Exercise set 2: Elastic scattering

Exercise 1

- Fultz & Howe problem 4.3

Exercise 2a

This exercise is divided into several part, where we will try to build a code together to simulate simple kinematical diffraction from clusters of atoms. The goal is to use the expression for the structure factor

$$I = |F(\Delta\mathbf{k})|^2 = |\sum_{j=0}^{N} \mathrm{f}_j e^{-2\pi i \Delta\mathbf{k}\cdot\mathbf{R}_j}|^2 \tag{1}$$

to write a simple Matlab script calculating the intensities of wavelets scattered from many atoms over a range of scattering vectors.

The script should take as input a list of atoms on the form

```
Z_1 x_1 y_1 z_1
Z_2 x_2 y_2 z_2
```

⋮

```
Z_n x_n y_n z_n
```

where x,y,z are the fractional coordinates of an atom, and Z is the atomic number. We can use VESTA to build a model of the system we are interested in, and to export such a list. It will need some minor manual editing.

We will make some assumptions that will simplify things a bit:

- We assume that the scattering strength of an atom is equal to its atomic number, and that it is independent of scattering angle.
- For simplicity, we will calculate only one plane in reciprocal space at a time, for example the h-k plane. However, it should be possible to specify the l value we wish to use.

Your task is to start writing snippets of code that we later can try to sew together to make a working code.

Exercise 2b

Make a working code based on 2a and use the script to simulate and plot diffraction from various size clusters of fcc Copper. For example a cluster of one unit cell and for 2x2x2, 3x3x3, and 5x5x5 unit cells. Try also with clusters that have different kinds of shapes, for example ones that are oblong. Discuss.