

ASSIGNMENT:SOLID STATE PHYSICS

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1 Theory

The Atomic Form Factor, or Atomic Scattering Factor, is a measure of the scattering amplitude of a wave by an isolated atom. The atomic form factor depends on the type of scattering, which in turn depends on the nature of the incident radiation, typically X-ray, electron or neutron. More precisely, here we consider that the incident radiation is scattered by a continuous distribution of "electron density" associated with each lattice point. This concept is in full accord with a wave-mechanical view of the process. It should be noted, however, that we are neglecting the scattering effect of the atomic nuclei, which interact much less strongly with the incident radiations like X-Rays. From the literature we have:

$$f(\mu) = \int_0^\infty 4\pi r^2 \frac{\sin(\mu r)}{(\mu r)} dr; \mu = \frac{4\pi}{\lambda} \sin\theta.$$

where this quantity which represents the ratio of the amplitude scattered by the whole atom to that scattered by a point electron on the lattice point is called the atomic scattering factor. As $\theta \rightarrow 0$, $\mu \rightarrow 0$ and $\frac{\sin(\mu r)}{(\mu r)} \rightarrow 1$ and hence

$$\lim_{\mu \rightarrow 0} = \int_0^\infty 4\pi r^2 \rho(r) = Z$$

The values of $\rho(r)$ must be obtained by evaluating, quantum mechanically, the "wave functions" of the atoms in the crystal.

Consider an electron in the ground state of a hydrogen atom. Since the electron could be found at any location where the probability density has an appreciable value, the charge it carries would not be confined to a particular location. Thus, when speaking of average properties of the electron in the atom, it is appropriate to speak of its charge distribution, which is proportional to its probability density. Since the probability density is independent of time in the ground state, so is the charge distribution. For the hydrogen atom in its lowest energy state the wave function is given by

$$\psi(r) = \frac{e^{-r/a_0}}{a_0^{3/2} \sqrt{\pi}}$$

where a_0 is the radius of the first Bohr orbit. The electron density of such an atom is given as $\rho(r) = \psi^* \psi = \frac{e^{-2r/a_0}}{\pi a_0^3}$

2 Coding

I used scilab to write a program for evaluating the integral for atomic scattering factor by using Gauss-Laguerre quadrature rule.

2.1 program code for calculating Atomic Structure Factor for the hydrogen atom in ground state.

```

clear;clc;close
function yy=gauss_laguerre(func,extra_parameters)//(lower,upper,func)
ret2=fscanfMat("60_pt_lag.dat");//reading data file storing nodes and weights
node=ret2(:,1);weight=ret2(:,2);
[lhs,rhs]=argn(0)
if rhs==1 then
    for i=1:size(weight,"r")
        func_at_nodes(i)=func(node(i))*exp(+node(i))
    end
elseif rhs==2 then
    for i=1:size(weight,"r")
        func_at_nodes(i)=func(node(i),extra_parameters)*exp(+node(i))
    end
end
yy=sum(weight.*func_at_nodes)
endfunction
//
function answer=integrand_asf(rval,muval)
a0=0.529177
if muval~=0 || rval~=0 then
    answer=(4*pi*rval**2)*(sin(4*pi*muval*rval)/(4*pi*muval*rval))*(exp((-2*rval/a0))/(pi*a0**3))
elseif muval==0 || rval==0 then
    answer=(4*pi*rval**2)*(exp((-2*rval/a0)/(pi*a0**3)))
end
endfunction
function gsf=geo_sf(frac_pos_mat,asf,hval,kval,lval)
sumis=0
for i=1:size(frac_pos_mat,"r")//number of rows would rep the no. of atoms in that crystal structure
    sumis=sumis+exp(i*(2*pi)*(hval*frac_pos_mat(i,1)+kval*frac_pos_mat(i,2)+lval*frac_pos_mat(i,3)))
end
gsf=asf*sumis
endfunction
//main program
theta=linspace(0.00000001,pi*3,1000)
lambda=1//1 angstrom
//mu=linspace(0,1)
for i=1:size(theta,"c")
    mu=(sin(theta(i)))/lambda
    myans(i,1)=mu/(sin(theta)/lambda)
    myans(i,2)=gauss_laguerre(integrand_asf,mu)
end
plot(abs(myans(:,1)),myans(:,2),"*b")
xgrid(4,0,1);
xlabel("$sin(\theta)/(\lambda)$","fontsize",4)
ylabel("$f(\mu)$","fontsize",4)
title("Atomic scattering factor for hydrogen plotted against sin(theta)/(lambda)","fontsize",4)
expt_data=fscanfMat("data_iucr_hydrogen_atom.dat")
plot(expt_data(:,1),expt_data(:,2),"-r")
legend("computationally","IUCR international table for crystallography analytical data")

```

2.2 Plot of the Result

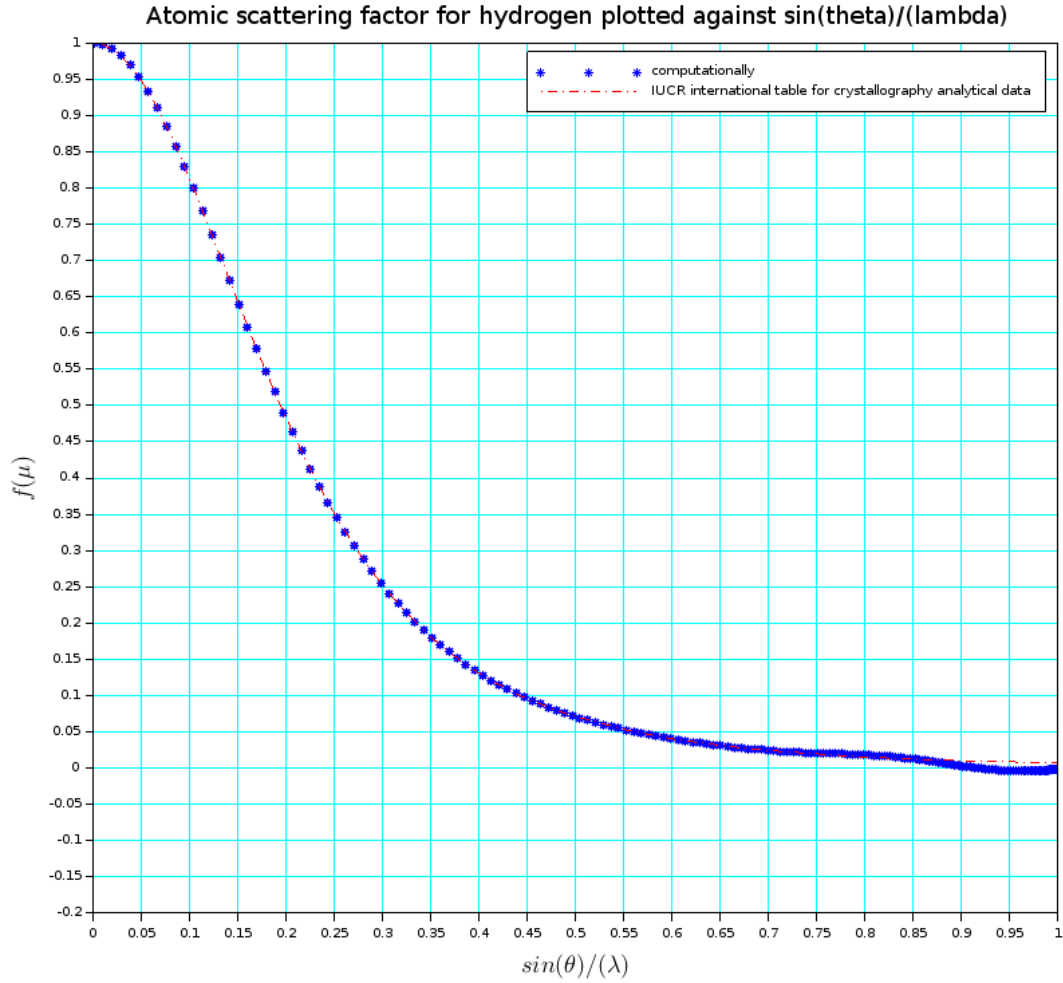


Figure 1: Atomic scattering factor the hydrogen in its ground state

3 Geometric structure factor

If we wish to predict the characteristics of radiation diffracted from crystals having complex unit cells containing more than one atom, such as the cubic cells for the b.c.c. and f.c.c. structures, we must account for the interaction of beams which are diffracted by the various atoms within the unit cell. If, for the $(h'k'l')$ reflection, we denote the ratio of the amplitude of the radiation scattered by the entire unit cell to that

scattered by a point electron at the origin by $F(h'k'l')$, then

$$F(h'k'l') = \sum_i f_i e^{2\pi i(h'x_i + k'l_i + l'z_i)}$$

where sum is taken over all the atoms in the unit cell and x_i, y_i, z_i represent the fractional positional coordinates of the i th atom.

The intensity of the diffracted beam is proportional to the square of the amplitude F , or, more accurately, since F is complex, to the square of the absolute value of F , which is F^*F , where F^* is the complex conjugate of F .

3.1 Code to evaluate the geometric structure factor.

```
function gsf=geo_sf(frac_pos_mat,asf,hval,kval,lval)
sumis=0
for i=1:size(frac_pos_mat,"r")//number of rows would rep the no. of atoms in that crystal structure
    sumis=sumis+exp(i*(2*pi)*(hval*frac_pos_mat(i,1)+kval*frac_pos_mat(i,2)+lval*frac_pos_mat(i,3)))
end
gsf=asf*sumis
endfunction
//
function storing=am_cal(thetaval,asf_corr_theta,frac_pos_within_ucell)
hvalue=[0,1,2,3,4];kvalue=[0,1,2,3,4];lvalue=[0,1,2,3,4]
value_intensity=0
index_st=0
for h=1:size(hvalue,"c")
    for k=1:size(kvalue,"c")
        for l=1:size(lvalue,"c")
            index_st=index_st+1
            //for i=1:size(frac_pos_within_ucell,"r")//size(kvalue,"c")
            value_intensity=value_intensity+abs(geo_sf(frac_pos_within_ucell,asf_corr_theta,hvalue(h)
            ,kvalue(k),lvalue(l)))*2;//abs(geo_sf(frac_pos_within_ucell,asf_corr_theta(5,1),hvalue(h)
            ,kvalue(k),lvalue(l)))*2;//abs(geo_sf(frac_pos_within_ucell,asf_corr_theta(j,1),hvalue(h)
            ,kvalue(k),lvalue(l)))*2;
            storing(index_st,:)=hvalue(h),kvalue(k),lvalue(l),value_intensity]
            //end
        end
    end
end
//end
endfunction
```

REFERENCES:

1.SOLID STATE AND SEMICONDUCTOR PHYSICS::JOHN PHILIP MCKELVEY