# **Outline of X-Ray Scattering**

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### X-ray sources

### X-ray Tubes<sup>1</sup>



The figure above shows a schematic of an x-ray tube. Electrons are accelerated from a large negative potential, through vacuum, onto a metal anode. Only a small fraction of the energy turns into x-rays and consequently the anode must be water cooled to remove the heat. When a high energy electron impinges on atoms in a metal there are two chief mechanisms by which x-rays are generated. A continuous spectrum of x-rays is generated by Brehmsstrahlung, which results from the acceleration of the electrons when they pass close to the atomic nuclei. The Brehmsstrahlung spectrum begins at close to zero energy and goes up to a maximum energy limited by the energy of the incident electron (corresponding to a single acceleration event, where the electron loses all its energy to a single photon). The other mechanism of electron energy loss is the production of characteristic x-rays which occurs when an electron knocks out an inner 1s electron (K shell) from an atom. When a higher quantum state electron falls down to fill the hole, an x-ray is emitted whose energy is given by the difference of the two atomic levels. The most common electron to fill the hole is the 2p electron (resulting in a  $k_{\alpha}$  x-ray) although there is also a fairly high probability for 3p electrons to fall into the hole as well (resulting in a  $k_{\beta}$  x-ray). The energy of this process can be modeled surprisingly well using the energy level formula from the Bohr model, with a slight modification to account for the presence of the remaining 1s electron:

(1) 
$$E_{k\alpha} = \frac{hc}{\lambda} = E_{2p} - E_{1s} \approx hcR_y \left(1 - \frac{1}{4}\right) \left(Z - 1\right)^2$$

Here Z is the atomic number and  $R_y$  is the Rydberg constant given by

(2) 
$$hcR_{y} = \frac{m_{e}e^{4}}{32\pi^{2}\varepsilon_{0}^{2}\hbar^{2}} \approx 13.6eV$$

The factor of  $Z^2$  from the Bohr formula is reduced to  $(Z-1)^2$  as an approximation of the shielding of the nucleus due to the other 1s electron. Electron-electron interactions can

<sup>&</sup>lt;sup>1</sup> Parts of this section are based on lectures given by Professor Peter Pershan at Harvard University in 1988.

only be partially represented by this shielding approximation, and to some extent the success of this formula is fortuitous. For example a similar formula to describe the energies of the  $k_{\beta}$  x-rays is not available. A handy source for tabulated x-ray energies is given in the "X-ray Data Booklet", which can be found on the web at <u>http://xdb.lbl.gov</u>.

The  $k_{\alpha}$  x-ray line is split into two lines by spin-orbit coupling. These lines are called (somewhat unimaginatively)  $k_{\alpha l}$  and  $k_{\alpha 2}$ . For Cu the magnitude of this splitting is 20 eV, which is quite small compared to the 8 keV energy of the k-alpha x-ray. It is possible to make an estimate of the  $k_{\alpha l}$  -  $k_{\alpha 2}$  spliting from the quantum formula for the energy level of an orbital in the presence of spin-orbit coupling. The formula below gives the energy shift to an orbital due to spin orbit coupling, it is derived in chapter 17 of Gasiorowicz [1];

(3) 
$$\Delta E \approx \frac{1}{2} m_e c^2 \Big[ (Z - 2) \alpha \Big]^4 \frac{1}{n^3} \bigg( \frac{1}{j + 1/2} - \frac{3}{4n} \bigg)$$

Here  $\alpha$  is the fine structure constant, *n* is the principle quantum number of the electron orbit and *j* is the total angular momentum.

We now consider the factor which determines how many x-ray will be emitted by an xray tube. This calculation is also of relevance to understanding the energy loss of any charged particle and is also of relevance in understanding electron microscopy, particle detection, and radiation damage. Most of the energy lost by a high energy electron does not go to create x-rays. Rather, the energy loss is primarily due to ionization of valence electrons, while the production of x-rays is mostly an incidental effect.

The energy transferred from a high energy electron to the valence electrons of a nearby atom can be estimated using the impulse approximation.

In this approximation neither the incident nor the scattered electron is assumed to move during the time of the interaction. We take the distance between the two electrons at closest approach to be *b*, called the impact parameter. The time of interaction is then approximately  $\Delta T = b/v$  where *v* is the velocity. This gives the momentum transferred to each electron via the total impulse

(4) 
$$\Delta P = F \Delta T = \frac{e^2}{4\pi\varepsilon_0 b^2} \frac{b}{v} = \frac{mc^2 r_0}{bv}$$

Here we use the classical electron radius  $r_0 \equiv e^2 / 4\pi \varepsilon_0 m_e c^2 \approx 2.82 \times 10^{-15} m$ . A more exact calculation differs by a factor of two from this result (See Homework Problem 4)

(5) 
$$\Delta P = \int F_{\perp} dT = \int F_{\perp} \frac{dx}{v} = \frac{2mc^2 r_0}{bv}$$

Using the latter result, the energy lost to the Z electrons in the atom is given by

(6) 
$$\Delta E \approx \frac{-Z\Delta P^2}{2m} = \frac{-Zm^2c^4r_0}{Eb^2}$$

To calculate the total amount of radiation by an electron we need to calculate the average of the radiation over collisions with all the atoms in the material occuring at various impact parameters.



#### Figure 2

Take the density of atoms to be  $\rho_N$ . The energy lost per unit length of the electron's path is given by

a(7) 
$$\frac{dE}{dx} = 2\pi \int_{b_{\min}}^{b_{\max}} \rho_N \Delta E_{Ionization} b db = \frac{-2\pi \rho_N Z r_0^2 m^2 c^4}{E} \ln\left(\frac{b_{\max}}{b_{\min}}\right)$$

Now consider the energy loss to Brehmsstrahlung. For details see Segre[2]. The method is to calculate the acceleration induced by the electric force on the electron when it passes close to an atomic nucleus. From the acceleration we can then estimate the power radiated. To simplest approximation we can assume that the change in the trajectory of the electron is negligible. Denote the distance of closest approach of the electron to the nucleus by the impact parameter *b*. The maximum acceleration is

Figure 3

(8) 
$$a_{\max} = \frac{F}{m_e} = \frac{Ze^2}{4\pi\varepsilon_0 b^2 m_e} = \frac{Zc^2}{b^2} \frac{e^2}{4\pi\varepsilon_0 m_e c^2} = \frac{Zr_0 c^2}{b^2}.$$

The Larmor formula gives the peak radiated power

(9) 
$$P_{rad} = \frac{2}{3} \frac{r_0 ma^2}{c} = \frac{2}{3} \frac{r_0^3 Z^2 mc^3}{b^4}$$

A crude estimation of the total power radiated can be made by multiplying the peak power, by the total time over which the electron is close to the nucleus  $\Delta T = b/v$ , with v the velocity of the electron. This gives

(10) 
$$\Delta E = P_{rad} \Delta T = \frac{2}{3} \frac{r_0^3 Z^2 mc^3}{b^3 v}.$$

The radiation will be emitted over a range of frequencies. The simplest approximation is a uniform distribution of power per unit frequency from v = 0 up to  $v = 1/\Delta T$ . This quantity is called the spectral density of radiation. To obtain this we divide eq. (10) by  $\Delta v = 1/\Delta T = v/b$  yeilding:

(11) 
$$\frac{dE_{brem}}{dv} = \frac{2}{3} \frac{r_0^3 Z^2 mc^3}{b^2 v^2} = \frac{1}{3} \frac{r_0^3 Z^2 m^2 c^3}{Eb^2}.$$

Here I have used  $E = mv^2/2$ . To obtain the total radiated energy per unit length per unity frequency interval we use the same procedure as before to obtain

(12) 
$$\frac{d^2 E_{brem}(v)}{dv dx} = 2\pi \int_{b_{\min}}^{b_{\max}} \rho_N \frac{dE_{brem}}{dv} b db = \frac{2\pi r_0^3 Z^2 \rho_N m^2 c^3}{3E} \ln\left(\frac{b_{\max}}{b_{\min}}\right)$$

We can combine the results of eq.(7) and eq. (12) to calculate the total Brehmsstrahlung radiated. We calculate the energy loss per unit distance using the ionization formula, and we then calculate the radiation produced per unit distance using the Brehmsstrahlung formula and integrate over the total energy of the electron. This gives

(13) 
$$\frac{dE_{brem}}{d\nu}(\nu) = \int_{E_{max}}^{n\nu} \frac{d^2 E_{brem}}{d\nu dx} \frac{dx}{dE} dE = (E_{max} - h\nu) \frac{Zr_0}{3c}.$$

Note, that the above formula is a bit of a cheat since  $b_{\min}$  and  $b_{\max}$  are not exactly the same for the ionization and Brehmsstrahlung processes, and thus would not exactly cancel in the evaluation of the integral in eq. (13). However, since the error occurs in a log term, it should be small. Note the significance that the Brehmsstrahlung radiation increases as the Z of the target increases.

We can further approximate the Brehmsstrahlung radiation in the limit of the electron energy much larger than the frequency being measured. In this case eq. (13) reduces to

(14) 
$$\frac{dE_{brem}}{d\nu} = \frac{Zr_0 E_{\max}}{3c}$$

This can be re-written in terms of the efficiency of the x-ray generator for Brehmsstrahlung, defined as the number of photons-out (per energy interval dv) per electrons in. The number of photons is equal to the energy radiated divided by the energy per photon (hv) giving:

(15) 
$$\frac{N_{photons}}{e^{-}} = \frac{Zr_0eV}{3hc}\frac{dv}{v} \approx 8 \times 10^{-10} ZV \frac{dv}{v}$$

The measured experimental value is  $1 \times 10^{-9} ZV dv / v$  which is in excellent agreement.

Now, consider the production of characteristic radiation. Production of characteristic radiation is best defined in terms of a cross section. Here we are most interested in the cross section to produce k radiation  $\sigma_k$ . The cross section is defined as the number of k electrons produced per second by an atom subject to an incident flux of  $\Phi \, e^{-}/m^2/s$ . This is given by[3]

(16) 
$$\sigma_k = \frac{2\pi r_0^2 (mc^2)^2 b_k}{EE_k} \ln\left(\frac{E}{E_k}\right)$$

Here  $b_k \sim 0.35$  is an empirical constant. Eq. (16) could also be derived approximately using eq.(7) (see problem 6). In the present case we have a single electron incident on an array of scatterers. If we consider an electron with velocity v incident on a section of the material of thickness dx then this is equivilent to an electron subject to a flux of scattering targets given by  $\Phi = \rho_N v$ . By symmetry the cross section for a beam of electrons scattering from an atom is the same as that for a beam of atoms scattering from an electron. We thus have the number of *k* x-rays produced per second given by

(17) 
$$\frac{dN_k}{dt} = \rho_N v \sigma_k$$

The number of k x-rays per unit length is then

(18) 
$$\frac{dN_k}{dx} = \rho_N \sigma_k$$

The total number of k-alpha photons produced by an electron from the time it enters the anode with energy E until the time it comes to rest is then given by,

(19) 
$$N_{k} = \rho_{N} \int_{E}^{E_{k}} \sigma_{k} \left( E \right) \frac{dx}{dE} dE$$

Since dE/dx as given in eq. (7) depends on  $b_{\min}$  and  $b_{\max}$  evaluation of the integral in eq. (19) requires estimates for these values. The maximum impact parameter is approximately the distance at which the energy transferred is just enough to ionize an electron,  $E_I$ . This gives

$$b_{\max} = \frac{\sqrt{2mc^2 r_0}}{\sqrt{EE_I}}$$

The minimum impact parameter is given by the value of a collision in which the all the energy of the electron is lost. This gives

$$b_{\min} = r_0 \frac{mc^2}{E}$$

Thus we find

(22) 
$$\frac{b_{\max}}{b_{\min}} \approx \sqrt{\frac{E}{2E_I}}$$

Putting this relation into eq. (19) gives

(23) 
$$N_{k} = \rho_{N} \int_{E}^{E_{k}} \sigma_{k} \left( E \right) \frac{dx}{dE} dE = \frac{2b_{k}}{ZE_{k}} \int_{E}^{E_{k}} \frac{\ln\left( E / E_{k} \right)}{\ln\left( E / 2E_{I} \right)} dE$$

Since  $E_k / E_I >> E / E_k$ , we can make the approximation

(24) 
$$\frac{\ln(E/E_k)}{\ln(E/2E_I)} \approx \frac{\ln(E/E_k)}{\ln(E_k/2E_I)}$$

The integral in equation (19) can now be evaluated. The result is

(25) 
$$\frac{N_k}{e^-} = \frac{2\omega_k b_k \left[ U \ln \left( U \right) - U + 1 \right]}{Z \ln \left( E_k / E_I \right)} \approx \frac{2\omega_k b_k}{Z \ln \left( E_k / E_I \right)} 0.37 (U-1)^{1.67} \text{ for } 1 < U < 5.$$

Here  $U = E / E_k$  and  $\omega_k$  is the fluorescence yield. The latter factor is needed because sometime instead of emitting an x-ray the atom can conserve energy by emitting a high energy electron termed an Auger electron.



Fig. 1-2. Fluorescence yields for K and L shells for  $5 \le Z \le 110$ . The plotted curve for the L shell represents an average of  $L_p$ ,  $L_p$ , and  $L_s$  effective yields.

Figure 2 Flourescence Yields (from the x-ray data booklet)

The actual flux is reduced by the absorption of the emitted x-rays within the anode of the x-ray tube. This depends on the depth at which electrons are absorbed, the takeoff angle of the x-rays and the absorption coefficient of the target material.

#### Problems

- 1. X-ray energies.
  - a. Compare the approximate energy of the  $k_{\alpha}$  lines based on eq. (1) with the exact values found in the x-ray data booklet for the elements Al, Cu, Sn and Au.
  - b. Try to extend the shielding approximation to make an estimate of the  $k_{\beta}$  energies. As before, compare your estimates with the tabulated values for Al, Cu, Sn and Au.
  - c. Discuss qualitatively why the shielding approximation works well for the  $k_{\alpha}$  but not the  $k_{\beta}$ .
- 2. Hyperfine Structure.
  - a. Due to the hyperfine splitting the energy of the atomic orbitals depends on the total angular momentum quantum number *j*. In the absence of a magnetic field the energy of an atomic state only depends on the magnitude of *j* and not its projection  $m_j$ . Use this to argue that the  $k_{\alpha}$  x-ray line should be split into two peaks,  $k_{\alpha 1}$  and the  $k_{\alpha 2}$ .
  - b. Use eq (3) to estimate the energy of the  $k_{\alpha 1} k_{\alpha 2}$  splitting for Al, Cu, Sn and Au and compare your result with the tabulated values.
- 3. In a simple resonance model for the k-alpha transition the line width of the transition, is determined by the Q-factor of the resonance. While for a simple harmonic oscillator the Q-factor is determined by friction, in an atomic transition, this friction actually comes about from the radiative-reaction force

(see J. D. Jackson chapter 17, [4]). Based on this model, the line-width is given by  $\frac{\Delta E}{E} = \frac{2\alpha E}{mc^2}$  Use this formula to estimate the line-widths for the k-alpha lines of Al, Cu, Sn and Au.

4. A more exact calculation of eq. (4) would employ an integral over the impulse. Assume that the path of the incident electron is un-deviated by the force of the atomic electron (a reasonable approximation for a high energy incident electron) and also assume that the atomic electron does not move over the time of the collision, thus all the longitudinal components of the force

cancel out. Show that  $\Delta P = \int_{-\infty}^{\infty} F dT = \frac{2mc^2 r_0}{bv}$ . Hint: Transform into an

integral over the path of the incident electron rather than over time, and then use Gausses Law to evaluate an equivalent integral over the surface of a cylinder with radius b.

- 5. Consider a collision of an electron with energy E with an atom at fixed impact parameter b. Calculate the ratio of energy lost to ionization to the energy lost to Brehmsstrahlung radiation integrated over all frequencies.
- 6. Use equation (7) to derive a formula for the cross section  $\sigma_k$  that is given in equation (16). How close does this come?
- 7. Rewrite eq. (13) Å in terms of  $\frac{dE_{brem}}{d\lambda}$  and sketch a plot of the intensity of

Brehmsstrahlung radiation as a function of wavelength.

- 8. Derive eq's (20) and (21).
- 9. An electron beam with a current of 30 mA and energy of 40 keV impinges on a thick molybdenum target. Calculate the number of k x-rays that would be expected to hit a detector subtending a solid angle of  $1 \times 10^{-7}$  steradians. Compare this with the actual measured flux for a molybdenum x-ray tube operated under similar conditions of ~  $5 \times 10^5$  phot/sec. Note that this calculation ignores the possibility of absorption of x-rays on their way out of the metal which would reduce the flux.

### Synchrotron sources

### **Bending magnets**

Synchrotron radiation occurs when a relativistic electron beam undergoes circular acceleration in a magnetic field. This radiation can be described using classical electromagnetic theory and a full treatment can be found in Jackson [4]. In the present context we will present a simplified derivation of the most important results of synchrotron radiation based on the discussion from chapter 2 of Als-Nielson [5].

In a synchrotron, electrons are accelerated to relativistic velocities and then confined in a circular orbit by the action of bending magnets. The acceleration from the circular motion causes the electrons to emit radiation, and relativistic effects shift the frequency of this radiation into the x-ray regime.

We begin our estimation of the amount of radiation emitted by a synchrotron source with the force on an electron in a magnetic field. This is given by:

(26) 
$$\vec{F} = e\vec{v} \times \vec{B} = \frac{dP}{dt}$$

Assuming circular motion this simplifies to

 $evB = \gamma mv^2 / r \,.$ 

The orbital frequency can then be calculated in a straightforward way,

(28)  $\omega_0 = v/r = eB/\gamma m = \omega_c/\gamma.$ 

Here we have defined  $\omega_c = eB / m$ , which is referred to as the cyclotron frequency.

Because the electron moves with relativistic velocities the observed frequency of the radiation is actually much higher. Recall the Lorentz transformations between two inertial reference frames given by

(29)  
$$\begin{aligned} x' &= \gamma(x - vt) \\ t' &= \gamma(t - vx / c^{2}) \\ y' &= y \\ z' &= z \end{aligned}$$

The transformation of velocity in the x and y directions can be found from taking differentials of eq. (29)

(30) 
$$\frac{dx'}{dt'} = \frac{\gamma dx - \gamma v dt}{\gamma dt - \gamma v dx / c^2} = \frac{dx / dt - v}{1 - v (dx / dt) / c^2} = \frac{v_x - v}{1 - v_x v / c^2}$$
$$\frac{dy'}{dt'} = \frac{dy}{\gamma dt - \gamma v dx / c^2} = \frac{dy / dt}{\gamma - \gamma v (dx / dt) / c^2} = \frac{v_y}{\gamma (1 - v v_x / c^2)}$$

Now consider a light wave emitted at angle  $\theta$  in the rest frame of a moving electron. In the lab frame the x and y components of its velocity can be calculated using eq. (30), for

each of the components. For velocities very close to the speed of light  $1 - \beta << 1$  the angle in the lab frame can be approximated as shown below:



#### Figure 4

From this one can see that the radiation emitted by a relativistically moving object is compressed into a cone of opening angle  $1/\gamma$ .

Now consider an electron radiating as it moves along a circular orbit.



#### Figure 5

Its radiation will only be seen for a short time when its cone of radiation is emitted within an angle  $1/\gamma$  of the horizon. Thus the observer will see a short pulse of light. In order to calculate the width of the pulse one has to be careful to include the fact that the light itself propagates at finite speed. (This is similar to the calculation employed in the derivation of the Doppler shift.) Thus, we calculate the difference in arrival times between light emitted from when the electron just emerges from the horizon, to light emitted from when the electron just sets again below the horizon. Between these two events, the electron has moved a distance  $d_e \approx c\beta / \omega_0 \gamma$  closer to the observer while the light beam emitted at the beginning of this time has moved a distance  $d_l = c / \omega_0 \gamma$  closer. Thus the difference in arrival times is given by:

(31) 
$$\Delta T = 2(c / \gamma \omega_0 - v / \gamma \omega_0) / c = 2 \frac{1 - \beta}{\gamma \omega_0} = 2 \frac{1 - \beta^2}{\gamma \omega_0 (1 + \beta)} \approx \frac{1}{\gamma^3 \omega_0}.$$

For the Advanced Photon Source  $\gamma = 14000$ , so the duration of this pulse is extremely short. In order to make up a very short radiation pulse, one need to include Fourier

components up to  $\omega = 1/\Delta T$ . Hence the spectrum of radiation is boosted to frequencies of order  $\omega_0 \gamma^3$ . Typically the radiation spectrum obtain from a synchrotron is scaled in terms of the critical frequency given by (32)  $\omega_c \equiv 3\gamma^3 \omega_0/2$ 

For the APS the critical energy  $E_c = \hbar \omega_c = 19.5 \text{keV}$ . (Note that the expression given in some earlier versions of Jackson differs slightly from the conventional definition, e.g.  $\omega_{crit} \equiv 3\gamma^3 \omega_0$ , however later editions have corrected the nomenclature to agree with the above definition).

The radiated power as a function of angle and frequency is a complicated function. However the limit of the total power integrated over all angles, as a function of frequency for  $\omega >> \omega_{crit}$  is relatively simple

(33) 
$$\frac{dI}{d\omega} = \sqrt{\frac{3\pi}{2}} \frac{r_0 \gamma mc^2}{c} \left(\frac{\omega}{\omega_{crit}}\right)^{\frac{1}{2}} e^{-\omega/\omega_{crit}}$$

This is the energy emitted per unit frequency per revolution of the electron around the ring. Thus the power falls off exponentially with frequency above the critical frequency.

# **Bend Magnet Spectrum**



#### Figure 6

The spectrum obtained from an Advanced Photon Source bending magnet. This curve was obtained from http://www-cxro.lbl.gov/optical\_constants/bend2.html .

The radiation from a synchrotron bending magnet differs from that of an x-ray tube in several important respects. The radiation is a continuous spectrum as opposed to sharp lines from the characteristic radiation. This can be important for applications involving absorption or resonant scattering. The radiation is collimated to an angle of order  $1/\gamma$ . The overall intensity of radiation is higher than that which can be produced by an x-ray tube chiefly because nearly all the energy used to create the x-rays goes into the x-rays themselves, rather than heat. One can still do quite a lot of diffraction experiments with an x-ray tube flux (typically around  $10^6$  photons/s ) and the additional flux from synchrotrons is often more useful for specialized experiments such as diffuse scattering, very high resolution scattering, or scattering from micro-crystals.

### Undulators

Magnets that are specially tailored to produce x-rays can produce more radiation than a uniform magnetic field.



This is typically done by arranging a series of alternating north and south magnetic poles. The electrons, rather than only emitting one pulse of radiation, will emit radiation each time they pass through a region of intense magnetic field. If the magnets are not close enough together, the radiation emitted from one set of magnet poles will not have a definite phase relationship with the radiation emitted from the other magnets. In this case, the net effect of such an arrangement is to produce the same spectrum as given by a bending magnet, then the radiation sums incoherently. The intensity of radiation is approximately N times the equivalent intensity from a bending magnet. This type of arrangement is called a wiggler, but wigglers are seldom used on modern synchrotron sources.

Much better performance can be obtained by arranging the magnets so as to scatter in phase. Since the electron beam must move slower than the light waves, the radiation from subsequent magnets must suffer a phase delay. The trick is to arrange the magnet spacing so that this phase delay is an integral number of wavelengths. This type of arrangement is called an undulator.



#### Figure 8

Consider the path of an electron shown above. The distance  $\lambda_u$  is the spacing between the poles of the magnet. The electron travels a slightly longer path, *s*, which follows the sinusoidal deflections induced by the magnets. The condition that the radiation from the

two magnet section is in phase requires that the time delay between the arrival of the light from the point *A* in fig. 8 and the arrival of the electron at point *B* be a multiple of the period of the light. The time for light to reach point *B* from point *A* is given by (34)  $\Delta T_{light} = \lambda_u / c$ 

The arrival time of the electron at point *B* is given by (35)  $\Delta T_{electron} = s / v$ 

The path length s can be determined from the maximum angle of deflection K (see Problem (10) and is given by

$$(36) s = \lambda_u \left( 1 + K^2 / 4\gamma^2 \right)$$

The condition for the radiation from the two magnets to be in phase is given by

(37) 
$$\lambda_{u} \left(1 + K^{2} / 4\gamma^{2}\right) / \beta - \lambda_{u} = n\lambda$$

Here, n is an integer. The required magnet spacing,  $\lambda_{\mu}$ , can then be solved for,

(38) 
$$\lambda_u = \lambda \frac{2\gamma^2}{\left(1 + K^2/2\right)}$$

Here I have used the approximation  $\gamma >> 1$ , so that  $1 - \beta \approx \frac{(1 - \beta)(1 + \beta)}{(1 + \beta)} \approx \frac{1}{2\gamma^2}$ 

The angle *K* can be derived from the curvature of an electron in a magnetic field and is given by (see problem 13)

(39) 
$$K = \frac{eB}{k_{\mu}mc}.$$

Here  $k_u = 2\pi / \lambda_u$ 



Figure 13: Aperture-limited spectral power (dotted curve) and cumulative power (dashed curve) for Undulator A at closed gap (10.5 mm) for the present low-emittance lattice. The aperture is 2.5 mm (h) x 1.0 mm (v) at 30 m from the source. The wiggler approximation is also shown (solid curve) using a *K* value of 2.79, corresponding to the peak magnetic field and a critical energy of 29.5 keV. Here,  $E_{10\%} = 11$  keV,  $E_{50\%} = 43$  keV, and  $E_{90\%} = 105$  keV. Note that  $E_{50\%}$  is larger than  $E_c$  here, showing that the spectrum is "harder" than what is expected from a bending magnet spectrum. The frequency-integrated power of 440 W is less than 10% of the total emitted power.

#### Figure 3

From http://www.aps.anl.gov/Facility/Technical\_Publications/techbulletins/tb45.pdf

The figure above shows the spectrum on-axis from an APS undulator A. of the (The APS creatively decided to name the first series of undulators "A"). Note that for a given magnet spacing there are also several harmonics which result from the condition that the phase difference is a multiple number of wavelengths.

The total power emitted by an undulator is the same as that emitted by a wiggler; however it is concentrated around the energies of the harmonics. At the harmonics it is of order  $N^2$  larger than the bending magnet intensity. Problems.

10. For a particle in circular motion, the total power radiated is given

by  $P = \frac{1}{4\pi\varepsilon_0} \frac{2}{3} \frac{q^2 a^2}{c^3} \gamma^4$ . Here, *a* is the acceleration in the laboratory frame of

reference. Use this formula to estimate  $\Delta E$ , the total energy emitted by an electron in a single pass by an observer. Next estimate the spectral power,

 $dE/d\omega$  under the assumption that  $\frac{dE(\omega)}{d\omega}$  is constant out to  $\omega_c$  and zero

above  $\omega_c$ .

- 11. At the Advanced Photon Source the energy of the electron beam is 7.0 GeV and the critical photon energy is 19.5 keV. Based on this, calculate the magnetic field within the bending magnets at the APS.
- 12. At the Advanced photon source the frequency with which electrons orbit the entire synchrotron, 1.7 MHz. Using the magnetic field strength from problem 11 calculate the orbital frequency expected. Explain why this number differes from the 1.7 MHz and why you not necessarily expect these values to be the same? (Hint, think about the details of how a synchrotron is constructed).
- 13. Path length for an electron through an undulator.
  - a. Show that the path length, *s* traveled by the electron between one maxima and the next is approximately equal to  $\lambda_u \left(1 + K^2 / 4\gamma^2\right)$  where  $K / \gamma$  is the maximum angular deflection of the curve, and the shape of the curve is assumed to be a cosine wave.
  - b. Show that the maximum angular deflection  $K/\gamma$  is related to the effective radius of curvature,  $\rho$ , via:  $\rho \approx 1/Ak_u^2$  where A is the amplitude of the sinusoidal oscillation of the electron. Use this result to show that  $K = \frac{eB}{k_u mc}$  Hint: If you need help see section 2.4 of Als-

Nielson, but you should be able to do this on your own!

14. Derive equation (38) from equation (37) using the approximations discussed in the text.

## X-ray Interactions with Matter

### **Dielectric Polarizability for X-rays**

We begin the discussion of x-ray interactions with matter by deriving an expression for the dielectric constant of a material. The following section is based on Chapter 8 of Griffiths [6].

Approximate an electron bound in a solid as a harmonic oscillator with resonance frequency  $\omega_0$  and damping coefficient  $\gamma$ . In the presence of an electromagnetic wave, the electron experiences a force, and satisfies the equation of a damped driven oscillator (40)  $m\ddot{y} + m\gamma \dot{y} + m\omega_0^2 y = qE_0e^{-i\omega t}$ .

We use here the usual complex representation of an electromagnetic wave. Using the ansatz  $y = y_0 e^{-i\omega t}$  yields the solution

(41) 
$$y_0 = \frac{qE_0/m}{(\omega_0^2 - \omega^2) - i\gamma a}$$

This results in an oscillating electric dipole moment, p = qy, given by

(42) 
$$p = \frac{q^2 E_0 e^{-i\omega t} / m}{(\omega_0^2 - \omega^2) - i\gamma\omega}$$

More generally, a density of  $\rho_N$  identical atoms per unit volume each with Z electrons, each with resonant frequency  $\omega_i$  has a dipole moment density given by<sup>2</sup>

(43) 
$$P = \rho_N \sum_{j=1}^{Z} \frac{f_j q^2 E_0 e^{-i\omega t} / m}{(\omega_j^2 - \omega^2) - i\gamma \omega}.$$

Here  $f_j$  is the oscillator strength of each electron in the atom. The oscillator strength of each electron is approximately 1. An exact calculation can be made using a proper quantum treatment. From this expression and using the definition  $P = \varepsilon_0 \chi E$  together with  $\varepsilon = \varepsilon_0 (1 + \chi)$  we arrive at

(44) 
$$\varepsilon = \varepsilon_0 \left( 1 + \frac{\rho_N}{\varepsilon_0} \sum_{j=1}^Z \frac{f_j q^2 / m}{(\omega_j^2 - \omega^2) - i\gamma\omega} \right)$$

Consider the limit (not always valid) that the frequency of the incident x-ray frequency is much larger than any of the resonance frequencies. In this case we can make the approximation

(45) 
$$\sum_{j=1}^{Z} f_j / \left[ (\omega_j^2 - \omega^2) - i\gamma \omega \right] \approx \left( \sum_{j=1}^{Z} f_j \right) / \omega^2$$

 $<sup>^{2}</sup>$  This is only true in the limit that the susceptibility is much less than one. However this is an excellent approximation for the case of x-rays.

The "f-sum" rule from atomic physics gives the result that  $\sum_{j=1}^{Z} f_j = Z$ . This in this limit

the dielectric constant simplifies to

(46) 
$$\varepsilon = \varepsilon_0 \left( 1 - \frac{\rho_N Z q^2}{\varepsilon_0 m \omega^2} \right) = \varepsilon_0 \left( 1 - \rho_N Z r_0 \lambda^2 / \pi \right)$$

In general, the x-ray frequency is not so large that the effects of resonances can be neglected. In this case, one writes for an atom collectively

(47) 
$$\sum_{j=1}^{Z} f_j = Z + f'(\omega) + if''(\omega)$$

(48)  $\varepsilon / \varepsilon_0 = 1 - \rho_N r_0 \lambda^2 [Z + f'(E) + if''(E)] / \pi$ 

The factors 
$$f'$$
 and  $f''$  are referred to as the anomalous scattering factors and can be  
looked up in tables. With the proper choice of  $f'$  and  $f''$  eq. (48) is completely general,  
and the assumption of a harmonic oscillator potential is no longer required. In general,  
 $f'$  and  $f''$  are small compared to Z, so that one can write an effective electron density

(49) 
$$\rho_e \approx \rho_N \left[ Z + f'(E) + if''(E) \right],$$

which is close to the actual electron density. We can then re-write eq. (48) more compactly

(50)  $\varepsilon / \varepsilon_0 \approx 1 - \rho_e r_0 \lambda^2 / \pi$ 

### The Far Field Scattering Pattern

We now consider how this oscillating dielectric constant causes the scattering of x-rays. An EM wave satisfies the wave equation

(51)  $\nabla^2 \vec{E} = \varepsilon \mu \partial^2 \vec{E} / \partial t^2.$ 

If we ignore polarization, we can approximate this as a scalar wave equation given by (52)  $\nabla^2 \psi = \varepsilon \mu \partial^2 \psi / \partial t^2.$ 

 $k^2 = \varepsilon \mu \omega^2$ 

 $\nabla^2 \psi + k^2 \psi = 0.$ 

Making the ansatz  $E(\vec{r},t) = \psi(\vec{r})e^{-i\omega t}$  and using the definition

eq. (52) becomes

(54)

For now, we will assume that magnetic effects can be ignored ( $\mu = \mu_0$ ). We can then substitute eq. (50) into eq.(53) to give

(55)  
This gives  
(56)
$$k^{2} = (1 - \rho_{e} r_{0} \lambda^{2} / \pi) (\omega^{2} / c^{2})$$

$$\nabla^{2} \psi + (k_{0}^{2} - 4\pi r_{0} \rho_{e} (\vec{r})) \psi = 0.$$

Let us represent the differential operator  $\nabla^2 + k_0^2$  by *L* and the also write  $f = 4\pi r_0 \rho_e(\vec{r})$ . In the absence of *f* we have  $L\psi_0 = 0$  and we would like to find a solution to  $L\psi = f\psi$ . If we can find the Green function which satisfies  $LG(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')$  then the solution to the full equation will be

(57) 
$$\psi = \int G(\vec{r}, \vec{r}') f(\vec{r}') \psi(\vec{r}') d^3 \vec{r}'$$

The Green function for eq. (56) is well known from electrodynamics and is given by

(58) 
$$G(\vec{r},\vec{r}') = \frac{e^{ik' |\vec{r} - \vec{r}'|}}{4\pi |\vec{r} - \vec{r}'|}.$$

The scattered field from eq. (56) can be found using the Green function for eq. (54). Even knowing the Green function, it is still not possible to solve eq. (58) since it is an integral equation involving  $\psi$  on both sides. However, we can find an approximate

solution using the first Born approximation by taking  $\psi \approx \psi_0 = E_0 e^{i\vec{k}\cdot\vec{r}}$  within the integral. The result for the scattered field is then given by

(59) 
$$\Psi_{s}(\vec{r}) \approx \Psi_{0} + r_{0} \int \frac{e^{i\vec{k}\cdot|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \rho_{e}(\vec{r}') E_{0} e^{i\vec{k}\cdot\vec{r}'} d^{3}\vec{r}'$$

Here, k' is the wavevector of the scattered radiation with magnitude  $k' = k = 2\pi / \lambda$ . We now take the origin of  $\vec{r}$  and  $\vec{r}'$  to be within the sample and note that the position  $\vec{r}$  represents the position where we are measuring the electric field, which we call the detector position (see fig. 4). We then have in the exponential:

(60) 
$$k' \left| \vec{r} - \vec{r}' \right| = \sqrt{r^2 - 2\vec{r} \cdot \vec{r}' + r'^2} \approx k'r - k'\vec{r} \cdot \vec{r}' / r = k'r - \vec{k}' \cdot \vec{r}'$$

In the denominator we can take  $|\vec{r} - \vec{r}'| \approx r$ , yielding

(61) 
$$\psi(\vec{r}) \approx \psi_0 + r_0 E_0 \frac{e^{ik'r}}{r} \int e^{-i(\vec{k}-\vec{k'})\cdot\vec{r'}} \rho_e(\vec{r'}) d^3\vec{r'}$$

The first term  $\psi_0$  represents the unscattered radiation and is generally not seen in the detector. The second term represents the scattered electric field which we represent with  $\psi_s$ .

In order to account for the polarization of light we need to multiply this result by a factor *P* to account for polarization. This factor is determined as follows: Take  $\hat{\epsilon}$  to be the polarization direction of the incident x-ray beam and take  $\hat{n} = \vec{r} / r$  to be the direction of the scattered radiation. Then

$$(62) P = \left| \hat{\epsilon} \times \hat{n} \right|^2$$

For the case of an unpolarized incident beam the polarization factor then becomes

$$P = \frac{1 + \cos^2(\theta)}{2}$$

Where  $\theta$  is the scattering angle.

The final result is then:

(64) 
$$\Psi_s(R) \approx r_0 P E_0 \frac{e^{i\vec{k}\cdot\vec{r}}}{r} \int e^{i\vec{q}\cdot\vec{r}'} \rho_e(\vec{r}') d^3\vec{r}' \quad .$$



#### Figure 4

Here we have defined a new variable,  $\vec{q}$ , defined by the difference between the incident and outgoing wavevectors of light,

(65)  $\vec{q} = \vec{k}' - \vec{k} = \vec{k}_{out} - \vec{k}_{in}$ 

The angle  $\theta$  defines the angle between the direction of *polarization* and the direction of the scattered light wave.



Figure 5 Definition of the scattering wavevector

This is the central result of x-ray scattering, the scattered x-ray intensity is proportional to the Fourier transform of the electron density. This result forms the basis by which the structure of materials can be extracted from the x-ray scattering.

### Absorption

For a plane wave moving in the x-direction the electric field can be written as

(66)  $\psi(x) = \psi_0 \exp\left[i\left(kx - \omega t\right)\right]$ 

The dielectric constant will generally not be a real number as can be seen from eq. (49) for the effective electron density. If we write

(67) 
$$k = \operatorname{Re}(k) + i \operatorname{Im}(k)$$

then the electric field intensity is given by

(68) 
$$\Phi(x) = \psi(x)\psi^{*}(x) = \Phi_{0}(x)\exp[-2\operatorname{Im}(k)x]$$

The intensity decays exponentially with an absorption length given by  $\Lambda = 1/2 \operatorname{Im}(k)$ . Since  $k = \omega/c = \sqrt{\mu \varepsilon} \omega$  we obtain

(69) 
$$\Lambda = 2\rho_N \lambda r_0 f''.$$

One can also describe absorption in terms of a cross section. This is especially useful when trying to make contact between x-ray scattering and neutron scattering. In terms of an absorption cross section,  $\sigma_a$ , we can use the relation  $dI/dx = -\sigma_a \rho_N I$  to obtain

(70) 
$$\sigma_a = \Lambda / \rho_N = 2\lambda r_0 f$$



### Figure 6

Above are shown the anomalous atomic scattering factors for the element copper. Note that the dispersion near the Cu k-alpha edge near 10,000 eV does not look at all like a simple harmonic oscillator resonance such as would be expected from (44). This is because instead of going from one bound quantum state to another bound state, the final state is the continuum. In addition, since the energy is quantized, there is no absorption below the edge. Note that, in this figure,  $f_2 = f$  and  $f_1 = f' + Z$ .

Absorption is frequently expressed in terms of mass-absorption coefficients (sometimes known as the mass attenuation coefficient which can be looked up in table on the web http://physics.nist.gov/PhysRefData/XrayMassCoef/cover.html, or in the x-ray data book. In this case one defines (71)

$$\Lambda = \rho \mu$$

So that we have (72)  $\mu = N_A 2\lambda r_0 f'' / A$ Here A is the atomic weight and  $N_A$  is Avogadros number. It is straightforward to generalize this notion to compound materials (73)  $\mu_{tot} = \sum_i m_i \mu_i$ 

Here  $m_i$  is the mass fraction of element *i* in the compound.

As can be seen from Figure 6 the absorption cross section has a large jump across the xray ionization threshold for a particular orbital. This jump is referred to as the edge. Above a K-edge the absorption typically decreases as  $\sigma_a \propto E^{-3}$  while the absorption at the k-edge for different elements goes approximately as Z<sup>4</sup>. Thus heavy elements absorb x-rays much more strongly than lighter ones.

### Scattering from Atoms

An x-ray detector measures the flux of photons  $I = E^* EA = \Phi A$ , e.g. the integral of the square of the electric field over the detector area. The value of the electric field (under the assumption that the detector is far away from the sample) can be found from the Born approximation via Eq. (64). , which is then given by

(74) 
$$\frac{\Phi(\vec{q})}{\Phi_0} \approx \frac{r_0^2 \cos^2\left(\theta\right)}{r^2} \left| \int e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) d^3 \vec{r} \right|^2$$

Here the wavevector transfer is defined by eq. (65).

Scattering measurements are typically defined in terms of differential scattering cross sections  $d\sigma/d\Omega$  with  $\Omega$  the solid angle of the detector. The differential scattering cross section is defined as the ratio of the scattered intensity  $N_s$  (photons/sec) measured in solid angle  $d\Omega$  to the flux  $\Phi_0$  (photons/s/m<sup>2</sup>) incident on the sample.

(75) 
$$I_s = \Phi_0 \Omega \frac{d\sigma}{d\Omega}$$

For an isolated atom the scattering cross section is obtained from eq. (74) and (75)

(76) 
$$\frac{d\sigma}{d\Omega} = Pr_0^2 \left| \int e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) d^3\vec{r} \right|$$

Here,  $\rho_e(\vec{r}) = \psi(\vec{r})^* \psi(\vec{r})$  is the atomic electron density distribution. The integral in eq. (76) is referred to as the atomic form factor defined by

(77) 
$$f \equiv \int e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) d^3\vec{r} \,.$$

For small q, the exponential can be approximated as unity, and we obtain f = Z; for larger q, f is generally less than Z. Values of the atomic form factors as a function of q can be found in tables. See, for example the web page

<u>http://www.isis.rl.ac.uk/ISISPublic/reference/Xray\_scatfac.htm</u>. The total scattering cross section from an isolated atom is given by the integral over eq. (76) over all angles. In the limit of small q one obtains,

(78) 
$$\sigma_{tot} = 8\pi r_0^2 Z^2 / 3$$

### Compton Scattering.

In addition to elastic scattering and absorption electrons will also scatter inelastically through Compton scattering. The distinction between elastic scattering and Compton scattering is that the energy of elastic (or Thompson) scattered electrons is un-modified, while Compton scattered electrons have their wavelength changed via

(79) 
$$\lambda = \lambda + (h/mc) \lfloor 1 - \cos(\phi) \rfloor$$

Here  $\phi$  is the scattering angle. Compton scattered photons can not interfere constructively and typically is seen as a diffuse background on scattering patterns. The intensity of the Compton scattering is related to the intensity of the coherent scattering

(80) 
$$f_{compton} = Z - \sum_{j=1}^{Z} f_j^2$$

The form factor for each individual electron in the atom is given by the integral over that electrons density,

(81) 
$$f_j \equiv \int e^{i\vec{q}\cdot\vec{r}} \rho_j(\vec{r}) d^3\vec{r} \,.$$

Problems.

- 15. Derive eq. (69)
- 16. Calculate the absorption length of 8-keV x-rays in a) Copper and b) GaAs using eq. (69)
- 17. Calculate how much NaCl would have to be dissolved in Water to double the absorption length at 8 keV.
- 18. Derive eq. (78)
- 19. (From chapter 1 of [7]. Suppose that the electron density for the three electrons in neutral Li can be represented by hydrogen-like expression of the form

$$\rho = \frac{e^{-(2r/a)}}{\pi a^3}$$

Where for each K electron  $a_K = 0.20$  Å and for the L electron  $a_L = 1.60$  Å. Calculate the atomic form factor using eq. (81). Note that for a spherically

symmetric atom you can re-write eq. (81) as  $f_e = \int_0^\infty 4\pi r^2 \rho(r) \frac{\sin(qr)}{qr} dr$ .

# Small Angle X-ray Scattering

In a material that consists of many atoms with inter-atomic correlations the integral expressed in eq. (76) can be generalized to include all electrons within the material. Thus the general cross section is given by

(82) 
$$\frac{d\sigma}{d\Omega} = Pr_0^2 V \rho_e S(\vec{q}) \,.$$

Here V is the sample volume,  $\rho_e$  is the average sample electron density and the structure factor is defined by

(83) 
$$S(\vec{q}) = \frac{1}{\rho_e V} \left| \int e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) d^3 \vec{r} \right|^2$$

Here the local density  $\rho_e$  is related to the averaged density by  $\rho_e = \langle \rho_e(r) \rangle_r$ . For the case of identical atoms, the atomic form factor f can be factored out giving:

(84) 
$$S(\vec{q}) = \frac{\left|f\right|^2}{\rho_e V} \left|\int e^{i\vec{q}\cdot\vec{r}} \rho_N(\vec{r}) d^3\vec{r}\right|^2.$$

In this case  $S(\vec{q})$  now represents the structure factor per atom. For materials with multiple different atoms the atomic form factor has to remain inside the integral. Sometimes, to make connection with neutron scattering, this equation is also written in terms of the "scattering length density"

(85) 
$$\rho_b = r_0 f \cos(\theta) \rho_N$$

In this case  $\rho_b$  is analogous to  $\rho_e$ . In most actual x-ray experiments the incident intensity is not measured, but rather the incident flux  $I_0$  (photons/sec). In this case one typically integrates over the area of the beam  $A_0$  and normalizes by the volume of the sample,  $V = A_0 \Lambda$ , with  $\Lambda$  thickness of the sample to obtain;

(86) 
$$I_s = I_0 \left(\frac{1}{V} \frac{d\sigma}{d\Omega}\right) \Lambda \Omega$$

The volume normalized cross section is sometimes referred to as  $\left(\frac{1}{V}\frac{d\sigma}{d\Omega}\right) = \frac{d\Sigma}{d\Omega}$ 

The differential scattering cross section per unit volume is then simply related to the structure factor via;

(87) 
$$\left(\frac{1}{V}\frac{d\sigma}{d\Omega}\right) = Pr_0^2 \rho_e S(\vec{q})$$

•

As a practical example, consider scattering from a colloidal suspension of particles of identical shape in water. If the particles are sufficiently large, then most of the scattering will be confined to small angles, and in this case  $P \approx 1$  and Eq. (87) simplifies to

(88) 
$$\left(\frac{1}{V}\frac{d\sigma}{d\Omega}\right) \approx r_0^2 S(\vec{q}) = \frac{r_0^2}{V} \left|\int e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) d^3\vec{r}\right|^2$$

Let  $\rho_0$  denote the electron density of the water. We can then write

(89) 
$$S(\vec{q}) = \frac{1}{V} \left| \int e^{i\vec{q}\cdot\vec{r}} (\rho_e - \rho_0) d^3\vec{r} + \rho_0 \int e^{i\vec{q}\cdot\vec{r}} d^3\vec{r} \right|^2 = \frac{1}{V} \left| \int e^{i\vec{q}\cdot\vec{r}} \Delta\rho d^3\vec{r} + (2\pi)^3 \delta^3(\vec{q}) \right|^2$$

If we ignore scattering along the direct beam direction,  $\vec{q} = 0$ , then we obtain

(90) 
$$S(\vec{q}) = \frac{1}{\Delta \rho_0 V} \left| \int e^{i\vec{q}\cdot\vec{r}} \Delta \rho(\vec{r}) d^3 \vec{r} \right|^2$$

Equation (90) is the starting point for the analysis of small angle scattering. This result applies the general scattering from all materials which have structure on large enough length scales that the scattering is confined to small angles.

In order to make further progress it is necessary to make assumptions about the system. If all the particles are identical, then we can write the density of particle i as

(91) 
$$\rho_i(r) = \left\langle \rho_p(\vec{r} - \vec{r}_i) \right\rangle_{\theta,\phi}$$

Here  $\vec{r}_i$  is the position of the center of mass of particle *i*. The symbol  $\langle \rangle_{a,b}$  represents

the averaging over all possible rotations of the particle. The function  $\rho_p(\vec{r})$  gives the electron density of an individual particle. If we make the assumption that the correlations between the positions of particles are independent of their relative rotations (which will become more accurate for dilute suspensions, but is frequently NOT a good assumption for concentrated solutions) then we can approximate Eq. (90) as the product

(92) 
$$S(\vec{q}) = N_p S_p(\vec{q}) | F(\vec{q})$$

Where the inter-particle structure factor  $S_p(\vec{q})$  is defined by

(93) 
$$S_p = S(\vec{q}) = \frac{1}{N_p} \left| \sum_i e^{i\vec{q}\cdot\vec{r}_i} \right|^2$$

And the particle form-factor (analogous to, but distinct from, the atomic form factor) is given by

(94) 
$$\left|F\left(\vec{q}\right)\right|^{2} = \left\langle \left|\int e^{i\vec{q}\cdot\vec{r}}\Delta\rho(\vec{r})d^{3}\vec{r}\right|^{2}\right\rangle_{\theta}$$

In most experiments, one should average over all possible particle orientations. In this case the density depends only on the magnitude of r and we can write

(95) 
$$F(q) = \iiint \Delta \rho(r) e^{-i\vec{q}\cdot\vec{r}} d^3\vec{r} = 4\pi \int \frac{r^2 \Delta \rho(r) \sin(qr)}{qr} dr.$$

In many cases, it is the particle form factor which is of chief interest. Note that since the form factor is averaged over orientation, this will only depend on the magnitude of the scattering vector. For a number of simple shapes the form factor can be calculated explicitly. For a sphere of radius *a*, we have

(96) 
$$F(q) = \Delta \rho V \left\{ 3 \frac{\left[ \sin(qa) - qa\cos(qa) \right]}{\left(qa\right)^3} \right\}$$

Form factors are usually written in terms of a normalized form factor  $\gamma(q)$  such that

(97) 
$$\gamma(q) = F(q) / \Delta \rho_0 V$$

This separates the form factor into a shape dependent part and a size dependent part. It can be shown that for any solid shape the form factor is related to the distribution of end to end vectors within the material. The form factors for most simple shapes can be looked up. A good summary is given in the International Tables for X-ray Crystallography.

Some useful limiting relationships can also be derived for either small or large q. As  $q \rightarrow 0 F(q) \rightarrow N_e^2$ . For q small the form factor approaches the Guinnier approximation

(98) 
$$F(q)^2 \xrightarrow[q \to 0]{} V^2 \Delta \rho_e^2 e^{-q^2 R_g^2/2}$$

Here  $R_{g}$  is the radius of gyration given by

(99) 
$$R_{g}^{2} = \frac{\int r^{2} \rho_{e}(r) d^{3} r}{\int \rho_{e}(r) d^{3} r}$$

For large q, we have the limit

$$\left(\frac{1}{V}\frac{d\Sigma}{d\Omega}\right) \xrightarrow{q \to \infty} \rho_{particles} \frac{2\pi r_0^2 \left(\rho_e - \rho_0\right)}{q^4} \frac{S}{V}$$
(100)

(Add a proof of this ...)

Here S/V is the ratio of surface area to volume and  $\rho_{particles}$  is the number of particles per unit volume.

(Put in a worked example of how to calculate the scattering from a suspension of spheres.)

Object	F(Q)	Reference
Gaussian Random Chain (Debeye form	$\frac{2N}{e^{-x^2}-1+x^2}$	[8]
factor)	$x^4 \left( \begin{array}{c} x \\ x \end{array} \right)$	
	$x = qR_g$	
Rigid Rod	$\frac{2N}{x}\int_{0}^{x}\frac{\sin(x)}{x}-\frac{N}{(x/2)^{2}}\sin^{2}(x/2)$	[8]
	x = qL	
Sphere	$N\left\{3\frac{\left[\sin\left(x\right)-x\cos\left(x\right)\right]}{x^{3}}\right\}$	
	x = qa	

In addition to the structure of the particles themselves, the small angle scattering can also be affected by correlations between different particles. Consider the case of a monoatomic liquid. We can define a pair correlation function,  $g(\vec{r_1}, \vec{r_2})$  which is the joint probability of finding particles at  $\vec{r_1}$  and  $\vec{r_2}$ .

(101) 
$$P(\vec{r}_1, \vec{r}_2) = \rho_N^2 g(\vec{r}_1, \vec{r}_2) dV_1 dV_2$$

For an isotropic media, only the magnitude of the separation  $r = |\vec{r_1} - \vec{r_2}|$  matters, we can write  $g(\vec{r_1}, \vec{r_2}) = g(r)$ . In this case  $g(r) \xrightarrow[r \to \infty]{} 1$  and  $g(r) \xrightarrow[r \to 0]{} 0$ 

Figure 7

Frequently one also defines the function h(r) = g(r) - 1, which removes the constant term from the Fourier transform. Figure 14 shows the expected g(r) for a simple monotonic liquid, such as liquid Xenon. The structure factor of scattering from this liquid will then be given by

(102) 
$$S(q) = \left[1 + \frac{\tilde{g}(q)}{V}\right]$$

Here we define the Fourier transform

(103) 
$$\tilde{g}(q) = \int e^{i\vec{q}\cdot\vec{r}} g(\vec{r}) d^3\vec{r} = \int_0^\infty \frac{g(r)r^2\sin(qr)}{qr} dr$$

The extra factor of 1 in the structure factor comes from the contribution of single atom scattering.

### Types of SAXS spectrometers

Below are shown two typical x-ray spectrometers used to measure small-angle scattering.





Typical resolutions from  $q=1 \text{ nm}^{-1}$  to  $q=0.01^{-1}$  for pinhole and to q=0.001 for Bonse-Hart.

## Thermal fluctuations

Consider an isotropic fluid, at large length scales the structure due to the individual particles will average out, however there will still be variations in density due to thermal fluctuations. One way to characterize the magnitude of fluctuations is to ask what the response would be to an externally imposed force field. This is an exact analogy of the dielectric susceptibility in a material. The mechanical susceptibility is the compressibility.

(104)

Here *v* is an external potential. However, if the force is non-uniform, one can define a q dependent susceptibility, typically defined in Fourier space as (105)  $\tilde{\chi}(q) = \Delta \tilde{\rho}(q) / \tilde{v}(q)$ 

 $\chi \equiv \Delta \rho / v$ 

One of the primary results of the fluctuation-dissipation theorem of thermodynamics is that the structure factor is related to the susceptibility via

(106)  $S(q) = k_b T \tilde{\chi}(q) / \rho_{particle}$ In the limit of  $q \to 0$  this implies (107)  $S(q) \xrightarrow[q \to 0]{} k_B T \rho_{particle} \kappa$ 

Here  $\kappa$  is the isothermal compressibility. (For details on this derivation, and for more details on x-ray scattering from colloids see chapters 11 and 14 of Hunter [9].)

# Scattering from a dilute polymer solution



A polymer in solution can be modeled as a segmented chain where the position of each segment executes a random walk with respect to the polymer. (For a reference see chapter 1 of Doe and Edwards [10])



The total length of the chain will then be given by the vector sum of all the displacements

(108) 
$$\left|\vec{R}\right|^2 = \left|\sum_{i=1}^N \vec{r_i}\right|^2 = \sum_{i=1}^N r_i^2 + \sum_{i \neq j} r_i r_j \cos\left(\theta_{ij}\right) = Nb^2$$

Hence  $R = \sqrt{Nb}$ . How will this scatter? Let  $|f(q)|^2$  represent the form factor of each monomer unit. The structure factor will be given by

(109) 
$$\frac{1}{N} \left\langle \left| \sum_{n,=1}^{N} \exp\left(i\vec{q} \cdot r_{n}\right) \right|^{2} \right\rangle_{angle} = \left\langle \sum_{m,n=1}^{N} \exp\left[i\vec{q} \cdot \left(\vec{r}_{m} - \vec{r}_{n}\right)\right] \right\rangle_{angle} = \sum_{n,m=1}^{N} \frac{\sin\left(q\left|\vec{r}_{m} - \vec{r}_{n}\right|\right)}{q\left|\vec{r}_{m} - \vec{r}_{n}\right|} \right\rangle$$

If we expand this for small q we obtain

(110)

(111) 
$$S(q) \approx \frac{1}{N} \left( 1 - \frac{1}{3} q^2 R_g^2 \right)$$

With

(112) 
$$R_{g}^{2} = \frac{1}{2N^{2}} \left\langle \sum_{n,m=1}^{N} \left| \vec{r}_{n} - \vec{r}_{m} \right|^{2} \right\rangle$$

In fact, the structure factor of the polymer chain can be solved exactly (see [10]) to give (113)  $S(q) = Nf(q^2R_g^2)$ 

With

(114) 
$$f(x) = \frac{2(e^{-x} - 1 + x)}{x^2}$$

Referred to as the Debye function.



A real polymer will not yield this structure factor because there is an additional constraint that the chains not cross. This makes the radius of gyration a little larger than expected. In fact, one finds a result closer to  $R_g \sim N^{0.588}$ . Interestingly, however, in a very dense melt, we obtain the result of eq. (108) again. This is because there is no way for a chain to distinguish its own members from those of its neighbors, and therefore the excluded volume effect is cancelled out. It is, however, not possible to measure the structure factor of a single chain within a melt using x-ray scattering since there is no what to isolate which chain does the scattering. However, with neutron scattering it is possible to deuterate a few selected chains, and hence measure the structure factor of individual chains within a melt.

Problems

- 20. Show that  $S(\vec{q}) \approx Z^2$  for a gas, when the positions of the atom centers are uncorrelated.
- 21. Consider a point a distance y away from a uniform beam of x-rays of intensity *I*. Assume that the result of problem 18 applies and further that the atomic structure factor of the gas can be ignored. Use eq. (76) to show that the intensity scattered into a detector of area *dA* is given by  $2Z^2r_0^2\rho IdA/y$  where

 $\rho$  is the number density of gas atoms.

- 22. A typical x-ray beam at the APS contains Consider  $10^{15}$  photons/s . Consider the passage of this beam through air (assumed to be N<sub>2</sub> gas).
  - a. Use the results of problem 19 to calculate the number of photons/sec scattered into a  $1 \text{ cm}^2$  detector located 1m from the an infinitely long pencil of beam.
  - b. Assume that you were, foolishly, sitting inside an x-ray enclosure 1 m from this beam. Suppose that the x-ray beam was completely absorbed within 1 mm of the surface of your skin, and assume that approximately 0.01 J of radiation per gm of material will give a lethal dose of radiation to your skin. How long would it take to acquire a lethal dose of radiation under these circumstances?
- 23. Show that  $S(\vec{q}) = \rho_{avg} \int e^{i\vec{q}\cdot\vec{r}} g(\vec{r}) d^3\vec{r}$  where the correlation function is defined

by 
$$g(\vec{r}) = \frac{V}{N^2} \int \rho_N(r') \rho_N(r-r') d^3 \vec{r'}$$
. Note that  $g(\vec{r})$  is defined so that it

becomes unity for un-correlated atoms.

- 24. Derive eq. (95)
- 25. Show that Eq. (100) is the limit of Eq. (96) at large q when averaged over a period of the oscillations.
- 26. Consider a colloidal suspension interacting with an external field. Using the Boltzmann distribution one can show that the local particle density at position r in an external field v(r) can be written as  $\rho(r)=\rho \exp(-W(r)/kT)$ . Here W(R) is the free energy (relative to a point where v(r)=0) of putting a molecule at r. The quantity W(R) has two contributions: (a) the direct interaction between the molecule and the external field, i.e. v(r) and (b) the effect which the presence of a molecule at r will have on the local density of molecules around r. The resulting excess of molecules (which may be positive or negative ) due to (b) also interacts with the external field and contributes to W(R). For a weak external field this second contribution has the form

 $\int \rho [g(\mathbf{r} - \mathbf{r'}) - 1] v(\mathbf{r'}) d\mathbf{r'} \text{ where } \rho [g(\mathbf{r} - \mathbf{r'}) - 1] v(\mathbf{r'}) d\mathbf{r'} \text{ is the excess}$ number of molecules at the volume element  $d\mathbf{r'}$  locate at  $\mathbf{r'}$  given that there is a molecule at  $\mathbf{r}$ , and  $g(\mathbf{r})$  is the correlation function. Assuming that  $v/kT \ll 1$ 

show that 
$$\rho(r) - \rho = \Delta \rho = -\frac{\rho v(\mathbf{r})}{kT} - \frac{\rho^2}{kT} \int [g(\mathbf{r} - \mathbf{r}') - 1] v(\mathbf{r}') d\mathbf{r}'.$$

27. Show that the Fourier transform of the equation in exercise 14 results in Eq. (106).

- 28. Show that Eq. (114) and (113) are consistent with Eq. (111).
- 29. Show that equation (112) can be re-written as  $R_g = \frac{1}{N} \left\langle \sum_{n=1}^{N} \left| \vec{r}_n \vec{r}_{cm} \right|^2 \right\rangle$ .



# **Surface Scattering**

We consider the scattering of x-rays from a flat interface between the vacuum and a material. For a reference to the treatment detailed here see Sinha [11]. Initially, let us assume that the surface is perfectly flat. We start with eq. (88) for the differential scattering cross section. Let the surface be at z=0. The electron density is described by a Heavyside function  $\rho_e(z) = \rho_{\infty}\theta(z)$ . Here  $\rho_{\infty}$  is the density deep within the material. Substition of this density profile gives for the integral in eq. (88),

(115) 
$$\int e^{i\vec{q}\cdot\vec{r}}\rho_e(\vec{r})d^3\vec{r} = \iiint dxdydz\rho_{\infty}\theta(z)\exp\left[i\left(q_xx+q_yy+q_zz\right)\right].$$

Using the relationship that

(116) 
$$\int_{-\infty}^{\infty} e^{iqx} dx = 2\pi\delta(q)$$

We can rewrite eq. (115) as

(117) 
$$\int e^{i\vec{q}\cdot\vec{r}}\rho_e(\vec{r})d^3\vec{r} = \rho_\infty 4\pi^2 \delta(q_x)\delta(q_y) \int_{-\infty}^{\infty} \theta(z)e^{iq_z z}dz$$

We can simplify this further using the integration by parts and the relationship that (118)  $d\theta(z)/dz = \delta(z)$ . This gives

This gives

(119) 
$$\int e^{i\vec{q}\cdot\vec{r}}\rho_e(\vec{r})d^3\vec{r} = \rho_\infty 4\pi^2\delta(q_x)\delta(q_y)\int_{-\infty}^{\infty}\frac{\delta(z)e^{iq_z z}}{iq}dz = \frac{\rho_\infty 4\pi^2\delta(q_x)\delta(q_y)}{iq}$$

Hence we have

(120) 
$$\left(\frac{1}{V}\frac{d\sigma}{d\Omega}\right) \approx \frac{r_0^2}{V} \left|\int e^{i\vec{q}\cdot\vec{r}} \rho_e(\vec{r}) d^3\vec{r}\right|^2 = \frac{r_0^2}{V} \frac{16\pi^4 \delta^2(q_x) \delta^2(q_y) \rho_0^2}{q_z^2}$$

In order to eliminate the delta functions we need to integrate this differential cross section over the area of the detector. The actual measured intensity is given by

(121) 
$$I(q) = \iint \Phi_0 \frac{d\sigma}{d\Omega} d\Omega = \iint \frac{I_0}{A_0} \frac{d\sigma}{d\Omega} d\Omega$$

We can write the solid angle in terms of the q-vector as shown in the diagram below.



In order to make further progress we must evaluate an integral of the form

(123) 
$$\int_{q_x - \Delta q_x/2}^{q_x + \Delta q_x/2} \delta^2(q_x) dq_x = \delta(0) = \infty?$$

However, in reality the sample is not infinite, so actually

(124) 
$$\delta(0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iq_x x} dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i0x} dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \xrightarrow{\text{finite sample size}} \int_{-L_x/2}^{L_x/2} dx = \frac{L_x}{2\pi}$$

Thus

(125)

$$\iint \frac{I_0}{A_0} \frac{d\Sigma}{d\Omega} d\Omega \approx \rho_0^2 r_0^2 \iint \frac{16\pi^4 \delta^2(q_x) \delta^2(q_y) \rho_0^2}{q_z^2} dq_x dq_y = \frac{I_0}{A_0} \frac{r_0^2 \rho_0^2}{V} \frac{16\pi^4}{q_z^2} \frac{A_{sample}}{4\pi^2} \frac{1}{k^2 \sin(\theta)}$$

Using  $A_{sample} / A_0 = \sin(\alpha)$ , and  $q_z = 2k \sin(\alpha)$  gives

(126) 
$$\frac{I_{scat}}{I_0} \equiv R(\theta) = \frac{16\pi^2 r_0^2 \rho_0^2}{q_z^4} \equiv \left(\frac{q_c}{2q_z}\right)^4$$

Here we have defined (for reasons that will become clear later)

(127) 
$$q_c^2 = 16\pi\rho_0 r_0$$

Since  $q_z = 2k \sin(\theta)$  equation (126) predicts that the scattering falls off as the fourth power of the angle for small angles. In addition, equation (127) predicts that the absolute magnitude of the scattering is proportional to the square of the electron density. However it can be seen that for very small angles the reflectivity is predicted to go above unity, which is not possible. The problem with the above derivation lies in the Born approximation, since this is only valid when the scattering is much smaller than the incident intensity. We will go on to derive a more exact solution shortly.

Before considering the exact solution consider the case of a non-sharp interface described by a density profile  $\rho(z)$ . In this situation eq. (119) becomes

$$(128)\int e^{i\vec{q}\cdot\vec{r}}\rho_e(\vec{r})d^3\vec{r} = \rho_\infty 4\pi^2\delta(q_x)\delta(q_y)\int_{-\infty}^{\infty}\frac{d\rho(z)}{dz}\frac{e^{iq_z z}}{iq}dz = \frac{4\pi^2\delta(q_x)\delta(q_y)}{iq}\int_{-\infty}^{\infty}\frac{d\rho(z)e^{iq_z z}dz}{dz}dz$$

And thus the differential scattering cross section becomes

(129) 
$$\frac{I_{scat}}{I_0} = \left(\frac{q_c}{2q_z}\right)^4 \left|\frac{1}{\rho_{\infty}}\int_{-\infty}^{\infty} \frac{d\rho(z)e^{iq_z z}dz}{dz}\right|^2$$

Here  $q_z = 4\pi \sin(\alpha)/\lambda$  thus we see that a measurement of the reflectivity as a function of angle yields the Fourier transform of the derivative of the density profile normal to the surface. For the case of a rough surface, the calculation is more complicated, but the result is essentially that the intensity is a measure of the average density profile over the coherence length of the x-rays on the surface. In addition a rough surface will scatter some intensity outside the specular condition. This can be described in the context of the distorted wave Born approximation which requires the more exact treatment of the wave solution given below.

As a simple example consider a surface with a density profile described by an error function, e.g.

(130) 
$$\frac{1}{\rho_{\infty}}\frac{d\rho(z)}{dz} = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-z^2/2\sigma^2}$$

Such a profile can result from random roughness such as capillary waves on a liquid or steps on the surface of a solid, or alternately it can represent a truly diffuse profile such as the interface between two polymers which slightly intermix. In this case eq. (129) give

(131) 
$$\frac{I_{scat}}{I_0} = \left(\frac{q_c}{2q_z}\right)^4 e^{-\sigma^2 q_z^2}$$

Thus for a surface with a Guassian derivative interfacial profile, the scattering intensity falls off as  $q_z^{-4}$  multiplied by a Gaussian falloff.

In order to do better than the Born approximation, one can try to find an exact solution to Maxwell's equations in the presence of an interface. We present here a simplified

derivation of Fresnel's laws of reflection and refraction, for the case of grazing incidence where polarization can be ignored.

Consider the reflection of an electromagnetic wave from the vacuum onto a material with index of refraction  $n_1$ . One can show from Huygen's principle that the angle of reflection is equal to the angle of incidence  $\alpha = \beta$  and that the transmitted beam is refracted according to Snell's law (where we define the angle  $\alpha$  with respect to the surface rather than with respect to the surface normal as is typically done for light)

(132) 
$$\cos(\alpha) = n_1 \cos(\alpha')$$

In addition, there is an angle where  $\cos(\alpha')$  would have to be greater than unity. Angles less than this correspond to total external reflection. We can calculate what this angle is by expanding the cosine term and using  $n \approx 1 - \rho_{N} Z q^{2} / 2\varepsilon_{0} m \omega^{2} = 1 - \rho_{e} r_{0} \lambda^{2} / 2\pi$ . This can also be written in terms of its real and imaginary components  $n = 1 - \delta + i\beta$ . If we ignore the absorption term  $\beta$  we can rewrite (132) for small angles as

(133) 
$$\begin{pmatrix} 1 - \frac{\alpha^2}{2} \end{pmatrix} = (1 - \delta_1) \left( 1 - \frac{\alpha^{\prime 2}}{2} \right)$$
$$\alpha^{\prime 2} = \alpha^2 - 2\delta_1$$

The critical angle thus occurs for  $\alpha_{c} = \sqrt{2\delta} = \lambda \sqrt{\rho_{e}r_{0}/\pi}$ 

(134)

We can re-write eq. (132) in terms of the sine of the angle as

(135) 
$$\frac{1 - \sin^2(\alpha) = n_1 \left(1 - \sin^2(\alpha')\right)}{\sin(\alpha') = \sqrt{\sin^2(\alpha) - \sin^2(\alpha_c)}}$$

Since the z-component of the wavevector  $k_{z0} = k \sin(\alpha)$  we then have for the magnitude of the wavevector inside the material  $k_{z1} = \sqrt{k_{z0}^2 - k_c^2}$ , here  $k_c = 2\pi\alpha_c / \lambda$ 

We can now derive the expected intensities from matching the boundary conditions across the interface. The z-dependence of the electric fields at the interface is given  $E_0 e^{ik_{0z}z}$  for the incident wave,  $E_r e^{-ik_{0z}z} = E_0 r e^{-ik_{z0}z}$  for the reflected wave and  $E_{t}e^{ik_{tz}z} = tE_{0}e^{ik_{tz}z}$  for the transmitted wave. The condition of continuity of the fields and their derivatives then gives for the amplitudes of the waves:

(136) 
$$r = \frac{k_{z0} - k_{z1}}{k_{z0} + k_{z1}}$$

and

(137) 
$$t = \frac{2k_{z0}}{k_{z0} + k_z}$$

The intensity of the transmitted and reflected waves are then given by  $|r|^2$  and  $|t|^2$ . In the limit of  $|r|^2 \ll 1$  we obtain

(138) 
$$\left|r\right|^{2} \approx \left(\frac{q_{c}}{2q_{z}}\right)^{4}$$

For the case of an interface with a density profile given by  $\rho(z)$  it can be shown using the distorted wave Born approximation that a better approximation than eq. (131) is

(139) 
$$\frac{I_{scat}}{I_0} \approx \left| \frac{k_{z0} - k_{z1}}{k_{z0} + k_{zi}} \right|^2 \left| \frac{1}{\rho_{\infty}} \int_{-\infty}^{\infty} \frac{d\rho(z)e^{iq_z z} dz}{dz} \right|^2 \equiv R_F \left| \frac{1}{\rho_{\infty}} \int_{-\infty}^{\infty} \frac{d\rho(z)e^{iq_z z} dz}{dz} \right|^2$$

Here  $R_F$  is the Fresnel reflectivity. Note that this is still an approximation and will not be accurate for small angles where multiple scattering becomes important.

An analogy between reflectivity and the 1-D Schrodinger equation. The 1-D wave equation for reflectivity can also be found from the scaler wave equation (eq. (54)  $\nabla^2 \psi - k^2 \psi = 0$ ). Let us asume we have a dielectric medium and a wave which only varies in the *z* direction, e.g. n(x, y, z) = n(z) and also that the wave has no variation in the y-direction, yielding a two-dimensional problem. We attempt a trial solution of the form:

$$\psi(x,z) = \phi(z)e^{ik_0 x \cos(\theta)} \tag{140}$$

Substituting into eq. (54) and taking out the common exponent we find

$$\frac{d^2\phi(z)}{dz^2} + \phi(z)k_0^2\cos^2(\theta) - k^2\phi(z) = 0$$
(141)

For x-rays, the index of refraction can be given in terms of the density of electrons,  $\rho_e$ , via  $n^2 = 1 - 4\pi r_0 \rho_e / k_0^2$  (using eq. (50) and noting that  $n^2 = \epsilon$ ) thus  $k^2 = k_0^2 - 4\pi r_0 \rho_e$ . We can then rewrite eq. (141) as:

$$\frac{d^2\phi(z)}{dz^2} - \left(k_z^2 + 4\pi r_0\rho_e\right)\phi(z) = 0$$
(142)

This is identical to the 1-D Schrödinger equation with  $\frac{2mV}{\hbar^2} \rightarrow 4\pi r_0 \rho_e$ .

#### Problems

- 30. Prove Eq. (122) in the limit of small angles.
- 31. Consider a surface of a material with average density  $\rho_2$  and a Gaussian surface width given by  $\sigma_2$ . A thin layer of material of thickness *d* and density  $\rho_1$  sits on top of this layer and the interface of this layer with the air is characterized by a Gaussian width  $\sigma_1$ . Calculate the reflectivity as a function of  $q_2$  in the limit of the first Born approximation.
- 32. Derive eqns. (136) and (137) from the continuity conditions.
- 33. Generalize eqns. (136) and (137) for the case where the incident wave is traveling through a medium with index  $n_0$
- 34. Derive the limit of eq. (138)
- 35. Derive eq. 132.

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