

your name(s) \_\_\_\_\_

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*Physics 851 Exercise #12 - Monday, Nov. 29*

Consider neutron scattering off a polonium target. Polonium is the only metal with a simple cubic structure. The distance between atoms is  $3.35 \text{ \AA}$ . The neutron scatters off the strong charge in the nucleus, with a cross section for a single nucleus being

$$\frac{d\sigma}{d\Omega} = \alpha.$$

The deBroglie wavelength,  $\lambda = 2\pi/p$ , of the incident neutrons is  $1.2 \text{ \AA}$  and the crystal is perfectly lined up along the  $xyz$  axes.

1. What is the energy of the neutrons in the beam?
2. Calculate the structure function,  $S(\vec{q}) = (d\sigma/d\Omega)/\alpha$ , as a function of the scattering angles  $\theta$  and  $\phi$ . Express your answer as a sum over lattice displacements  $\delta\vec{a}$ . Write the sum as a product of three one-dimensional sums, rather than as a single sum over three indices. Use symmetries to replace complex phase factors with sines and cosines.
3. If the momentum transfers  $\vec{q}$  are not perfectly measured, terms in the sums such as  $\cos(\vec{q} \cdot \vec{a})$  are altered,

$$\cos(\vec{q} \cdot \vec{a}) \rightarrow \cos(\vec{q} \cdot \vec{a})e^{-a^2\sigma_q^2/2},$$

where  $\sigma_q$  is a measure of the experimental resolution, and would become zero for perfect resolution. Write a program to perform the sum above, including the correction for finite resolution and assume  $\sigma_q = 0.25 \text{ \AA}^{-1}$ .

4. Display your result as a density plot vs. the scattering angles  $\theta$  and  $\phi$  in radial coordinates, where the polar angle  $\theta$  is the radial coordinate. If you bin the scattering angles into 2-degree bins (90 bins for  $\theta$  and 180 bins for  $\phi$ ) it should be sufficient.
5. What happens in the limit that the resolution  $\sigma_q \rightarrow 0$ .

Useful information: The momentum transfer,  $\vec{q} = \vec{k}_i - \vec{k}_f$ , in terms of scattering angles:

$$q = 2k \sin(\theta/2), \quad q_z = k(1 - \cos \theta), \quad q_x = -k \sin \theta \cos \phi, \quad q_y = -k \sin \theta \sin \phi.$$

Lattice sites separated by more than 20 cells can be neglected with this value of  $\sigma_q$ .