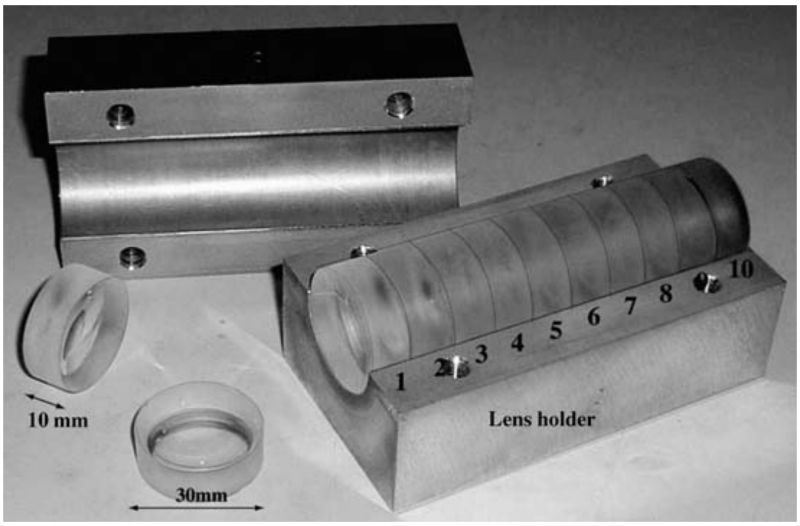
- Neutron guides can also be used as focusing devices. Suggest a shape to:
  - focus a parallel beam on a point-like sample?
  - focus a point like source on a point-like sample?

Solution

For nickel, the index of refraction n is smaller than 1, hence, for a focusing lens we need a biconcave shape instead of the biconvex shape for visible light. For the same radius of curvature r on both sides, the focal length of a thin lens is:

$$f = \frac{r}{2}\frac{1}{n-1}$$

This results in a radius of $r = 0.34$mm. As most neutron beams have a cross section of a few cm^2, such a lens can not be reasonably used in real experiments.
However, stacks of lenses could be used instead of single lenses. for an array of N lenses the total focal length is given by $F_{tot} = f/N$. This means, that for a given f_{tot} the radii of each single lens scales with N (with $N = 100$ lenses $r = 34mm$). At the SANS-J-2 beamline at JRR-3 in japan such a stack of lenses made from MgF_2 is employed with $N = 70$ and $r = 25$mm, which is showed in the image below.



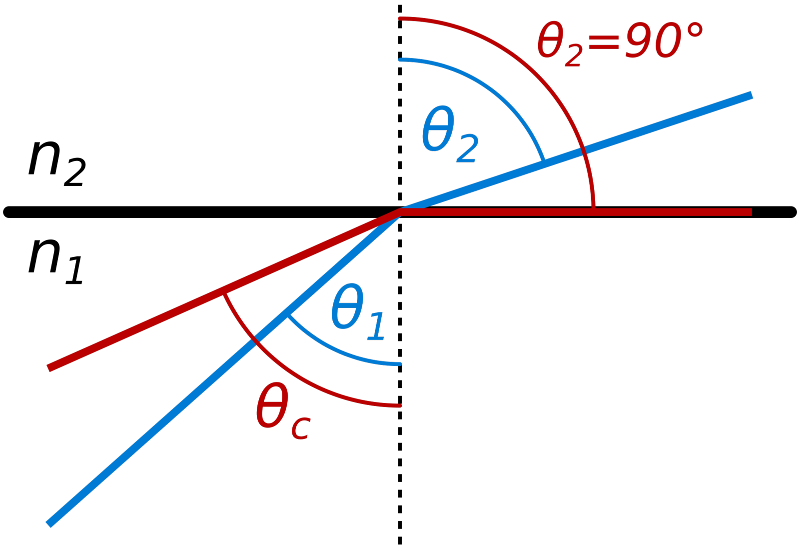
In a waveguide, neutrons are guided by total reflection, on an interface from an optically thicker region (vacuum, $n = 1$) to an optically thinner region (nickel, $n < 1$). The geometry is shown below. Refraction for neutrons follows Snell's law just like optics:

$$n_1 \cdot \sin\theta_1 = n_2 \cdot \sin\theta_2$$

The critical angle for total reflection θ_c can be calculated by setting $\theta_2 = 90°$:

$$\theta_c = \arcsin\frac{n_2}{n_1}$$

For the vacuum-nickel interface and a neutron wavelength $\lambda = 6$Åthis gives $\theta_c = 89.678°$(or 0.322°measured against the surface).



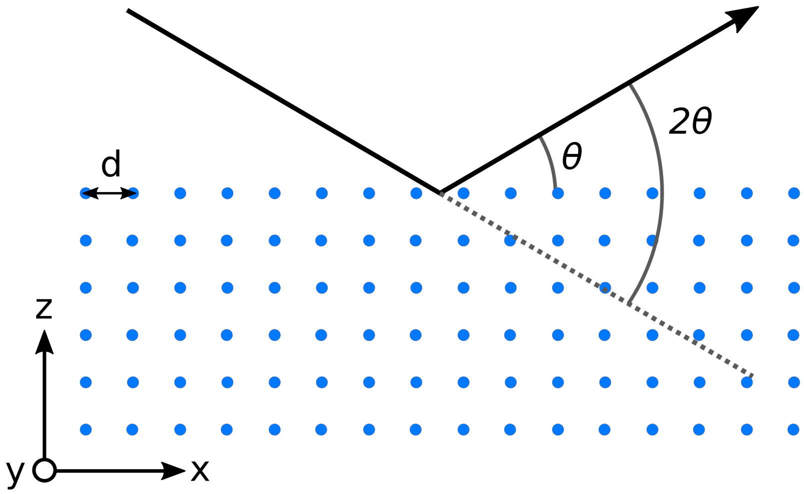
For larger wavelengths λ, the deviation of a materials refractive index from 1 becomes larger as well. Accordingly, the critical angle θ_c gets lower as well and more neutrons can be reflected. For this reason, at the FRM-II, all instruments using a waveguide look at the cold source and use neutrons with a large λ.

both curved neutron guide are used to filter fast neutrons and gamma radiation. In a straight guide, both can just pass through, but in curved guides, they have to be reflected at lest once which decreases the background drastically. The advantage of s-shaped over c-shaped guides is, that there is no possibility for unwanted particles to pass through by a series of reflections under very shallow angles at the outer wall. Additionally, a c-shaped guide distorts the beam profile (because it is curved only in one direction) while in an s-shaped guide the effect of both curvatures cancels each other.

In order to act as a focusing device, the neutron guide has to have a parabolic shape for a focus from parallel beam to point-like sample or an ellipsoidal shape for a focus from point-like source to point-like sample.

4. Bragg Scattering

Bragg Scattering (constructive interference from a periodic structure) is a very important process in neutron experiments, either to investigate unknown structures (crystal lattices) or to use known structures to select specific neutron wavelength (monochromator).



- Assume a cubic crystal lattice with lattice parameter d and neutrons with wavelength λ and derive Bragg's law (with n an integer number):

$$2 \cdot d \cdot \sin\left(\frac{2\theta}{2}\right) = n \cdot \lambda \tag{1}$$

- How does the scattering intensity depend on the number of atoms in x-, y- and z- direction?

- Numerically compute the angular dependence of the scattering intensity for neutrons with $\lambda = 1\text{Å}$, on a crystal with lattice parameter $d = 4\text{Å}$ and 1,10,100 and 1000 lattice planes in z-direction.

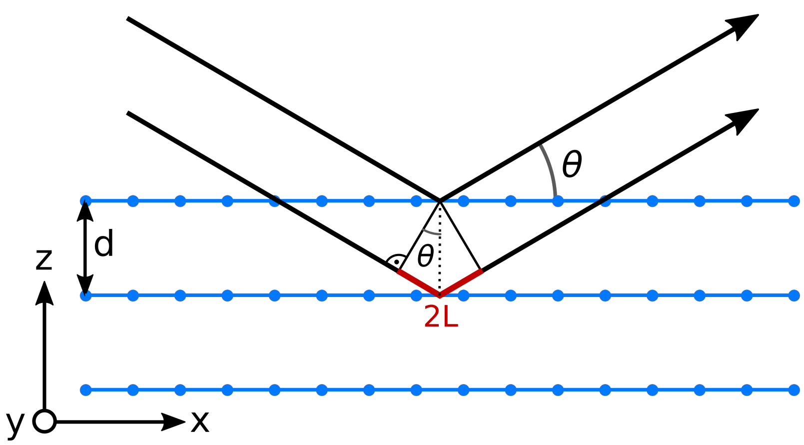
Solution

For Bragg scattering, one has to consider the difference of the optical path δ between scattered waves from two adjacent lattice planes. For maximum intensity in a certain direction θ the path difference must be equal to multiples of the wavelength:

$$n \cdot \lambda = \delta$$

Here, n is an integer. δ can be constructed geometrically, as shown in the image below where $\delta = 2L$, and L is the opposite side of a right triangular with d as the hypotenuse and angle θ. Using trigonometric functions the Bragg equation can be formulated:

$$n \cdot \lambda \delta = 2 \cdot L = 2 \cdot d \cdot \sin\theta$$



Generally, the amount of scattering centers in any direction increases the intensity of Bragg scattering. In addition, the amount of scattering planes in z-direction enhances the sharpness of Bragg beaks. The next part of the exercise illustrates how the overall angular dependence of scattering with increasing crystal planes changes.

In order to compute the scattering intensity under arbitrary angles θ one needs to add up the amplitudes of all scattered waves contributing to the signal and take into account the phase shift ϕ between adjacent scattering planes. ϕ can be easily calculated from the additional optical path δ by relating it to the wavelength λ:

$$\phi = \frac{2 \cdot \pi}{\lambda} \delta$$

In general, the intensity I of a plane wave is given by the square of its amplitude.

$$I = A^2 \propto (\exp(i(...)))^2 \propto \begin{pmatrix} \cos(...) \\ \sin(...) \end{pmatrix}^2$$

We use here, that the waves scattered in a certain direction look like plane waves (even though the scattering process itself is assumed to be spherically symmetric) which is represented by the imaginary exponential function. For computational reasons, however, we represent the wave by its vector representation of the real and imaginary part. The argument of the functions is just indicated by dots ... because for us only the phase shift ϕ between waves is important. The Intensity of N scattered waves is now given through the sum of their amplitudes:

$$I_{tot} = (A_0 + A_1 + ... + A_{N-1})^2 = \begin{pmatrix} \cos(0 \cdot \phi) + \cos(1 \cdot \phi) + ... + \cos((N-1) \cdot \phi) \\ \sin(0 \cdot \phi) + sin(1 \cdot \phi) + ... + sin((N-1) \cdot \phi) \end{pmatrix}^2$$

Where $\phi(\theta)$ is Angular dependent. In experiment, the angular dependence is often displayed in terms ot the momentaum transfer Q:

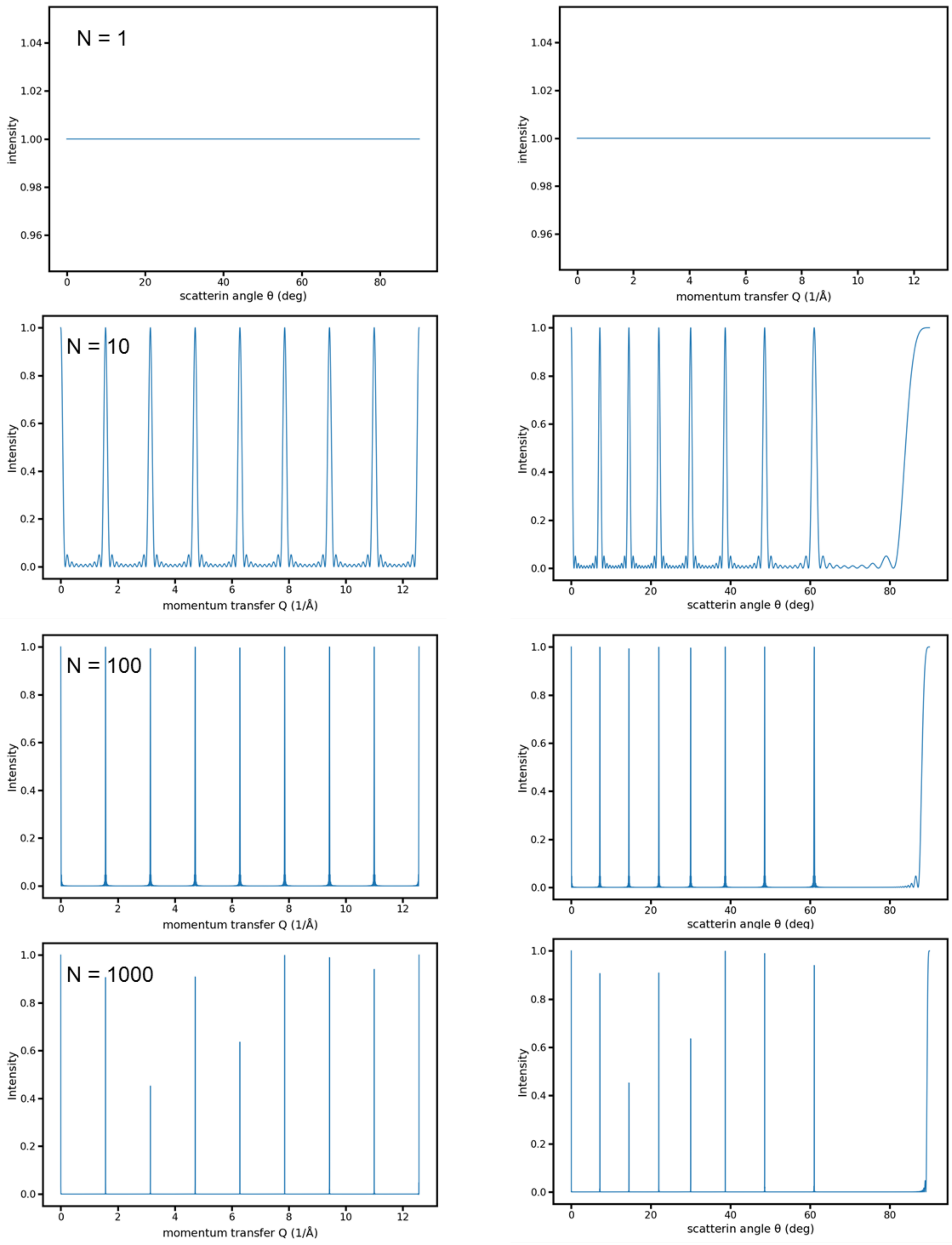
$$Q = \frac{4\pi}{\lambda} \sin(\theta)$$

Shown below are the resulting images and exemplary code for the computation written in **Python 2.7**.

For only one scattering plane, the Intensity is equal in each direction, representing the spherical symmetry of the process. For increasing number of planes, the Bragg peaks stay at the same position, but get better defined in terms of θ or Q. In between the peaks, some intensity pattern can be seen for low N, which vanishes however, with increasing planes. The different hight of Bragg peaks for $N = 1000$ is just an artifact due to sampling in the image, all peaks have the same maximum intensity.

```
#Bragg scattering computation

import numpy as np
import matplotlib as mlp
import matplotlib.pyplot as plt

# this is just my personal way for predifining plots
mlp.rcParams['axes.linewidth'] = 3
mlp.rcParams['xtick.major.width'] = 3
mlp.rcParams['xtick.major.size'] = 8
mlp.rcParams['ytick.major.width'] = 3
mlp.rcParams['ytick.major.size'] = 8
```

```
mlp.rcParams[’mathtext.default’] = ’regular’
mlp.rcParams[’lines.markersize’] = 8
mlp.rcParams[’lines.markeredgewidth’] = 1.5
mlp.rcParams[’axes.titlesize’] = 18
mlp.rcParams[’axes.labelsize’] = 18
mlp.rcParams[’legend.fontsize’] = 14
mlp.rcParams[’xtick.labelsize’] = 16
mlp.rcParams[’ytick.labelsize’] = 16

d = 4. # lattice plane distance in Angstrom
Wl = 1. # neutron wavelength in Angsrom

Theta = np.linspace(0,90,10001) # scatterin angle in degrees
Q = 4*np.pi*np.sin(np.pi*Theta/180.)/Wl # momentum transfer in 1/Angstrom
phi = 2*np.pi*2*d*np.sin(np.pi*Theta/180.)/Wl # phaseshift between adjacent planes

N = 10 # number of scattering planes

# initialise the scattered wave amplitude
x = 0 # real part of the amplitude
y = 0 # imaginary part of the amplitude

# add up all contributing waves
for n in range(N):
x += np.cos(n*phi)
y += np.sin(n*phi)

# calculation of the intensity
# I have normalized the intensity with N so that all images have the same scale
I = (x**2 + y**2)/N

# graphical visualization
name = ’Bragg Scattering - 1’
plt.figure(name, figsize=(10, 7), dpi=120)
fig = plt.gcf()
fig.set_tight_layout(True)
plt.plot(Theta,I)
plt.xlabel(r’scattering angle θ (deg)’)
plt.ylabel(’intensity I’)

name = ’Bragg Scattering - 2’

plt.figure(name, figsize=(10, 7), dpi=120)
fig = plt.gcf()
fig.set_tight_layout(True)
plt.plot(Q,I)
plt.xlabel(’momentum transfer Q (1/Å)’)
plt.ylabel(’intensity I’)
```


N = 1
intensity
1.04
1.02
1.00
0.98
0.96
0
20
40
60
80
scatterin angle θ (deg)
intensity
1.04
1.02
1.00
0.98
0.96
0
2
4
6
8
10
12
momentum transfer Q (1/Å)
N = 10
Intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
12
momentum transfer Q (1/Å)
Intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
scatterin angle θ (deg)
N = 100
Intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
12
momentum transfer Q (1/Å)
Intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
20
40
60
80
scatterin angle θ (deg)
N = 1000
Intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
12
momentum transfer Q (1/Å)
Intensity
1.0
0.8
0.6
0.4
0.2
0.0
0
20
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60
80
scatterin angle θ (deg)