your name(s)____

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Physics 851 Exercise #12

Consider neutron scattering off a polonium target. Polonium is the only metal with a simple cubic structure. The distance between atoms is 3.35 Å. 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 Åand 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 θ and ϕ. 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 σ_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 $\sigma_q = 0.25$ Å^{-1}.
4. Display your result as a density plot vs. the scattering angles θ and ϕ in radial coordinates, where the polar angle θ is the radial coordinate. If you bin the scattering angles into 2-degree bins (90 bins for θ and 180 bins for ϕ) 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:

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

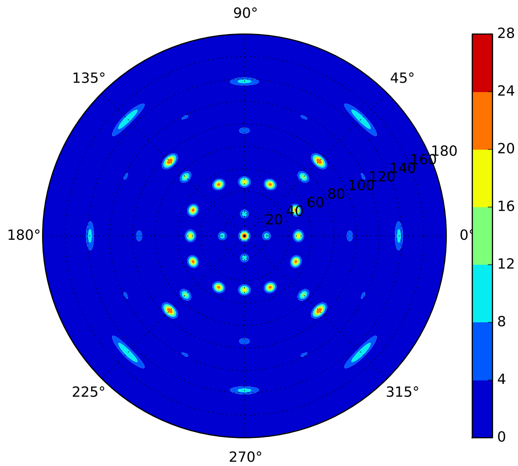
Lattice sites separated by more than 20 cells can be neglected with this value of σ_q.

Solutions:
1. $\lambda = 0.12$ nm, $pc = 2\pi\hbar c/\lambda = 10311$ eV. Use $\hbar c = 197.327$ eV nm. $E = (pc)^2/2mc^2 = 0.0568$ eV. Use $mc^2 = 939.6\times 10^6$ eV.

2.

$$\begin{aligned}
S(\vec{q}) &= s_x s_y s_z,\\
s_x &= 1 + 2\sum_{n\geq 1}\cos q_x x,\\
s_y &= 1 + 2\sum_{n\geq 1}\cos q_y y,\\
s_z &= 1 + 2\sum_{n\geq 1}\cos q_z z.
\end{aligned}$$

3. See next page



4.

5. peaks become infinitely narrow and sharp

```
import matplotlib.pyplot as plt
from matplotlib.lines import Line2D
import numpy as np
import os
from pylab import *
from matplotlib import ticker
from matplotlib.ticker import ScalarFormatter
import matplotlib.cm as cm
pi=np.pi
na=20
da=3.35
lambdan=1.2
p=2.0*pi/lambdan
sigmaq=0.25
sigmaq2=sigmaq*sigmaq
ntheta=90
nphi=180
theta=arange(0,ntheta+1)
theta=theta*pi/ntheta
phi=arange(0,nphi+1)
phi=phi*2.0*pi/nphi
FormFactor=np.ndarray(shape=(ntheta+1,nphi+1),dtype=float)
p=2.0*pi/lambdan
for itheta in range(0,ntheta+1):
  ctheta=cos(theta[itheta])
  stheta=sqrt(abs(1.0-ctheta*ctheta))
  qz=p*(1.0-ctheta)
  for iphi in range(0,nphi+1):
    qx=-p*stheta*cos(phi[iphi])
    qy=-p*stheta*sin(phi[iphi])
    qmag=sqrt(qx*qx+qy*qy+qz*qz)
    sx=0.0
    #for iax in range(-na,na+1):
    for iax in range(0,na+1):
      ax=iax*da
      dx=1
      if iax>0:
        dx=2
      sx+=dx*np.cos(qx*ax)*exp(-0.5*sigmaq2*ax*ax)
    sy=0.0
    for iay in range(0,na+1):
      ay=iay*da
      dy=1
      if iay>0:
        dy=2
      sy+=dy*np.cos(qy*ay)*exp(-0.5*sigmaq2*ay*ay)
    sz=0.0
    #for iaz in range(-na,na+1):
    for iaz in range(0,na+1):
      az=iaz*da
      dz=1
      if iaz>0:
        dz=2
      sz=sz+dz*np.cos(qz*az)*exp(-0.5*sigmaq2*az*az)
    FormFactor[itheta][iphi]=sx*sy*sz
```

```
fig,ax = plt.subplots(subplot_kw=dict(projection='polar'))
cax = ax.contourf(phi, 180*theta/pi, FormFactor, cmap=cm.jet)
plt.colorbar(cax)
plt.savefig('polonium.pdf',format='pdf')
#os.system('open -a Preview polonium.pdf')
plt.show()
quit()
```