1

Basic Physics of X-ray Interactions in Matter

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1.1 Preface

It is the nature of human curiosity to always explore new frontiers. Questioning, observing, and modeling nature are the ingredients for advancement and progress. Observing nature requires gauges and obviously our senses to be well-adjusted instruments to encompass the environment for survival, in the first place, but also for pleasure and for medical diagnostics. A medical doctor would use all his senses to evaluate the status of his patient. The human eye brain system, for example, is designed to detect electromagnetic radiation, which can be also considered as a fluence of neutral particles, so-called photons. Under normal conditions at least some 20 optical photons are required to fire a signal on our retina, which is not that sensitive. In return, the human eye possesses adaptively a luminance range of $10^{14}$, which is a fantastic number. Moreover, the human eye is able to distinguish millions
of colors, which is also a great thing. However, this works only within a frequency range from 400 to 800 nm, while the entire spectrum of electromagnetic waves from AC currents over radio waves to X-rays and gamma rays comprises 23 orders of magnitude. In order to increase our fairly limited window of visibility, special instrumentation is required to detect (but also to generate) this, for our senses are not able to resolve electromagnetic radiation. In other words, we need to shift the associated wavelength to a range accessible to our eyes. This instrumentation would measure physical parameters of particles and radiation such as arrival time, energy, momentum, and position. In order to do so we need to study in detail (what concerns this chapter) and subsequently exploit the underlying mechanism of interaction of radiation with matter. In diagnostics, basically, three frequency bands are used to generate medical images. These are ultrasound to radio waves (20 kHz–GHz) which find applications in medical sonography and magnetic resonance imaging (MRI), X-rays, in the energy interval between some keV and 150 keV, and eventually γ-rays, in the energy interval between some hundreds of keV to some 1000 keV. In this chapter, we will concentrate on the interactions of radiation with matter, with special regard to imaging methods used in medical physics. The chapter is sub-divided into two sections: The first section is a summary of the most important points for readers new in the field, and a selection of the most important equations, which certainly will be useful for the subsequent chapters. The second section (Appendix A) contains a flavor of mathematical development of equations for readers with particular interest in the matter, where I tried to aggregate methods and deductions that can be found in textbooks of classical electrodynamics (Born and Wolf 1999; Jackson 1999; Zangwill 2013) and quantum mechanics (Heitler 1954; Bethe and Salpeter 1957; Messiah 1966; Landau and Lifshitz 1977; Awadalla 2015) and which are sometimes not easy to spot. Due to space constraints in some cases, intermediate steps are waived, but I hope the reader may follow the argument anyway and, in the worst case, refer to the textbooks. Due to the correspondence principle and due to the zero rest mass of the photon, most of the calculations can be executed using classical electrodynamics. In some cases, relativistic or quantum mechanical corrections have been applied, though.

1.2 Introduction

As early as the eighteenth century it was shown by macroscopic observations that the attenuation of visible light relates to the properties of the material through which the light is traveling (Lambert 1760; Beer 1852).

Following the arguments of Beer (1852), we assume a monochromatic wave field traveling in a direction \( \vec{k} = k \cdot \hat{e}_r \) (\( \hat{e}_r \) being the unit vector of length 1 pointing into the x-direction) parallel to the x-axis and impinging perpendicularly onto a material sample, which is divided into thin slices of the thickness, \( \Delta x \) (Figure 1.1). According to Figure 1.1a and as demonstrated in Section A.1.2 we note that the incident intensity is proportional to the square of amplitude \( I \cdot E_r \) of the wave field. We also assume \( \Delta x \) is sufficiently thin (\( \Delta x \rightarrow dx \)) that one particle in a slice cannot obscure another particle in the same slice when viewed in the x-direction. The radiant intensity \( dI(x') \) that emerges from a slice is reduced, compared to the intensity that entered \( I' \), by

\[
\frac{dI'}{I'} = -\mu \cdot I(x') \cdot dx
\]

(1.1)

where \( \mu \) is the linear attenuation coefficient, whose numerical value is material dependent. Equation 1.1 is a homogenous differential equation of first order, which can be solved by the separation of the variables and by subsequent partial integration, thus

\[
\int_{I_0}^{I} \frac{dI'}{I'} = \ln(I) - \ln(I_0) = \ln \left( \frac{I}{I_0} \right) = -\int_{0}^{x'} \mu(x') \cdot dx'
\]

(1.2)

yielding

\[
I(x) = I_0 \cdot e^{-\int_{0}^{x} \mu(x') \cdot dx'}
\]

(1.3)

which is nowadays referred to as the Lambert–Beer law. According to Figure 1.1, we notice that the radiant intensity, \( I(x) \), is proportional to the square of the attenuated amplitude, \( I \cdot E_r \).

If we know the material distribution \( \mu(x) \) along the path of the
light, the line integral in the exponent can be accomplished. This line integral is sometimes referred to as the “ray sum.”

We should remember that light in a vacuum always travels at the same speed, \( c \). As shown in Einstein’s special relativity theory (Einstein 1905a), whenever light propagates in a vacuum, its speed possesses that exact value, no matter in which reference system it is measured. As we will see later, as light travels through materials it will slow down. For instance, the propagation or phase velocity, \( v \), of light in water is only \( v = \frac{3}{4} c \). Therefore, it is not surprising that, in some dielectric (thus electrically polarizable) materials, light will propagate more slowly than high energetic charged particles such as electrons might do. This means that, under certain circumstances, the speed of electrons (although still less than \( c \)) can definitely outstrip the speed of light in these materials. If this is the case, the so-called Cherenkov radiation (Cherenkov 1934) will be emitted. Although the Cherenkov effect is mostly used in high energy physics, nuclear physics, and astrophysics, more recently Cherenkov radiation has been used in in-vivo imaging for the detection of labeled biomolecules (Lui 2010).

The amount by which light slows in a given material is described by the index of refraction, \( n \), which in first order we can define through the so-called dispersion relation (Equation A.18), as \( \ln n = c/v \), which for water would be 1.33. In a naïve view, we can now argue that the radiant wave field is retarded due to the reduced speed of light in the material when compared to a (coherent) reference wave propagating in vacuum. In other words, their relative phases are shifted, which results in a change of propagation direction of the radiant wave field. As indicated in Figure 1.1, this means that the radiant light defined by its propagation vector, \( \vec{k} \), changes its direction with respect to the direction of the incident wave field, \( \vec{k} \), by the so-called refraction angle, \( \Delta \theta_r \).

### 1.3 Macroscopic Description of Interactions of X-rays with Matter

Similar to visible light, Röntgen (1895) observed that, also, the attenuation of X-rays in matter as measured as exposure on a photographic film followed the Lambert–Beer law. However, utilizing different substances, he did not succeed in reflecting or refracting X-rays at that time, and was uncertain if it was possible to deflect X-rays at all. He stated “Doch ist die Sache sehr unsicher, und die Ablenkung ist, wenn überhaupt vorhanden, jedenfalls so klein, dass der Brechungsexponent der X-Strahlen in den genannten Substanzen höchstens 1.05 sein könnte” [“But the thing is very uncertain, and the deflection is, if present at all, in any case so small that the refractive index (exponent) of the X-rays could be at most 1.05 in those substances”] (Röntgen 1895, p. 5). As we will see later, the refractive index, \( n \), for X-rays is indeed very close to unity, which explains why it took several decades to develop the first X-ray lenses and to adapt well-known optical concepts such as phase contrast or dark field imaging to imaging modalities utilizing X-rays.

We identify the transmission, \( T \), of X-rays passing through a slab of matter with thickness \( x \) as

\[
T = \frac{I(x)}{I_0} = e^{-\int_0^x \mu(x) \, dx}
\]  

(1.4)

We notice that the highest intensity of X-rays impinges in the very first infinitesimal layer of matter. In a patient, we can identify the latter in most of the cases as the patients’ skin, which then gets most of the radiation. The X-rays will then be attenuated exponentially in the subcutaneous layers (Figure 1.1b). We should also note that the integral in the exponential of Equation 1.4 is commutative.

Therefore, the transmission of X-rays when passing through compound materials characterized by their specific absorption coefficient, \( \mu(x) \), is independent from the relative order of these materials. In other words, each permutation in the relative order of skin, bone, soft tissue, connecting tissue, and fat within a patient should attain the same transmission. As we will see later in the microscopic description of absorption of X-rays, this is not always the case. We should also note that the absorption or attenuation \( A \) is given by

\[
A = 1 - T
\]  

(1.5)

For a discrete contribution of \( N \) materials in matter, the integral in the exponential of Equation 1.4 can be approximated by a sum, and we get

\[
T = \frac{I(x)}{I_0} = e^{-\sum_{i=1}^{N} \mu_i \Delta x_i}, \quad \text{with} \quad x = \sum_{i=1}^{N} \Delta x_i
\]  

(1.6)

In the special case for a single material possessing a constant attenuation coefficient, \( \mu \), we see that Equation 1.3 turns into \( I(x) = I_0 \cdot e^{-x \mu} \). Thus, knowing the thickness of the sample together with the measurement of the incident and radiant X-ray intensities, respectively, we are then able to determine the attenuation coefficient through

\[
\frac{-\ln(T)}{x} = \mu
\]  

(1.7)

once we apply an appropriate geometry. This will be discussed later in Section 1.4.8.

We can ask ourselves at which absorber thickness, \( x_{1/2} \), the initial intensity drops by 50%, which means we look at \( -\ln(T) = -\ln(0.5) \) and, according to Figure 1.1b, this would be exactly where the transmission crosses the absorption.

\[
\frac{-\ln\left(\frac{1}{2}\right)}{\mu} = \frac{\ln(2)}{\mu} = \Lambda \cdot \ln(2) = x_{1/2}
\]  

(1.8)

The dimension of the quantity \( \Lambda = \mu^{-1} \) is a length and is referred to as the mean free path.

We have to keep in mind that both \( I_0 \) and \( I(x) \) are measurable quantities, which are prone to statistical errors and, therefore, should be strictly interpreted as mean values \( \langle I_0 \rangle \) and \( \langle I(x) \rangle \), together with their associated variances. Up to now we merely considered the wave nature of X-rays. Due to the wave–particle duality we have to understand X-rays also as particles with zero rest mass, which we, hence, will refer to as quanta or photons. The good thing is that, due to this particle wave duality, together with the null rest mass of the photon, we can understand most
of the phenomena using classical electrodynamics. As we will see, particle parameters such as the energy, \( E \), and the momentum, \( \vec{P} \), are linked to wave parameters (the angular frequency, \( \omega = 2 \cdot \pi \cdot \nu \), and the wave vector, \( \vec{k} \), \( | \vec{k} | = 2 \cdot \pi / \lambda \), where \( \nu \) is the frequency and \( \lambda \) is the wavelength) through the Planck–Einstein relations (Cohen-Tannoudji et al. 1973):

\[
E = h \cdot \nu = h \cdot \omega
\]

\[
P = h \cdot \vec{k}
\]  

(1.9)

where \( h \) denotes Planck’s constant (or the quantum of action \( h = 6.626 \cdot 10^{-34} \text{ J} \cdot \text{s} \)) and \( h = \hbar / (2 \cdot \pi) \) is the reduced Planck constant. It is noteworthy that the Planck constant has dimensions of physical action; such as energy multiplied by time, or momentum multiplied by distance \( (\Delta x \cdot \Delta P) \), which would translate into an angular momentum. In this context, we should remember the uncertainty principle, which was introduced by Heisenberg (1927). The uncertainty principle asserts a fundamental limit to the precision with which certain pairs of complementary physical properties (or operators in quantum mechanics) of a particle, such as position, \( \Delta x \), and momentum, \( \Delta P \), can be known simultaneously, in other words

\[
\Delta x \cdot \Delta P \geq \frac{\hbar}{2}
\]

(1.10)

Since time is to energy as position is to momentum, we might rewrite Equation 1.10 naïve to

\[
\Delta t \cdot \Delta E \geq \frac{\hbar}{2}
\]

(1.11)

However, here we have to be careful, since quantum mechanics knows an energy operator (the Hamiltonian), but a time operator does not exist. In spite of the missing time operator, the time-energy uncertainty relation can be proven anyway (Messiah 1966). Therefore, Equation 1.11 is reasonable as a definition for time uncertainty, because it gives the shortest time scale in which we will be able to notice changes in the energy states.

In the particle picture of X-rays, the aforementioned mean intensities should, therefore, equalize mean numbers of photons, together with the associated variances. To obtain photon numbers, we have to divide the mean intensity by the specific photon energy, \( h \cdot \omega \), thus we get \( \langle N(x) \rangle / (h \cdot \omega) = \langle N(x) \rangle \). Inserting this equivalence, for instance, into Equation 1.6, we get

\[
T = \frac{\langle N(x) \rangle}{\langle N_0 \rangle} = e^{\sum \xi \Delta t}.
\]

(1.12)

We should note that the absorption process of photons in a matter is governed by the Poisson statistics (Poisson 1837), which assume the existence of small enough subintervals for which the probability of an event occurring twice is “negligible.” For the Poisson distribution, the probability, \( P(k) \), of observing \( k \) events in an interval is given by:

\[
P(k) = \frac{n^k \cdot e^{-n}}{k!},
\]

(1.13)

in which \( k \geq 0 \) is an integer, \( \eta \) is the mean value, and \( k! \) is the fractional of \( k \). The first practical application of the Poisson statistics was presented by von Bortkiewicz (1898). He presented here his famous analysis of “Die durch Schlag eines Pferdes im preussischen Heere Getöteten.” [“Those killed in the Prussian army by a horse’s kick.”] The Poisson statistics applied here, since the sample size was reasonably large (all the soldiers of the Prussian army), but the actual events (killed by a horse’s kick) were rare. Interestingly the mean value and the variance of a Poisson-distributed random variable are both equal to \( \eta \). This means if we measure \( \eta = \langle N(x) \rangle \) photons after passing through a slab of matter with thickness \( x \) the error in our measurement in terms of the standard deviation (the square root of the variance) will be \( \sqrt{\langle N(x) \rangle} \). Therefore, the relative error of our measurement of the radiant numbers of photons \( \delta \langle N(x) \rangle \) is given by

\[
\delta \langle N(x) \rangle = \frac{\sqrt{\langle N(x) \rangle}}{\langle N(x) \rangle} = \frac{1}{\sqrt{\langle N(x) \rangle}}
\]

(1.14)

We now can define the inverse of the relative error as the signal to noise ratio (SNR):

\[
\text{SNR} = \frac{1}{\delta \langle N(x) \rangle} = \sqrt{\langle N(x) \rangle}
\]

(1.15)

Since in medical imaging \( \langle N(x) \rangle \) is the number of X-rays escaping from the patient (typically 9%), which is forming the exposure on the image receptor, the relative error in the resulting radiograph decreases with increasing intensity. Accordingly, the SNR increases with increasing intensity. This matches our daily experience that we can read a book better the more ambient light we have available.

For a Poisson process, hits occur with a known long-term average rate, \( \xi \), of hits per unit time. The Poisson distribution would let us find the probability of getting some particular number of hits. Now, instead of looking at the number of hits, we consider the random variable, \( L \), which is the time we have to wait for the first hit \( (k = 0) \). The probability that the waiting time, \( t \), is greater than a given time value, \( L \), is then

\[
P(L > t) = \frac{(\xi \cdot t)^0 \cdot e^{-\xi t}}{0!} = e^{-\xi t}
\]

(1.16)

keeping in mind that \( 0! = 1 \). This implies that in a Poisson process the probability of two consecutive hits increases with decreasing waiting time between two hits. Typical examples are airplane crashes, which follow the Poisson statistics, since the sample size is again large, while the occurrences of the events are rare. This means, once an airplane has crashed we will find a high probability that a second accident will happen a short time afterwards.

The fact that X-rays occur rather temporal “packed” than equally distributed in time has some implications on systems possessing significant processing times. In particular, this applies to image receptors, which require some inherent and so-called dead time, \( \tau_p \), to process a photon detection event. We will come back to this aspect later.
So far, we have been concerned with monochromatic wave fields only. However, the electromagnetic fields emitted by a physical source are never strictly monochromatic, and even the narrowest emission lines possess a certain energy bandwidth. As shown in Section A.3, the spectral distribution of an X-ray tube, \( P(E) \), can be energetically fairly wide. It is a sensitive assumption that the linear attenuation coefficient, \( \mu \), is not only material specific, but will also vary with the X-ray energy. If we subdivide the spectral distribution, \( P(E) \), into \( K \) discrete energy steps of \( \Delta E \), we can identify \( I_\gamma \) for each of the respective energies, \( E_\alpha, \gamma = 1, K \), and \( K \) as \( I_\gamma(E) = P(E) \cdot \Delta E \). In case our image receptor integrates over all energies, Equation 1.3 will become

\[
I(E,x) = \sum_{\gamma=1}^{K} P(E_\gamma) \cdot e^{-\int_{E_\gamma}^{E_\gamma'} \mu(E,x') \, dx'} \cdot \Delta E \quad (1.17)
\]

or, for a discrete distribution of \( N \) different elements in the sample:

\[
I(E,x) = \sum_{\gamma=1}^{K} P(E_\gamma) \cdot e^{-\sum_{i=1}^{N} \mu(E_i,\Delta x_i) \cdot \Delta x_i} \cdot \Delta E \quad (1.18)
\]

For each of the \( K \) energy steps we find an equation of the type

\[
I(E_\gamma,x) = P(E_\gamma) \cdot \Delta E \cdot e^{-\sum_{i=1}^{N} \mu(E_i,\gamma) \cdot \Delta x_i} \cdot e^{-\mu(E_\gamma,\Delta x_\gamma) \cdot \Delta x_\gamma}, \ldots, \cdot e^{-\mu(E_\gamma,\Delta x_N) \cdot \Delta x_N} \quad (1.19)
\]

or in terms of the transmission per energy interval

\[
-\ln(T(E_\gamma,x)) = -\ln \left( \frac{I(E_\gamma,x)}{P(E_\gamma)} \right) = \mu(E_\gamma,\Delta x_1) \cdot \Delta x_1 + \mu(E_\gamma,\Delta x_2) \cdot \Delta x_2 + \cdots + \mu(E_\gamma,\Delta x_N) \cdot \Delta x_N \quad (1.20)
\]

We can consider \( \mu(E_\gamma,\Delta x_i) \) as known values, which are available in specific databases (see Table C.1 in Appendix C) for arbitrary chemical elements and X-ray energies, respectively. If the number of energy steps, \( K \), is equal to the number, \( N \), of elements in the sample, thus \( K = N \), we will obtain a system of \( N \) equations comprising \( N \) (normally) unknown \( \Delta x_i \). Since we can, in principle, measure \( T(E_\gamma,x) \), we yield a system of \( N \) equations with \( N \) unknowns which can be written in the following matrix equation

\[
\begin{pmatrix}
-\ln(T(E_1,x)) \\
-\ln(T(E_2,x)) \\
-\ln(T(E_N,x))
\end{pmatrix}
= \begin{pmatrix}
\mu(E_1,\Delta x_1) & \cdots & \mu(E_1,\Delta x_N) \\
\vdots & \ddots & \vdots \\
\mu(E_N,\Delta x_1) & \cdots & \mu(E_N,\Delta x_N)
\end{pmatrix}
\begin{pmatrix}
\Delta x_1 \\
\vdots \\
\Delta x_N
\end{pmatrix}
\quad (1.21)
\]

A matrix inversion of the \( \mu \) matrix would allow us to solve for the unknown \( \Delta x_i \), as long as the elements of the \( \mu \) matrix are linearly independent. We will see later that, under certain circumstances, such matrix inversion is possible. Let us assume that the thorax of a patient consists of lung (air), bone (Ca), and soft tissue (water) only. Let us further assume that we are using three different and reasonable small X-ray energy intervals in which the absorption coefficients of air, Ca, and water are linearly independent. Executing three transmission measurements would allow us then to solve for the different thicknesses of air, Ca, and water, which can be identified as a lung, a bone, and a soft tissue image, respectively. This is the basic idea of spectral imaging, which, from the instrumental point of view, is challenging but accomplishable. These small X-ray energy intervals can be attained by optical methods, in which a monochromator would select the respective energy band. With the recent progress in detector technology, the necessary energy discrimination of X-rays can also be achieved by energy dispersive image receptors. This implies, however, that each single photon has to be analyzed according to its energy, which requires some processing time, \( \tau_p \). Recalling the time distribution of Poisson events (Equation 1.16), detector based spectral imaging works only as long as \( \tau_p \ll \xi^{-1} \).

Since the density, \( \rho \), and the attenuation coefficient, \( \mu \), are element or compound specific, it makes sense to normalize \( \mu \) to the respective density. The resulting \( \mu/\rho \) is called the mass absorption coefficient, which then is independent from the state of matter of the element or compound. This requires a subsequent multiplication with the real density of the solid, liquid, or gaseous phase, to estimate the final transmission. Using this mass absorption coefficient, \( \mu/\rho \), Equation 1.21 can be rewritten as

\[
\begin{pmatrix}
-\ln(T(E_1,x)) \\
-\ln(T(E_2,x)) \\
-\ln(T(E_N,x))
\end{pmatrix}
= \begin{pmatrix}
\frac{\mu}{\rho_1}(E_1,\Delta x_1) & \cdots & \frac{\mu}{\rho_1}(E_1,\Delta x_N) \\
\vdots & \ddots & \vdots \\
\frac{\mu}{\rho_N}(E_N,\Delta x_1) & \cdots & \frac{\mu}{\rho_N}(E_N,\Delta x_N)
\end{pmatrix}
\begin{pmatrix}
\Delta x_1 \\
\vdots \\
\Delta x_N
\end{pmatrix}
\quad (1.22)
\]

where the indices, \( i \), for the density, \( \rho_i \), refer to the material with the thickness \( \Delta x_i \). This implies that the measurable change in intensity arises also from changes in the density, \( \rho_i \), of the object.

When dealing with polychromatic radiation and not having the possibility of spectral imaging, we need to think of something else to characterize the absorption length of a substances. This brings us to the so-called Half-Value Layer (HVL), which is defined as the layer thickness, which reduces the incident beam intensity by 50%. Recalling Equation 1.8, it is defined as \( \ln(2)/\mu \). From our previous discussion, it is clear that the HVL depends on the spectral distribution, \( P(E) \), and of course on the type of tissue. For most soft tissues, according to the average energy of the X-rays, the HVL ranges from 4 to 8 cm.

### 1.4 Microscopic Description of Interaction

So far, we just treated macroscopic observations in naïve models. To understand the effect on propagation of a wave field in detail we have to consider microscopic effects on the atomic level which are summarized in Figure B.1 in Appendix B. We anticipate that...
the mass absorption coefficient is proportional to the so-called atomic cross-sections. The cross-section can be considered as the likelihood of an interaction when an incident wave field or particle beam impinges on a target object consisting of discrete particles. In the following we will denote a cross-section with \( \sigma \), which is measured in units of an area, thus cm\(^2\). This definition makes a lot of sense if we think of an example from daily life such as archery, where we use a bow and arrow to hit a target possessing a certain area. It is clear that the intrinsic likelihood to hit the bull’s eye (small center area) normalized to the total number of arrows used in the trail is lower than hitting the outer (larger outer ring area). Moreover, we will see that we have to deal with different kind of interactions, \( \sigma \), of photons with matter. Recalling that the number, \( N_A \) (Avogadro = Loschmidt number (Loschmidt 1865)) of constituent particles (atoms or molecules) in a mole of matter is a scaling factor between macroscopic and microscopic (atomic scale) observations of nature, we can deduce that:

\[
\frac{\mu}{\rho} = \frac{N_A}{A \cdot u} \cdot \sigma = \frac{N_A}{A \cdot u} \sum_i \sigma_i \tag{1.23}
\]

where \( A \) is the atomic mass number, and \( N_A = 6.022140857(74) \times 10^{23} \text{ mol}^{-1} \). Here \( u \) is the atomic mass unit, which is the mass of an atom/molecule expressed in units of 1/12 of the mass of a single \(^{12}\text{C} \) atom at rest. These and other constants used in throughout this chapter are listed in Appendix D.

One should verify that the dimension of Equation 1.23 is given in cm\(^2\)/g. In order to understand the concept of different cross-sections, we have to start with the atom in the first place.

### 1.4.1 Atom Models

In the following we will consider most of the time the relatively simple Bohr model (Bohr 1913). In spite of its shortcomings, the model’s success is due to its explanation of the spectral emission lines of atomic hydrogen and it solved the problems associated with the Rutherford model (Rutherford 1911), in which the atom consists of a central charge or nucleus holding most of the atomic mass surrounded by a cloud of presumably orbiting electrons.

We know from Section A.1 and especially from Equation A.37 that point charges such as electrons exposed to non-relativistic acceleration, \( \vec{a} \), radiate electric fields. We saw there that the instant power radiated per unit area by the accelerated electron in the \( \vec{n} \) direction, which we can measure at \( \vec{r} \), is described by the Poynting vector, \( \vec{S} \),

\[
\vec{S}(\vec{r}, t) \sim \frac{\vec{a} \cdot \vec{n} \sin^2(\theta)}{l^2} \cdot \vec{n} \tag{1.24}
\]

where \( \theta \) denotes the angle between \( \vec{a} \) and \( \vec{n} \). We note that the radiated power decreases with the square of the inverse distance from the accelerated point charge (\( l \)) and increases with the square of its acceleration. Due to the \( \sin^2(\theta) \) term, we will observe in the far field a donut shaped emission pattern known as dipole radiation (see Figure 1.18). Since, in Rutherford’s atom model, the orbiting electrons would be subject to high angular acceleration, \( \vec{a} \), they would constantly emit dipole radiation (Figure 1.2a), which means they would constantly lose energy. As a consequence, the orbiting electrons would spiral towards the nucleus and, subsequently, annihilate after a very short time, which is not observed, since we are still able to write and read books. Bohr (1913) proposed his quantized, but one-dimensional shell model (Figure 1.2b) of the atom to explain how electrons can have stable orbits around the nucleus. This model includes that electrons in atoms orbit the nucleus only at certain discrete distances (stationary orbits), without radiating. These distances are associated with certain energy levels or shell energies. In Bohr’s model, bound electrons in an atom can only change their energy by the transition from one allowed orbit/shell to another one (Figure 1.2b). As is shown in Section A.1.5, the energy of the \( n \)th shell (\( n = 1, 2 \ldots \)) in hydrogen like atoms is given by

\[
E_n = -R \cdot \frac{Z^2}{n^2} = -13.6 \text{eV} \cdot \frac{Z^2}{n^2} \tag{1.25}
\]

whereas each shell can hold up to \( 2 \cdot n^2 \) electrons. In Equation 1.25, \( R \) is also known as Rydberg constant in units of energy with a numerical value of approximately 13.6 eV. From Equation 1.25, we see that the binding energy decreases with the inverse square
of the principle quantum number. For the outer shells or larger \( n (n \rightarrow \infty) \) the binding energy of the electrons approximates zero, which means we can consider those as free electrons. Electrons in the innermost K-shell \( (n = 1) \) are most tightly bound to the nucleus, which is indicated by the greatest negative binding energy. Regarding the binding energies for poly electron atoms, a widespread simplification is that the effective charge of the nucleus decreases by 1 when an unpaired electron is screening it. Moseley (1913) presented his empirical formulae to calculate K- and L-shell energy levels for poly electron atoms, and Equation 1.25 turned into

\[
E_a = -13.6 \text{eV} \cdot a \cdot \frac{(Z - b)^2}{n^2} \quad (1.26)
\]

where \( a \) and \( b \) are constants, both 1 for \( n = 1 \). Using this formula for a poly electron atom such as oxygen \( (Z = 8) \) the characteristic binding energy of the K-shell of 666.4 electron volts (eV) is overestimated by approximately 20% \( (E_K = 550 \text{ eV}; \text{Bearden and Burr 1967}) \), but gives at least the right order of magnitude. We also note that the binding energy scales with the square of the atomic number. This means, for high \( Z \) materials like in a \( ^{235}\text{U} \) atom \( (Z = 92) \), we can obtain substantial K-shell binding energies such as 112.6 keV \( (E_K = 115.6 \text{ eV}; \text{Bearden and Burr 1967}) \).

The binding energies calculated according Equation 1.26 for the K- and the L-shell versus the atomic number are shown in Figure 1.3. As we see in the examples, the simple model approximates at least within an order of magnitude the real binding energies as found in literature (Bearden and Burr 1967) or in databases (Henke et al. 1993).

We can also use Equation 1.25 to calculate the energy change, \( \Delta E \), associated to an electron transmission from shell \( i \) to shell \( j \), which is given as

\[
\Delta E = E_i - E_j = 13.6 \text{eV} \cdot Z^2 \cdot \left( \frac{1}{j^2} - \frac{1}{i^2} \right) = \hbar \cdot \omega \quad (1.27)
\]

This energetic change is associated with the absorption \( (j < i) \) or emission \( (j > i) \) of electromagnetic radiation. In 1888, Rydberg devised a similar Rydberg formula, which was used to predict the wavelengths of photons emitted by changes in the energy level of an electron in a hydrogen atom (Ritz 1908). In order to calculate the energy of the emission lines, and inspired by Rydberg, Moseley (1913) found empirically that

\[
E(K_\alpha) = \hbar \cdot (3.29 \cdot 10^{15}) \cdot 3 \cdot \frac{(Z - 1)^2}{4} \quad E(L_\alpha) = \hbar \cdot (3.29 \cdot 10^{15}) \cdot 5 \cdot \frac{(Z - 7.4)^2}{36} \quad (1.28)
\]

We should note that, if we are able to measure the energy of a given K, L, or M line then we are capable of determining the
atomic number of the element producing that line, which brings us back to the earlier discussion of spectral imaging (Equation 1.22) (Figure 1.4).

Although Bohr’s model was successful at describing binding energies and emission lines in the hydrogen atom, it failed to predict the exact binding energies for others. Moreover, it is a one-dimensional model that describes the size of the orbit only by the quantum number, \( n \), as we have seen in Section A.1.5. We calculated the orbit, \( R \), using Equation A.59, as \( R = a_0 \cdot n^2 / Z \), where \( a_0 = 0.53 \cdot 10^{-8} \text{ cm} \) is the Bohr radius. Since the model does not foresee an upper limit in the quantum number, \( n \), this means that a hydrogen atom (\( Z = 1 \)) could possess substantial spatial extensions. For instance, for \( n = 1000 \) we would get \( R = 0.53 \cdot 10^{-3} \text{ mm} = 0.53 \mu\text{m} \), which in fact is not observed. In addition, the particle view of Bohr’s atom model impeded the explanation of the observed fine and hyper fine structures in the emission lines, which were partially solved by de Broglie (1925) and eventually by Schrödinger (1926). Similar to the particle-wave dualism of light particles, electrons also possess wave-like properties. By rearranging the momentum Equation 1.9, de Broglie (1925) found a relationship between the wavelength, \( \lambda \), associated with an electron and its momentum, \( P \), through the Planck constant

\[
\lambda = \frac{\hbar}{|P|} \quad (1.29)
\]

In this view, electrons bound to an atom can be considered as standing waves where the lowest possible energy is equivalent to the fundamental frequency of its wave function. Higher energy states are then similar to harmonics of the fundamental frequency. These standing wave functions represent the eigenstates of the Hamiltonian operator for the energy and are solutions of the Schrödinger equation (Schrödinger 1926) (see Section A.5). According to the uncertainty principle, this also implies that electrons are never found in a single point location, although the probability of interacting with the electron at a single point can be estimated from its wave function. To explain the observed phenomena and the solution of the Schrödinger equation requires more than just a principle quantum number, \( n \). In fact, Schrödinger’s model allows the electron to occupy three-dimensional space. As we show in Section A.5, this requires a wave function of the type \( R(\vec{r}) = N_j \cdot e^{i \phi} \cdot P_\ell^m(\cos(\theta)) \cdot e^{i m \phi} \) and, subsequently, three quantum numbers to describe the orbitals in which electrons can be found. The multiplicative functions and their associated quantum numbers describe the size, shape, and orientation in space of the orbitals of an atom.

In contrast to the principle quantum number, \( n \), which is (like in Bohr’s model) coupled to the radial component of the wave function and describes the size of the orbit, the angular momentum quantum number, \( \ell \) (the polar component), and the magnetic quantum number, \( m \ell \) (the azimuthal component) are required. The angular quantum number (\( \ell \)) describes the shape of the orbital. As depicted in Figure 1.5, orbitals have shapes that are described as spherical (\( \ell = 0 \)), and with some imagination polar (\( \ell = 1 \)), or cloverleaf (\( \ell = 2 \)). They can even take on more complex shapes as the value of the angular quantum number becomes larger. There is only one way in which a sphere (\( \ell = 0 \)) can be oriented in space. For higher angular numbers and, subsequently, more complex shapes, the orbitals can point in different directions. We, therefore, need the magnetic quantum number, \( m \ell \), to describe the orientation in space of the particular orbital. This is called the magnetic quantum number because the effect
of different orientations of orbitals was first observed in the presence of a magnetic field. There are certain rules that govern the allowed combination of quantum numbers. All quantum numbers are positive integers, whereas \( n \) must be greater than zero (\( n = 0 \) is forbidden). The angular number ranges from 0 to \( n - 1 \). If \( n = 3 \) this means \( \ell \) can be 0, 1, or 2. The magnetic quantum number, \( m_\ell \), can be any integer between \(-\ell \) and \( \ell \). If \( \ell = 1 \), \( m_\ell \) can either be \(-1\), 0, or 1. Orbitals that have the same value as the principal quantum number form a shell. Orbitals within a shell are divided into subshells that have the same value of the angular quantum number. Some conventions describe shells and subshells in which subshells that have the same value of the angular momentum form a shell. Orbitals within a shell are divided into subshells that have the same value of the angular number, \( m_\ell \), whereas the principal quantum number, \( n \), can be 0, 1, or 2. The magnetic quantum number, \( m_\ell \), can be 0, 1, or 2. The magnetic quantum number, \( m_s \), can be \( \pm \frac{1}{2} \) for an electron with spin \( \frac{1}{2} \) or \( \pm \frac{1}{2} \) for an electron with spin \( \frac{1}{2} \). These opposite spin states are also called spin pairing. In the ground state, \( 0s \), electrons are tightly bound to the nucleus, while in the higher orbitals electrons can be considered as almost free electrons. As before in Bohr’s atom model, electrons can change their energetic level within the shells, which we identify with absorption, excitation, and emission. Since the energy states are well defined, we can find for each process an associated lifetime, \( \Delta \tau \), which is defined by the (energy) uncertainty relation (Equation 1.11). For instance, a 3s electron of a vaporized sodium atom is excited within femtoseconds (\( 10^{-15} \) s) and vibrational relaxations (remember we are thinking now of molecules) of excited state electrons to the lowest energy state in the order of picoseconds (\( 10^{-12} \) s) or, more precisely, from \( 10^{-14} \) s to \( 10^{-11} \) s. The fluorescence from the S1 to the S0 state is in the order of nanoseconds to some tenths of microseconds (\( 10^{-9} \) s–\( 10^{-7} \) s). The emission of longer wavelengths and the return to the ground state occurs within nanoseconds. If a change in electron spin is involved, the lifetime of the excited state is prolonged, and can be in the order of seconds to minutes. Because of the high specificity, spatial resolution and extreme sensitivity of the emission profiles, techniques that use fluorescence are rapidly emerging in cell biology, genetics, and in general preclinical in-vivo imaging. We should add that fluorescence is excessively used in imaging detector technology, since it allows shifting wavelength from the X-ray regime into the optical regime and the subsequent detection with optical sensors such as charge coupled devices (CCDs) or complementary metal–oxide–semiconductors (CMOS imagers).

### 1.4.2 Incoherent Thomson Scattering

After the excursion in the world of atom models, we can turn towards the microscopic view of interaction of radiation with matter, and subsequently towards cross-sections. When a wave field of frequency, \( \omega_0 \), and wavelength, \( \lambda \), impinges on an isolated atom, it can interact in a different manner with the bound electrons in this atom. For weakly bound electrons in the outer orbitals of the atom, and a long wavelength (compared to the Bohr radius) of the incident radiation (Section A.1.4), the electron would be accelerated along the polarization of the wave, \( \hat{\Pi}_0 \), similar to a cork bouncing on water waves (Figure 1.6a). While doing so, the cork will be a source of spherical waves which propagate with the same frequency as the
incident wave field. Since the electron undergoes a continuously changing but periodic acceleration, this bouncing electron emits dipole radiation with the same frequency, $\omega_0$, and wavelength, $\lambda_0$, of the incident radiation. The quantity that we are eventually interested in is the flux of energy per surface element generated by the oscillating electron normalized to the energy flux of the incident radiation, which is referred to as a differential cross-section. In other words, the differential cross-section is given by:

$$\frac{d\sigma}{d\Omega} = \frac{\text{energy emitted per solid angle by the electron}}{\text{energy flux of the electromagnetic radiation}}$$  \hspace{1cm} (1.30)

which basically describes the angular distribution of the scattering event. For a weakly bound electron, we calculated the differential cross-section in Section A.1.4, and we obtained, according to Equation A.52, a polarized incident wave field

$$\frac{d\sigma_{th}}{d\Omega} = \frac{n_0^2}{4 \pi \varepsilon_0 c^2 \cdot m^2  \cdot \pi^2} \cdot \sin^2(\theta)$$  \hspace{1cm} (1.31)

where $\theta$ denotes the angle between the polarization, $\vec{n}_0$, and the direction, $\vec{n}$, of an observer, as indicated in Figure 1.6a. The $\sin^2(\theta)$ factor defines the typical donut shaped emission pattern of the radiated fields when seen from a distant point, $\vec{r}$. Regarding the multiplicative factor, one should verify that the dimension of such metrics is given in m$^2$ and, therefore, really can be considered a cross-section. This result was first obtained by J.J. Thomson in 1906 and is, therefore, referred to as the “Thomson scattering cross-section.” To evaluate the order of magnitude of the total Thomson cross-section, we need to integrate over the solid angle (Equation 1.31) as we do in Equation A.54 and we obtain, accordingly,

$$\sigma_{th} = \frac{8 \pi}{3} \cdot n_0^2.$$  \hspace{1cm} (1.32)

The quantity $e^2/4 \pi \varepsilon_0 m c^2 = 2.8 \cdot 10^{-13}$ m is the value of the so-called “classical electron radius,” $r_0$, which can be understood as the radius of a spherical shell of total charge, $e$, whose electrostatic energy equals the rest mass energy of the electron. We can, therefore, consider an electron, when scattering radiation, as a solid sphere with a radius of the classical electron radius order. The total Thomson cross-section $\sigma_{th} = 0.665 \cdot 10^{-24}$ cm$^2 = 0.665$ barn is independent from the wavelength of the incident radiation, which indicates that the scattering of electromagnetic waves on weakly bound or free electrons is the same across the entire spectrum of wavelengths from microwaves to X-rays. However, we should keep in mind that, according to the correspondence principle, the Thomson cross-section remains valid only at low frequencies, when the photon momentum $P_{\gamma}$ can be neglected.

### 1.4.3 Incoherent Compton Scattering

When the wavelength is of the order of the Bohr radius, $\lambda \sim a_0$, or smaller, the electron with the mass $m$ will not just bounce up and down anymore, as assumed previously, but will receive a momentum transfer of the incident wave field, which is given by

$$P_{\gamma} = \omega_0 \cdot h/c.$$  \hspace{1cm}

In the cork–water picture, this means that the ripples of the water wave field are pushing the cork in a forward direction. We saw before when discussing Thomson scattering that the frequency and, subsequently, the energy of incident and radiated photons are equal. Therefore, no energy transfer on the electron took place. Now, when the photon momentum is in the order of $m \cdot c$, we have to correct the classical Thomson cross-section accordingly. Such corrections for scattering on electrons are needed for photon energies of the order of tens or hundreds of keV, which is the energy range used in diagnostic X-ray imaging. In this case our photon-electron scattering can be considered as a two-body process, where we have to obey momentum and energy conservation. Using relativistic kinematics, we were able to obtain the differential cross-section for a Compton scattering process on a free electron possessing the mass $m$ in Section A.1.7. Also, taking the electron spin into account we ended up with the so-called “Klein–Nishina differential cross-section,” which is given by

$$\frac{d\sigma_{Kn}}{d\Omega} = \frac{n_0^2}{2 \cdot \left(1 + \frac{1}{1 + \gamma \cdot (1 - \cos(\theta))} \cdot \left(1 + \cos^2(\theta) + \frac{\gamma^2 \cdot (1 - \cos(\theta))^2}{1 + \gamma \cdot (1 - \cos(\theta))} \right) \right).$$  \hspace{1cm} (1.33)

with $\gamma = \hbar \cdot \omega_0 / (m \cdot c^2)$, where $\omega_0$ is the frequency of the incident photon, and $\theta$ is the angle between the scattered photon and the emitted Compton electron. The energy transfer onto the electron is maximized when the incident photon is backscattered, thus for $\theta = \pi$. The angular distribution of the differential Compton scattering cross-section is depicted in the form of a polar plot in Figure A.4 for different energies of the incident photon. In comparison, we added the trace of the Thomson differential cross-section to the graph, which is symmetrical for forward and backward scattering. The area enclosed by the contour of the Thomson cross-section can be interpreted as the frequency of the emitted radiation normalized to the frequency of the incident photon. Since no energy transfer takes place in a Thomson scattering process, the ratio is unity and, subsequently, the enclosed area is maximized. We can see that the differential cross-section becomes more concentrated in the forward direction as the

![FIGURE 1.7 Probability density function for Compton scattering versus the photon scattering angle.](image-url)
photon energy increases and the enclosed area decreases. For 20 MeV photons, we have a very narrow angular distribution in forward direction, with little backscattering contribution. When for a given scattering angle the photon energy increases, the fraction of the energy transferred to the scattered photon decreases, which is manifested by the decreasing area. Therefore, for a high incident photon energy, the majority of the energy is transferred to an electron. This effect becomes noticeable at the energies of the X-rays used in radiology (from 20 keV up to ~150 keV); however, predominantly the energy is still transferred to the scattered photon. Using the probability density function (PDF) (Equation A.94) that we calculate in Section A.1.7, we can describe the directional distribution of secondary radiation from a Compton scatter process. The relative probabilities of Compton scattering are shown versus the scattering angle for seven X-ray energies (Figure 1.7). Also, here we included the directional distribution of a Thomson process for comparison. The probability is still almost symmetric at 20 keV, which points in the forward direction when the incident energy increases.

As we can see in Figure 1.7, in the range used for clinical radiography, the scattered X-rays are emitted predominantly in the lateral direction, and change insignificantly as the incident photon energy is increased. Consequently, the fraction of Compton scattered X-rays emitted laterally between 45° and 135° can be significant, and sufficient shielding for personnel involved in clinical radiography is mandatory.

As described in Equation A.92, integrating over the solid angle we attained the total Compton scattering cross-section. For the low energy limit, \( E_i^l \ll m \cdot c^2 \), where the incident photon energy is much smaller than the rest energy of the electron and the high energy limit, \( E_i^h \gg m \cdot c^2 \), we can approximate the Compton cross-section with

\[
\sigma^C_{\text{low}} = \sigma^S_{\text{Th}} \cdot (1 - 2 \cdot \gamma) \tag{1.34}
\]

and

\[
\sigma^C_{\text{high}} \propto \ln \left( \frac{E_i^h}{E_i^l} \right), \tag{1.35}
\]

respectively. This means in the low energy limit, thus for \( \gamma \rightarrow 0 \), we end up with the Thomson cross-section. In the high energy limit the Compton cross-section approximates zero. For a Compton event on a poly electron atom of atomic number, \( Z \), we can assume that the cross-section increases by exactly the factor \( Z \) (i.e., \( \sigma^C_{\text{atom}} = Z \cdot \sigma^C \)), since we have \( Z \) electrons as potential scatterers available. As is shown in Equation A.90 during a Compton process, the incident photon energy is only partially transferred to the electron. It is, therefore, quite natural to define something like an energy cross-section as

\[
\sigma_{ES} = \frac{E_i^l}{E_i^h} \cdot \sigma^C \tag{1.36}
\]

And, subsequently, an energy absorption cross-section

\[
\sigma_{EA} = \sigma^C - \sigma_{ES}. \tag{1.37}
\]

The latter is relevant for absorption processes and gives us the probability to find a given transferred kinetic energy of the electron, \( E_{\text{kin}} = E_i^l - E_i^h \). If we were able to determine simultaneously this energy of the Compton electron and the position of the Compton scatter event within a suitable (scatter) detector and measure subsequently the position of the scattered photon in a second photon absorption detector, then we would know the origin of the incident photon along an elliptical base of a cone in the image plane (Figure 1.8).

The opening angle of the cone is equal to the Compton scattering angle, which, according to Equation A.89, is given by

\[
\cos(\theta) = \frac{E_{\text{kin}} \cdot (1 + \gamma) - \gamma}{\gamma \cdot (E_{\text{kin}} - 1)} \tag{1.38}
\]

when rearranging the equation for \( \cos(\theta) \). If the photon was emitted for instance by a radioactive source as one of many, then all possible directions of incident photons form associated cones with an axis along the scattered photons, whereas the apex lies on the interaction point within the scatter detector. The intersection of different cones formed by consecutive events eventually reproduces the position of the source in the image plane. This is the principle of a so-called (fully electronic) Compton Camera, which finds application in nuclear medicine and in single photon emission tomography (SPECT) to reveal radioactive tracer elements within a patient. For the sake of completeness, we should mention that we could invert the Compton process, which means to invert the direction of arrows in Figure 1.6. Instead of hitting an electron at rest we could shoot a high energy electron onto a low energy photon. The electron then would partially transfer its energy onto the photon, which then is shifted towards higher frequencies, such as to higher energies. This process plays an important role in astrophysics (Wilson et al. 2000), but more recently also on the search for compact high brilliant X-rays sources beyond synchrotron radiation (Graves et al. 2014).

Subsequent to a Compton scattering event we remain with an ionized atom, a photon with reduced energy and a free electron with a certain kinetic energy in the final state. The further
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1.4.4 Coherent Rayleigh Scattering

Up to now we have just considered weakly bound electrons, thus electrons in the outer shells of an atom. In the following we want to investigate what is happening when a wave field with the frequency \( \omega_0 \) impinges on a bound electron, which we view as being bound to the nucleus via a spring with a natural angular frequency \( \omega_r \). In the case of Thomson scattering, we assume that the wavelength of the incident radiation is reasonably large in comparison with the classical electron radius. The oscillating electric field of a light wave acts on the charges within a particle, causing them to move at the same frequency. The particle, therefore, becomes a small radiating dipole whose radiation we see as scattered light. We also assume that the electron is reasonably attracted to its orbit, and does not bother to leave it. In other words, once the wave field deflects the electron, it is pulled back to its orbit with a damping rate, \( \gamma_e \), which we assume is much smaller than \( \omega_0 \). In this case, we can apply Newton’s second law of motion of the form,

\[
m \frac{d^2 \vec{r}}{dt^2} + m \cdot \gamma_e \frac{d\vec{r}}{dt} + m \cdot \omega_a \cdot \vec{r} = -e \cdot \vec{E},
\]

(1.39)

where \( m \) is the electron mass, \( e \) the electron charge, and \( \vec{E} \) is the electric field of the incident radiation. Following the steps described in Section A.1.6, we find, for the cross-section of bound electrons,

\[
\sigma = \sigma_m \cdot \frac{\omega_0^4}{(\omega_a^2 - \omega_0^2)^2 + (\gamma_a \cdot \omega_0)^2},
\]

(1.40)

where \( \sigma_m \) again denotes the Thomson cross-section. The angular distribution is the same as in the case of Thomson scattering. We also note that, as the frequency of incident and emitted radiation is the same, therefore no energy transfer takes place. In the resonant case when the incident frequency is equal to the oscillating frequency of the electron (thus \( \omega_a = \omega_0 \)), Equation 1.40 reduces to

\[
\sigma = \sigma_m \cdot \frac{\omega_0^4}{\omega_0^2 + (\gamma_a / 2)^2}.
\]

This cross-section is named after Lord Rayleigh (John Strutt), “Rayleigh scattering cross-section” (Strutt 1871), and depends on the inverse fourth power of the wavelength of the incident radiation. This finding enabled Strutt in 1871 to explain the origin of the blue color of the sky and the polarization of sunlight. Among other applications, such as remote temperature sensing, Rayleigh scattering is important in the field of optical fiber transmission (thus, in the development of endoscopes) and in medical applications of (optical) lasers. Absorption and scattering of laser beams are important in diagnostics and therapy. In the former, Rayleigh scattering is used to elucidate particle sizes with respect to the wavelength of the laser in biological tissues. For lasers in the ultraviolet range, Rayleigh scattering increases sharply at the resonant energy \( h \cdot \omega_0 \) (Lorentzian line shape of halfwidth \( \gamma_a / 2 \)) as the laser wavelength decreases. In this fashion, we can tune the penetration depth of the laser and, subsequently, can treat near superficial cancers, shrink tissues, or control bleeding. While Rayleigh scattering is certainly of great value in these applications, it has a deleterious effect on traditional absorption based medical imaging, where the detection of scattered radiation is undesired, since it causes image blur and decreases the signal to noise ratio in the radiograph. The likelihood of a Rayleigh scattering event increases with decreasing X-ray energy, and, as we will see in the following section, increases with the atomic number of the absorber.

FIGURE 1.9 Model for coherent scattering (a) and photoelectric effect (b).
We now translate the concept of bound electrons to a poly electron atom, as indicated in Figure 1.9a. We observed an atom with the nucleus of charge $Z\cdot e$ located in the origin of a coordinate system from a distant point $\vec{r}$. We do not stress here the point that the wavelength, $\lambda$, must be large in comparison to the extension of the atom, since such an assumption does not hold for high energy X-rays. However, we allow the electron to sit at different coordinates, $\Delta \vec{r}_n$. As for the single electron in the external wave field propagating along the $x$-direction, the electrons start to bounce according to the polarization of the electric field, and start to emit dipole radiation at the same wavelength, $\lambda$, as the incident radiation. Due to the fact that we allow different positions of the electron, the propagation distance of each electron, $\vec{r}_n = \vec{r} - \Delta \vec{r}_n$, to the point of the observer at $\vec{r}$ might be slightly different, which results in a shift of the relative phases $\varphi_n = i \vec{k}_n / \lambda$. Therefore, we expect that in the general case the phase of the radiated fields emitted from electrons at position $\Delta \vec{r}_n$ and $\Delta \vec{r}_{n+1}$ are shifted by the amount $\Delta \varphi = (\Delta \vec{r}_n - \Delta \vec{r}_{n+1}) / \lambda$ when observed from a far distance. Due to this phase shift, we might observe a destructive or non-destructive interference of the emitted wave fields in the far field, depending on the angle $\theta$ under which we observe the atom. Following the steps in Section 1.1 we found, for the total cross-section for coherent scattering in forward direction,

$$\sigma_{coh} \sim \frac{8 \cdot \pi}{3} \cdot r_0^2 \cdot Z^2 = \sigma_{Th} \cdot Z^2 \quad (1.42)$$

In contrast to Thomson scattering, where the incident field works on independent electrons, here the $Z^2$ factor appears, since all $Z$ electrons of the atom contribute coherently to the scattered fields. As an aside, we should draw our attention on the quantity $\Delta \vec{k} = \vec{k} - \vec{k}_0$, which is the difference of the propagation vector of the incident radiation and the propagation vector of the scattered fields towards the observer. According to Figure 1.9a, we can see that

$$|\Delta \vec{k}| = 2 \cdot \frac{\vec{k}_0}{\lambda} \cdot \sin(\theta), \quad (1.43)$$

which can be identified as Bragg’s law (Bragg and Bragg 1913):

$$n \cdot \lambda = 2 \cdot d \cdot \sin(\theta) \quad (1.44)$$

for crystal diffraction, when $|\Delta \vec{k}| = 2 \cdot \pi \cdot n / d$ and $d$ is the spacing of the crystal lattice, $|\vec{k}_0| = 2 \cdot \pi / \lambda$ and $n$ is an integer number. Equation 1.43 explains why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence $\theta$ when we have non-destructive interference. Although Bragg’s law was used to explain the interference pattern of X-rays scattered by crystals, diffraction has been developed to study the structure of all states of matter with any beam, for example ions, electrons, neutrons, and protons, with a wavelength similar to the distance between the atomic or molecular structures of interest. Bragg diffraction is observed only in a small band of incident angles in the order of microradians. A microradian is the angle under which you observe a 1 mm high coin in a distance of 1 km, thus really small. This narrow angular range is called the Darwin width (Darwin 1914) of the reflection, and is in the first order approximation proportional to the wavelength of the incident radiation and, subsequently, inverse proportional to the energy. This effect is extensively used to select narrow energy bands from broad range X-ray sources, whereas the instrument is referred to as a monochromator.

### 1.4.5 Photo Effect

If the energy of the incident photon, $\hbar \cdot \omega$, is greater than the binding energy of a bound electron in a specific shell, $E_{\text{B}}$, of an atom, the photon can be completely absorbed, transferring all its energy to the electron. For energy and momentum conservation, such an effect is not possible on free electrons, but it requires the Coulomb field of the heavy nucleus absorbing the recoil. This mechanism is called the “photoelectric effect” (Figure 1.9b). Here, the photon is exciting the electron from its initial bound state, $\varphi_i$ into a final state, $\varphi_f$. The final state is usually an ionized atom and a free electron, such as an electron wave, is emitted from the atom. Due to energy conservation, the difference between the photon energy and the binding energy is transformed into kinetic energy of the now unbound $E_{\text{kin}} = \hbar \cdot \omega - E_{\text{B}}$ electron, while the photon annihilates. We are now interested in the cross-section of the photoelectric effect which, in analogy to Equation 1.30, we define as

$$\frac{d\sigma}{d\Omega} = \frac{\text{energy absorbed per unit time in } \varphi_i \rightarrow \varphi_f}{\text{energy flux of the electromagnetic radiation}}. \quad (1.45)$$

Following the steps in Section 1.4.5 we ended up with the cross-section of the photoelectric effect being given by

$$\sigma_{PE} = \frac{32}{\epsilon ^2} \cdot \alpha^4 \cdot Z^3 \cdot \sigma_{Th}, \quad (1.46)$$

where $\alpha = e^2 / (\hbar \cdot c) = 1 / 137$ is the fine structure constant, $\sigma_{Th}$ is, according to Equation 1.32, again the Thomson cross-section, and $\epsilon = m \cdot c^2 / (\hbar \cdot \omega)$ is the reduced photon energy. To obtain this result, we applied some restrictions. Equation 1.46 holds valid only for the following approximations, also known as the non-relativistic Bohr approximation (Marmier and Sheldon 1969).

First of all, we considered only light, hydrogen like atoms in the 1 s state with small atomic numbers, Z. Moreover, we assumed that we are far enough from the photoelectric thresholds where the binding energy, $E_{\text{B}}$, of the electron is small compared to the photon energy. Finally, we restricted ourselves to the case that the ejected electron is non-relativistic, which in general holds for incident photon energies up to 50 to 150 keV, thus in a range which is used for diagnostic X-ray imaging. In this energy range, the cross-section drops rapidly with the energy of the photon. For higher photon energies ($\epsilon \ll 1$, thus $E_{\text{B}} > 1$ MeV) the energy dependence is smaller and decreases linearly with the reduced photon energy. In this case, the cross-section is given by

$$\sigma_{PE} = \frac{4 \cdot \pi \cdot r_0^2}{\epsilon} \cdot \alpha^4 \cdot Z^3. \quad (1.47)$$
The $Z^2$ dependence in our approximation implies that this interaction is favorable for poly electron atoms. However, we should remember that we neglect the $Z^2$ in the denominator of Equation A.146 and this correction depends on the incident photon energy. The higher it was, the higher are the atomic numbers allowed in this approximation. Therefore, we would expect the exponent of $Z$ to vary between 4 and 5 in the energy range from 0.1 MeV to 5 MeV. In any case the proportionality to higher powers of the atomic number $Z$ tells us that high $Z$ materials are absorbing X-rays much better than light materials, since the cross-section is coupled to the mass absorption coefficient by Equation 1.23. For instance, the composition of the mineral component of bones can be approximated as hydroxyapatite ($\text{Ca}_10(\text{PO}_4)_6(\text{OH})_2$) and possesses, therefore, an effective atomic number, $Z_{\text{eff}}$ bone $\sim$ 13.8. In contrast, fat is composed basically of carbon ($Z = 6$) and hydrogen ($Z = 1$), which results in $Z_{\text{eff}}$ fat $\sim$ 6. This means that bone features a cross-section four times higher than fat, which explains why bones are dominant in X-ray imaging.

The effective atomic number we used in this context is equivalent to the atomic number, but is calculated for compounds (e.g., water) and mixtures of different materials (such as tissue and bone). Apart from utilizing simple mass-weighted averages, there are different approaches to calculate $Z_{\text{eff}}$. A coarse (and not always accurate) method to calculate the effective atomic number was proposed by Murty (1965), where $Z_{\text{eff}} = \sum i f_i Z_i^{29}\rho$, where $f_i$ denotes the fraction of the total number of electrons associated with each element, and $Z_i$ is the atomic number of each element in the compound of mixture. More accurate methods, for instance Taylor et al. (2012), include interaction cross-sections to determine the effective atomic number of some tissues and contrast agents (Table 1.1).

The strong $Z$ dependence of the photoelectric cross-section is also the reason why chemical elements such as iodine ($Z = 53$), xenon ($Z = 54$), and barium ($Z = 56$) are utilized as contrast agents in X-ray imaging. These elements have high atomic numbers and are therefore more likely to absorb X-ray photons, making them useful for imaging purposes.

TABLE 1.1
Effective Atomic Numbers for Some Tissues and Contrast Agents

<table>
<thead>
<tr>
<th>Material</th>
<th>$Z_{\text{eff}}$</th>
<th>$\rho$ [g/cm$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>7.42</td>
<td>1.0</td>
</tr>
<tr>
<td>Air</td>
<td>7.64</td>
<td>0.00129</td>
</tr>
<tr>
<td>Fat</td>
<td>5.92</td>
<td>0.91</td>
</tr>
<tr>
<td>Muscle</td>
<td>7.46</td>
<td>1.0</td>
</tr>
<tr>
<td>Bone</td>
<td>13.8</td>
<td>1.85</td>
</tr>
<tr>
<td>Iodine</td>
<td>53.0</td>
<td>4.94</td>
</tr>
<tr>
<td>Barium</td>
<td>56.0</td>
<td>3.5</td>
</tr>
</tbody>
</table>

FIGURE 1.10 Cross-section and mass absorption coefficient for the photoelectric effect versus the photon energy for xenon.

and they correspond to the binding energies of electrons within their respective shell. The energy threshold for which the photoelectric effect becomes possible on the most tightly bound electrons in the K-shell is called “K-edge”; the one on the less tightly bound L-shell is called L-edge. Successive edges (M-edge, ...) are defined in a similar way. Since for the K-shell ($n = 1$) we have just one orbital ($\ell = 0$), the K-edge possesses only one peak, while for the L-shell ($n = 2$) we have three possible orbitals ($\ell = -1, 0, 1$) and, subsequently, three different peaks with slightly different energy (Figure 1.10). Interestingly, the jump of the cross-section when moving from the L- to the K-edge (or more precisely the ratio $\kappa$ of the cross-sections before and after the jump) decreases with the atomic number $Z$ due to the electron shielding effect and can be quoted with $\kappa = 8.7$ for $Z = 20$ and $\kappa = 4.8$ for $Z = 80$. To enhance the effect of contrast agents, we should, therefore, use not too heavy elements possessing higher ratios, such as iodine ($Z = 53$) or barium ($Z = 56$), with $\kappa \sim 6$.

Utilizing high-resolution spectrometers employing for instance the Bragg reflection (Equation 1.44), we can observe resonance structures in the order of 10% just above the absorption edges. The technique is called extended X-ray absorption fine structure (EXAFS) (Sayers et al. 1971), and allows one to quantify the chemical state, the temperature, or in general the atomic environment of the atom on which the photoelectric absorption took place. Recently, EXAFS has found entry in many biomedical applications such as the systematic analysis of the biochemical effect of magnetic properties of iron oxide nanoparticles (Levy et al. 2011), which are used as contrast agents in magnetic resonance imaging and, more recently, in X-ray imaging.

As a consequence of the photoelectric absorption on an inner shell (but also subsequent a Compton process), we remain with an ionized, thus excited, atom in an intermediated state. Apparently, the atom is not very happy about this situation, and wants to return as soon as possible (or at least within picoseconds to nanoseconds) into its ground state. As we saw before in Section 1.1 an electron from the $i$th shell can substitute the missing electron in the $j$th shell ($j > i$), whereas the nascent energy (Equation 1.27) is emitted as characteristic fluorescence radiation with a characteristic energy of $E_{\text{fluoresc}} = 13.6 \text{eV} \cdot Z^2 \cdot (1/\ell^2 - 1/j^2)$. Since the momentum was already transferred during the absorption
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FIGURE 1.11 Yield for the emission of fluorescence photon and Auger electrons.

process at time scales of femtoseconds, the fluorescence radiation is emitted isotopically in the entire solid angle, thus into $4 \cdot \pi$. The fluorescence process cascades down to the outer shells, whereas fluorescence radiation is emitted with always-longer wavelengths until the atom grabs a free electron somewhere from its vicinity and relaxes in its ground stage. The emitted fluorescence radiation can be absorbed by other atoms or by the same atom on which the photo effect originally took place. In this case an electron in the outer shells of the same atom reabsorbs high energetic fluorescence radiation from an inner shell transition. As a consequence, a second photo effect takes place with the subsequent emission of a so-called Auger electron (Auger 1923). If the photo effect took place on the K-shell, and the missing electron was substituted by an L-shell electron, then the kinetic energy of the Auger electron is given by

$$E_{\text{Auger}} = E_K - 2 \cdot E_L.$$  \hspace{1cm} (1.48)

This kinetic energy is (as the wavelength of the fluorescence) element-specific and, for barium, this would be 9.91 keV. The probability that the excited atom relaxes via the emission of a fluorescence photon or the ejection of an Auger electron depends on the atomic number, $Z$. As the atomic number increases, the shell electrons are more tightly bound, which is lowering the Auger emission probability. Since we just have two relaxation processes, subsequently the probability of the fluorescence emission increases. Several semi-empirical equations have been developed to calculate the fluorescence yield for a wide range of atomic numbers.

According to Hanke et al. (1985), the fluorescence yields for K- and L-shell transitions can be approximated with

$$\zeta_K = 0.337 - 6 \cdot 10^{-2} \cdot Z + 3.3 \cdot 10^{-3} \cdot Z^2$$ \hspace{1cm} (1.49)

and

$$\zeta_L = 0.04 - 4.6 \cdot 10^{-3} \cdot Z + 1.2 \cdot 10^{-4} \cdot Z^2 - 1.9 \cdot 10^{-7} \cdot Z^3$$ \hspace{1cm} (1.50)

and are shown versus the atomic number in Figure 1.11. The probability of an Auger process is then $\zeta_{k,l}^{\text{Auger}} = 1 - \zeta_{k,l}$.

The kinetic energy $E_{\text{Auger}} = h \cdot \omega - E_p$ of the ejected photoelectron can be substantial. Due to momentum conservation, the photoelectron is emitted in the first place mainly in a forward direction, whereas the angular distribution is given by Equation A.149 and shown in Figure 1.12 and, subsequently, is traveling through matter. During its travels, it will be the subject of energy loss due to ionization (knock on electrons) and radiative processes (bremsstrahlung) on atoms in the vicinity (see Figure A.6). We should adopt the view that, after each collision, the electron might change its direction, but, for energy and momentum conservation, on average, it will be directed in the forward direction anyway.

During this “directed random walk” through matter, it will generate secondary charges and lose its energy, whereas its energy loss is governed by the collision stopping power (Equation A.107) and radiative stopping power (Equation A.113), as is seen in Section A.4. Eventually, the photoelectron will thermalize and will be grabbed by an ionized atom. In Figure 1.13, we depict the situation using data generated by the ESTAR (see Table E.1 in Appendix E) database from the National Institute of Standards and Technology (NIST) (Berger 1992). Shown here is the energy

FIGURE 1.13 Stopping power and range versus the kinetic energy of electrons for brain tissue.

FIGURE 1.12 Relative number of photoelectrons per unit solid angle versus the emission direction relative to the incident photon.
loss or better the stopping power given (in MeV · cm²/g) versus the electron energy (in MeV) in brain tissue (density ρ ~ 0.99−1.2 g/cm³, so basically 1). Multiplying the stopping power with the brain density, this means that a 10 keV photoelectron is losing ~20 MeV per cm. Since we just have an energy of 10 keV available, the electron will travel about one per mille of a cm, thus 20 μm until it rests.

However, we should note that the range we quote here describes the entire length of the electron track. The projected electron range for instance on an axis parallel or perpendicular to the initial photon direction can be substantially smaller. A good rule of thumb for the projected electron range perpendicular to the photon direction, thus the lateral spread, is given by the empirical formula of Katz and Penfold (1952):

\[ \sigma_\perp = 1.5 \cdot 10^{-6} \cdot \frac{E_{\text{kin}}^{1.75}}{\rho} \text{ cm}^2 \cdot \text{keV}^{1.75} \]  

(1.51)

which would give us, for 10 keV, approximately 840 nm, thus two orders of magnitude less.

For low electron energies, the radiative energy loss can be neglected and the collision energy loss is predominant. At roughly 100 MeV we hit a so-called critical energy, where both contributions are equal. This matches our findings in Section A.3 and specifically Equation A.117 when assuming an effective atomic number of brain tissue of about Z eff = 5.5. For higher electron energies above the critical energy, the brain tissue would predominately radiate and subsequently become an X-ray tube.

As an aside, let us come back to the Auger electrons. Because of their low energy and, subsequently, their relatively small range in tissue, these Auger electrons are excellent candidates to generate double strand breaks in the DNA of the cancer cell, which subsequently leads to their apoptosis. However, it requires mid-range or heavy atoms (from bromine to platinum) incorporated into the DNA (such as cisplatinum) or at least close to the DNA to attain therapeutic effects, which are not easy to obtain. In the case of barium, using Equations 1.48 and 1.51, thus \( E_{\text{kin}} = 9.91 \text{ keV} \rightarrow \sigma_\perp \approx 900 \text{ nm}, \) we are dealing with a range of the Auger electron of about 1 μm, which is in the order of the size of the cell nucleus. With the increasing use of nanometer sized particles, which can be incorporated into cells by phagocytosis or endocytosis (Menk et al. 2011), Auger electron based tumor therapy will certainly have an impact in the near future.

On its random walk the photoelectron generates an average \( n_{\text{el}} = (\hbar \cdot \omega - E_\gamma)/w_{\text{ion}} \) charge, whereas \( w_{\text{ion}} \) is the required energy to generate a free ion and electron pair. Typically, \( w_{\text{ion}} \) is in the order of 30 eV for gases and roughly an order less for solid states (3.6 eV for Si). If we account also for the emitted fluorescence we will end up with

\[ n_{\text{el}} = \frac{\hbar \cdot \omega}{w_{\text{ion}}} \]  

(1.52)

Due to these correlations and applying error propagation, the final error is with \( \sigma(n_{\text{el}}) = \sqrt{F \cdot n_{\text{el}}} \), smaller than predicted by Poisson statistics. The material depending factor, \( F \), is called the “Fano-factor” (Fano 1947) and ranges from 0.08 to 0.32 (for silicon \( F = 0.115 \)). It effectively reduces the error in the measurement of the photon energy using spectroscopic X-ray detectors, based on photon to charge conversion. The final energy resolution, \( \Delta E \), we can obtain is given by

\[ \Delta E = 2.355 \cdot \sqrt{F \cdot w_{\text{ion}} \cdot E_\gamma + \sigma_{\text{ele}}^2}, \]  

(1.53)

where \( \sigma_{\text{ele}} \) is the electronics noise in terms of electron volts, and the factor 2.355 is the conversion from \( \sigma_{\text{rms}} \) to full width at half maximum (FWHM). Just to give you an idea, the FWHM of the fluorescence line at 5898.75 eV of an ion (⁰⁵Fe) source. Such detectors working on the Fano limit are widely used to elucidate the energy of characteristic fluorescence lines and, subsequently, the chemical composition of samples or more recently in spectral imaging.

### 1.4.6 Pair Production

For the sake of completeness, but without further deduction from fundamental equations, we will briefly discuss another high energy photon interaction (>MeV) that takes place in the vicinity of the Coulomb field of a nucleus or of an electron. At these energies, Einstein’s mass energy equation (Einstein 1905b), \( \hbar \cdot \omega = m \cdot c^2 \), becomes relevant, telling us that we can convert energy (or photons) into matter, and vice-versa. For energy, momentum, and charge conservation, such conversion has to satisfy some conditions. Since the photon is neutral, the total charge generated in the process must add up to zero. This is possible because of the positron, which is the anti-particle of the electron, such as it possesses identical mass, but a positive electron charge, which was proposed first by Dirac (1928). As an electron–positron pair producing in free space cannot simultaneously satisfy conservation of energy and momentum, it requires the Coulomb field of the nucleus or another electron to absorb the recoil. In order to satisfy the kinematics, the energy of photon \( E_\gamma \) must be higher than a threshold value

\[ E_\gamma \geq 2 \cdot m \cdot c^2 + 2 \cdot \frac{m^2 \cdot c^2}{M} \approx 2 \cdot m \cdot c^2, \]  

(1.54)

where \( M \) denotes the mass of the nucleus and \( m \) the mass of the positron and electron, respectively. Since \( M \gg m \), we can approximate the threshold energy with the right hand side of Equation 1.54, at least for the pair production in the Coulomb field of the nucleus. In other words, in this case, we need to have at least twice the rest mass of the electron. If the pair production takes place in the vicinity of another electron, thus, we have to substitute \( M \rightarrow m \), and the threshold energy is then given by:

\[ E_\gamma \geq 4 \cdot m \cdot c^2. \]  

(1.55)

This process, however, is less probable than the pair production in the Coulomb field of the nucleus. If the photon energy
is substantially greater than the rest mass of the electron, 
\[ E_e \gg m \cdot c^2, \]
then the cross-section is given by (Heitler 1954):
\[
\sigma_{\text{pair}} = 4 \cdot Z^2 \cdot \alpha \cdot n_e^2 \cdot \left( \frac{7}{9} \cdot \ln \left( \frac{183}{Z} \right) \right) \approx \frac{1}{54} \]
\[
\approx \frac{7}{9} \left( 4 \cdot Z^2 \cdot \alpha \cdot n_e^2 \cdot \ln \left( \frac{183}{Z} \right) \right) = \frac{7}{9} \cdot \frac{A}{N_A} \cdot x_0, \tag{1.56}
\]
where \( x_0 \) is the radiation length of the electron, defined in Section A.3.

As a side remark, the inverse process is referred to as position–
electron annihilation that finds applications for example in posi-
tron–electron tomography (PET) (Ter-Pogossian et al. 1975), an
indispensable instrument in functional imaging, oncology, and
neuroimaging. Here a circular arrangement of suitable detectors
reveals a pair X-rays that are generated during the annihilation
process. The sources of the required positrons are \( \beta^+ \) emitting
and biologically active molecules such as fludeoxyglucose, which
are injected into the body and accumulate in regions of the body
with increased metabolic activity, such as cancers of active parts
in the brain.

### 1.4.7 Photo–Nuclear Interactions

When the wavelength is substantially smaller than the Bohr
radius, \( \lambda < a_0 \) (for instance the associated wavelength for 10 MeV
photons is \( \approx 12.4 \cdot 10^{-15} \) m), the incident wave field can interact
with the nucleus, which possesses spatial extensions in the range
of 1.75 fm (1.75 \( \cdot 10^{-15} \)) for hydrogen to about 15 fm (15 \( \cdot 10^{-15} \) m)
for uranium. Baldwin and Klaiber (1947) observed that, at high
excitation energies of about 15 to 20 MeV, the nucleus acts as a
strong absorber of the incident photons. This phenomenon was
named the giant nuclear resonance (GNR). These resonances are
called giant because of their great strength, with 50% to 100%
of the theoretical limit concentrated in a compact energy region.

To understand this type of interaction, we have to have a closer
look at the composition of the nucleus. We briefly discussed
Rutherford’s atom model before. He came up with this model
as a consequence of experimental results when he was shooting\n\( \alpha \) particles through thin gold foils, from which he deduced that
only the presence of a very strong force could explain the deflec-
tion of the massive and fast moving \( \alpha \) particles at very large
angles. This justified the idea of a nuclear atom with a dense
center of positive charge and mass. Our present understanding
is that the nucleus of an atom consists of neutrons and protons,
which in turn are built up by three even more elementary parti-
cles, so-called quarks. Similar to molecules that are held together
by electromagnetic force, composite nuclear particles made of
quarks—the so-called hadrons—are held together by a nuclear
strong force. Triple quark hadrons such as protons and neutrons
are referred to as baryons, while two quark particles are called
mesons. The nuclear strong force has a very short range, but
extends far enough from each baryon so as to bind the neutrons
and protons together against the repulsive electrical force stem-
ing from the positively charged protons. Eventually, the strong
force drops to zero just beyond the edge of the nucleus that lets
the nucleus appear Z-fold positively charged. At this point only
the Coulomb force is seen by the negative charge of the electrons,
which eventually holds them in their orbits. We can imagine the
nucleus as a drop of incompressible nuclear proton/neutron fluid
of very high density. This liquid drop model was first proposed by
Gamow (1928) and then further developed by Weizäcker (1935),
who came up with the semi-empirical mass formula (SEMF)
which allow one to estimate the mass and various other proper-
ties of an atomic nucleus from its number of protons and neutrons
and explains the spherical shape of most nuclei. According to
this model, a stable nucleus holds almost a constant density and
therefore the nuclear radius \( R \) can be approximated by
\[
R = \pi_0 \cdot \frac{1}{A^{1/3}} \tag{1.57}
\]
where \( \pi_0 = 1.25 \) fm is the diameter of the proton and \( A \) the
atomic mass number, thus the sum of \( Z \) protons and \( N \) neutrons.

An incident electromagnetic wave with sufficiently short wave-
length will change the charge distribution inside the liquid drop
and generate elementary modes of oscillations of the whole
nucleus (see Section A.8). This occurs systematically in most,
if not all, nuclei. It can cause a radial swelling and ebbing of
the liquid sphere, thus a radial oscillation (monopole), dipole, quad-
rupole, and higher order pole oscillations of the nucleus, which
eventually could explain the observed peak in the photosorption
probability, thus the GNR. It was Goldhaber and Teller (1948) who interpreted first the GNR as the excitation of a col-
clective nuclear vibration in which all the protons in the nucleus
move collectively against all the neutrons, providing a separation
between the centers of mass and charge, thus creating a giant
electric dipole moment (GDR). The latter is the best known of
all giant resonances in which protons and neutrons oscillate with
opposite phase producing a large electric dipole moment, which
acts as an effective antenna for \( \gamma \)-rays. This implies that we can
also here use the instruments of classical electrodynamics to esti-
mate the associated cross-sections. Using a similar approach as
in Section A.1.6 to describe the scattering on bound electrons,

![FIGURE 1.14 Giant nuclear resonance for uranium. (The data used in this plot were taken from Baldwin, G.C. and G.S. Klaiber. 1947. Photo-fission in heavy elements. Physics Review 71:3–10; Data obtained from the Xcom data.)](image-url)
we could find in Section A.8 that the cross-section for the GDR is given by

\[
\sigma_{\text{GDR}}(E) = \frac{\sigma_{\text{GDR}} \cdot E^2}{\left( E^2 - E_{\text{GDR}}^2 \right)^2 + E^2 \cdot \hbar^2 \cdot \Gamma_{\text{GDR}}^2},
\]

(1.58)

which is nothing else but a Lorentzian resonance profile (Figure 1.14), similar to scattering on bound electrons (Equation 1.40) where \( \sigma_{\text{GDR}} \) is the maximum and \( E_{\text{GDR}} \) and \( \Gamma_{\text{GDR}} \) are the mean energy and width of the distribution. Empirically, the atomic mass number, \( A \), dependence of the excitation energy of the GDR is intermediate between \( A^{-1/6} \) and \( A^{-1/3} \), and can be reproduced by a two parameter expression

\[
E_{\text{GDR}} = 31.2 \cdot A^{-1/3} + 20.6 \cdot A^{-1/6}[\text{MeV}]
\]

(1.59)

For medium or heavy nuclei, Equation 1.59 can be approximated with \( E_{\text{GDR}} \sim 78 \cdot A^{-1/3}[\text{MeV}] \). The width of the GDR is typically 4 MeV for medium and heavy but spherical nuclei, which can broaden to 8 MeV for non-spherical nuclei. In nuclei with a large deformation, the GDR splits into two components corresponding to oscillations along and perpendicular to the symmetry axis. In that case, the GDR cross-section is well reproduced by the sum of two Lorentzian components (Figure 1.14). In real life, we can simulate photonuclear interaction by placing non-Newtonian liquids such as Oobleck, which is a non-toxic suspension of starch on a powerful subwoofer. Depending on the power and frequency of the subwoofer, the Oobleck will deform in the aforementioned oscillation modes, but beyond a certain threshold explode and spit all over the place. This can happen during GNR as well. The absorption of a \( \gamma \)-ray induces a GDR, which eventually breaks up by emitting secondary particles. The emitted particle may be neutrons, protons, alpha particles, and heavy ions, which will—as Oobleck—spit all over the place. This is a serious problem in radiotherapy, in which MeV \( \gamma \)-rays are used to cure otherwise untreatable forms of cancer. Often, linear particle accelerators (LINACs) are utilized to generate high energy \( \gamma \)-rays, which are then the source of photon nuclear interactions within the LINAC or within the patient, with the subsequent emission of secondary particles. Since the range of charged particles (electrons, protons, and \( \alpha \) particles), as seen in Section A.4, is fairly limited, they can be easily shielded, at least when generated in the LINAC head. Eventually, it is the neutral photo-neutron that causes trouble. The propagation of these photo-neutrons in the treatment room can lead to an increase in the patients’ and staff’s exposure to dose. The radiobiological effects of such photo-neutrons can be up to 20 times higher than those of photons with a similar energy. Long-term survivors of radiation therapies are at increased risk to develop treatment-induced side effects, such as radiogenic second cancer, complications of the cardiovascular and central nervous systems, fertility problems, and a myriad of other toxicities (Newhauser et al. 2016).

### 1.4.8 Total Absorption Cross-Section

Having now determined the cross-sections of the major players for the interaction of photons with matter, we can use Equation 1.23 to calculate the total mass absorption coefficient summing all cross-sections and multiplying it with \( N_A / A \), thus the number of atoms

\[
\mu = \frac{N_A}{A} \cdot (\sigma_{\text{coh}} + \sigma_{\text{en}} + \sigma_{\text{PE}} + \sigma_{\text{pair}})
\]

(1.60)

Here we included in the incoherent cross-section \( \sigma_{\text{coh}} = \sigma_{e} + \sigma_{\text{atom}} \), and both the atomic Compton and the Thomson cross-sections. Moreover, we summed the cross-sections of pair production in the Coulomb field of the nucleus and the electron. We saw that the various cross-sections possess quite different dependencies from the energy of the incident photon and the atomic number of the target. Therefore, we expect, for Equation 1.60, a quite complicated curve progression versus the photon energy, which is different for each chemical element or compound. We should be prudent when dealing with Compton scattering. As we discussed in Section 1.4.3, we have to distinguish between the energy cross-section (Equation 1.36) and the energy absorption cross-section (Equation 1.37). If we use the

---

**FIGURE 1.15** Mass attenuation for brain tissue versus the photon energy. We used the XCOM (Berger and Hubbell 1987) database here. Regarding pair production, \( N_e \) indicates the pair production in the field of the nucleus (\( N \)) and in the field of an electron (\( e \)).

**FIGURE 1.16** Difference of the mass absorption coefficient and the energy mass absorption coefficient for bone versus the photon energy.
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former (Equation 1.60), \( \mu \) is sometimes referred to as the mass attenuation coefficient, while using the latter it is sometimes called the mass absorption coefficient (Figure 1.15).

Apart from the difference in the Compton energy and energy absorption cross-sections, respectively, we should also recall that, for the other interactions, not all of the energy carried by the photon is necessarily transferred to matter. This is important for dosimetry, where it is important to know how much of the energy, \( \Delta E \), carried by X-rays of energy, \( E_x \), is eventually absorbed by a material of mass, \( \Delta M = \rho \cdot \Delta V \). For an infinitesimal layer of skin, we can directly calculate the so-called skin dose, \( D_{\text{skin}} \):

\[
D_{\text{skin}} = \frac{\Delta E}{\Delta M} = \frac{\Delta (\varphi_0 \cdot E_y \cdot (1 - T))}{\rho \cdot A \cdot \Delta x} = \frac{\varphi_0 \cdot E_y \cdot d \left( 1 - e^{-\alpha_{\text{skin}} x} \right)}{\rho} \approx \frac{\varphi_0 \cdot E_y}{\rho} \cdot \mu_{\text{skin}}
\]

(1.61)

where \( \varphi_0/A \) is the photon fluence (photon per area, \( A \), which should not be confused with the atomic mass, \( A \)), \( T \) is the transmission, as defined in Equation 1.4, and \( \Delta x \) is the extension of the volume into the propagation direction (x-direction) of the photons. For small volumes, \( x \to 0 \) and \( \Delta x \to dx \), we can approximate the exponential by its first order Taylor expansion and execute the differentiation. It therefore makes sense to define a mass energy absorption coefficient, \( \mu_{e/m} \) (Hubbell 1982) that is related to the sum of the kinetic energies of all those primary charged particles released by photons per unit mass (KERMA) (ICRU 1980). For the KERMA we can directly exclude coherent and Thomson scattering, since—as we discussed above—during those processes no energy transfer takes place. High energy fluorescence radiation might escape out of a regarded volume, \( A \cdot \Delta x \), while low energy fluorescence might create collective excitation like phonons or plasmons, which, therefore, will not contribute to the energy balance (Figure 1.16).

The energy mass attenuation coefficient is, therefore, given by the sum of weighted cross-sections (Hubbell 1982)

\[
\mu_{\text{en}} = \frac{N_A}{A \cdot u} \cdot (f_{\text{mech}} \cdot \sigma_{\text{mech}} + f_{\text{PE}} \cdot \sigma_{\text{PE}} + f_{\text{Pair}} \cdot \sigma_{\text{Pair}}),
\]

(1.62)

where \( f_{\text{PE}} = 1 - E_{\text{fluor}}/E_x \), \( f_{\text{Pair}} = 1 - (E_x - E_{\text{fluor}})/E_x \), and \( f_{\text{Pair}} = 1 - (2 \cdot m \cdot c^2 + E_{\text{fluor}})/E_x \). As we see, the weighting factors neglect the energy of the fluorescence, which is normalized to the energy of the incident radiation. Regarding the weighting factor of the Compton scattering, we recognize the factor \( E'_x / E_x \) that appeared previously in the energy absorption cross-section (Equation 1.37).

Multiplying Equation 1.62 with the photon fluence, \( \varphi_0/A \), and the photon energy, will directly yield the KERMA.

1.4.9 Complex Refractive Index and Atomic Scattering Factors

Summarizing up to now, we see that we can subdivide the interaction of photons (at short wavelengths) with matter into processes with and without energy transfer. These are also referred to as resonant (photo effect, Compton effect, and pair production) and non-resonant (Thomson and coherent scattering) processes, whereas the resonant bit proceeds—as we saw—via an intermediate excited state. This intermediate state relaxes by production of fluorescence radiation and Auger electrons, which have energies characteristic of the atom. To describe these two classes of effects in a simple macroscopic model, a single quantity such as the refractive index, \( n \) (\( n \) being a real number), is not sufficient. Our ancestors, therefore, packed everything into a complex refractive index, \( n = 1 - \delta + i \cdot \beta \), and this was truly a brilliant idea. They called the parameters \( \delta \) and \( \beta \) the refractive index decrement and the absorption index, and they refer to non-resonant and the resonant processes, respectively. To understand the effect of moving from a real to a complex index of refraction, we assume a plane wave with amplitude, \( E_0 \), and frequency, \( \omega \), propagating in the x-direction, \( (\vec{k} = k \cdot \hat{\epsilon}_x) \). The one-dimensional solution that solves the general wave (Equation A.6) and is given by Equation A.16 is:

\[
\vec{E}(x,t) = \vec{E}_0 \cdot e^{-i(\omega t - k x)},
\]

(1.63)

having the dispersion relation (Equation A.18) given by

\[
\frac{\omega}{k} = \frac{c}{n} \Rightarrow k = \frac{\omega \cdot n}{c}.
\]

(1.64)

For long wavelength photons, \( n \) is a real number and is greater than unity, and that explains refraction due to the reduced speed of light in that material. Substituting now the complex index of refraction into the right hand side of Equation 1.64, we get \( k = \omega/(1 - \delta + i \cdot \beta)/c \) and substituting this wave number into Equation 1.63 gives:

\[
\vec{E}(x,t) = \vec{E}_0 \cdot e^{-i(\omega t - k x)} = \vec{E}_0 \cdot e^{-i\omega t} \cdot e^{i\frac{\omega x + \delta x}{c}} \cdot e^{-\frac{\beta x}{c}},
\]

(1.65)

Since the intensity is the time averaged modulo (thus \( E^* \cdot E \), where the asterisk denotes the complex conjugate) of the pointing vector, all imaginary terms in Equation 1.65 cancel out, while the real terms remain, and we obtain:

\[
|\vec{E}(x,t)|^2 = \frac{\varepsilon_0}{\mu_0} \cdot \frac{\vec{E}_0 \cdot \vec{E}_0}{2} e^{\frac{4\pi \beta x}{c}} = \frac{\varepsilon_0}{\mu_0} \cdot \frac{\vec{E}_0 \cdot \vec{E}_0}{2} e^{\frac{4\pi \beta x}{c}},
\]

(1.66)

whereas we used the relation \( \omega/c = 2 \cdot \pi/\lambda \) in the exponential function on the right hand side. According to Equation A.50, we can identify the coefficient in front of the exponential on the right hand side as the intensity of the undisturbed wave field, which we denote with \( T_0 \); therefore we get

\[
|\vec{T}(x)| = T_0 \cdot e^{\frac{4\pi \beta x}{c}},
\]

(1.67)
which is the Lambert–Beer law (Equation 1.3) for a slab of a single material of thickness $x$. With a direct comparison of the argument of the exponential, this means we can rewrite the attenuation coefficient, $\mu$, in terms of the absorption index, $\beta$; thus $\mu = 4 \cdot \pi \cdot \beta / \lambda$. After the quite painful calculations in Section A.1.6, we were also able to show that the complex index of refraction $n$ is related to the atomic scattering factors in forward direction, $f_0^0$ and $f_2^0$, through:

$$n(\omega_0) = 1 - \frac{r_0 \cdot n_a \cdot \lambda^2}{2 \cdot \pi} \left( f_0^0(\omega_0) - i \cdot f_2^0(\omega_0) \right) = 1 - \delta + i \cdot \beta,$$

(1.68)

where $r_0$ is the classical electron radius and $n_a$ is the number of atoms of per unit volume (see Equation A.80) which is directly proportional to the electron density. Typical electron densities are for muscle $3.36 \cdot 10^{23}$ electrons/gram, for fat $3.16 \cdot 10^{23}$, and for bone $5.55 \cdot 10^{23}$.

The direct comparison gives us $\delta = f_0^0(\omega) \cdot r_0 \cdot n_a \cdot \lambda^2 / (2 \cdot \pi)$ and, accordingly, $\beta = f_2^0(\omega) \cdot r_0 \cdot n_a \cdot \lambda^2 / (2 \cdot \pi)$. Using the latter, we can express $\mu$ in terms of the atomic scattering factor, $f_2^0$, as

$$\mu = \frac{2 \cdot f_2^0(\omega) \cdot r_0 \cdot \lambda}{A \cdot m_a},$$

(1.69)

and, subsequently, using the relation between $\mu$ and the cross-section (Equation 1.23)

$$\sigma_a = 2 \cdot r_0 \cdot \lambda \cdot f_2^0.$$

(1.70)

We used the subscript $a$ to emphasize that we are dealing here exclusively with absorption cross-sections. Certainly, we can also employ a transmission measurement of a well-known absorber of thickness $x$ at a well-known wavelength, $\lambda$, to determine $\mu$ according to Equation 1.69, but the precise experimental determination of the linear absorption coefficient is not trivial at all. When rearranging Equation 1.70, we can derive $f_2^0$ from the atomic photoabsorption cross-section, thus $f_2^0 = 2 \cdot r_0 \cdot \lambda \sigma_a$, and this is how databases are normally calculating the scattering factors.

Obviously, as for the absorption cross-section, the amplitude of $f_2^0$ depends on the photon energy, and it increases sharply at the absorption edges of the scattering atoms, at least in the energy range interesting for radiography (10–150 keV). Owing to the so-called Kramers–Kronig relationships (Kronig 1926; Kramers 1927), which couples the real part of a complex quantity to its imaginary part, we can calculate $f_0^0$ once we have determined $f_2^0$

$$f_0^0(\omega) = Z + \int_0^\infty \frac{\omega' \cdot f_2^0(\omega')}{\omega^2 - \omega'^2} \cdot d\omega' - \Delta f_1$$

(1.71)

where $\omega$ is the determination frequency (or energy) and $\Delta f_1$ is a relativistic correction term that can be neglected for soft X-rays. In other words, for each $\omega$ we choose we have to accomplish the integration over all possible frequencies, $\omega'$. Actually, we do not have to do this, since accessible databases, for instance from the Center of X-ray Optics (CXRO) (Henke et al. 1993), did that already for us. As depicted in Figure 1.17a, distal to the absorption edges, the amplitude of $f_0^0$ varies smoothly with the photon energy. The real and imaginary parts have very different dependences on the photon energy. In the energy regime from 10 to 30 keV, the energy dependence of $f_2^0$ for soft tissue is dominated by that of the photoelectric cross-section, thus, according to Equation 1.46, $f_2^0 \propto E^{-\gamma/2}$, while $f_2^0$ is, according to Equation A.71, driven by $\omega_0^2 - \omega^2$, thus $f_2^0 \propto E^{-\gamma}$, except in the vicinity of absorption edges. Also shown in the graph of Figure 1.17a is the ratio $f_2^0(\omega) / f_2^0(\omega)$, which is in the order of $10^3$ to $10^4$ in the energy regime from 10 to 30 keV.

This means that, for soft tissue, the non-resonant processes (thus Rayleigh and coherent scattering) outstrip the resonant processes (photoelectric absorption and Compton scattering) by orders of magnitudes, and explains why Rayleigh/coherent scattering has such a deleterious effect on traditional absorption based medical imaging. If not suppressed by anti-scatter grids, it just generates image blur in radiographs. We should add that the situation is a bit different in the vicinity of absorption edges, as we note in Figure 1.17b, where we depict the atomic scattering factors for bone. Here the ratio $f_2^0(\omega) / f_2^0(\omega)$ is not as dramatic as...
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for soft tissue. That does not imply that coherent scattering is not useful. In fact, elastically scattered waves interfere, and this is the basis for studies of atomic and molecular structures by X-ray diffraction and small angle X-ray scattering. Both techniques find a wealth of applications in the biomedical field (Chance et al. 1994). To give a flavor, X-ray diffraction has been predominantly used to elucidate the human genetic code and the structure of macromolecules/viruses, while small angle X-ray scattering is applied to clarify semi-ordered structures such as cell membrane structures or to understand the working principle of muscles. Coherent scattering even allows one to generate holographic images on the atomic level (Gog et al. 1998). Moreover, when used in the right way, coherent scattering can yield a wealth of information in medical imaging, as we will see in the following.

1.4.10 Absorption Imaging and Phase-Contrast Imaging

Let us return to the one-dimensional wave field described by Equation 1.65. If we observe the right hand side, we recognize the three exponential factors where the imaginary part, \( e^{-\omega t} \), describes the wave propagation in vacuum, the decay (real part), \( e^{-\lambda x} \), as we saw is responsible for absorption, and the imaginary part, \( e^{i\phi} \), is the phase shift due to the medium. This means that the phase of the wave field is shifted by the amount

\[
\Delta \phi = \frac{2 \pi}{\lambda} \cdot \Delta x \quad (1.72)
\]

when travelling through a slab of homogenous material with the thickness \( \Delta x \) with respect to a wave field that is propagating undisturbed (see Figure 1.1a). For non-homogenous materials we obviously have to integrate over the refractive index decrement, \( \delta(x, y, z) \), thus

\[
\Delta \phi = \frac{2 \pi}{\lambda} \cdot \int \delta(x, y, z) \cdot dx = \rho_0 \cdot \lambda \cdot \int \rho(x, y, z) \cdot dx. \quad (1.73)
\]

In principle, this phase shift can be measured utilizing so-called interferometers (Michelson 1881). The basic idea of such an interferometer is to split an electromagnetic wave into two equal parts using what is called a beam splitter. In the optical regime, a beam splitter would be a half transparent mirror. Both beams propagate onto secondary mirrors and from there to an image receptor. While the so-called reference beam propagates undisturbed through air or similar, the second beam shines through something we want to measure and which induces the phase shift. When the two light beams are superimposed at the image receptor, they interfere, and the phase difference between them creates a pattern of light and dark areas, which are referred to as interference fringes. By measuring the fringes, we can retrieve the phase shift with great accuracy.

At present, most of the X-ray technologies in medical imaging rely primarily on the resonant part, \( f_0^2 \), of the incident radiation, and do not depend on its phase, since the latter cannot be derived directly from an intensity measurement, as we saw from Equation 1.67. Let us now consider an ideal absorption measurement of monoenergetic X-rays of the energy \( E_\gamma \), where only the total attenuation of the direct beam is observed, and all non-resonant effects (scattering) are rejected (Figure 1.18). We now ask ourselves what are the requirements to visualize a detail, which might be a tumor, embedded in similar tissue using X-rays. The medical application would be, for instance, mammography. The detail (for the ease of calculation a cube with edge length \( w \)) occupies a volume of \( w^3 \) and is characterized by its energy mass absorption coefficient, \( \mu_e \), and its density, \( \rho \). The energy mass absorption coefficient of the embedding tissue of the similar density, \( \rho_0 \), is \( \mu_0 \). If \( \phi_0 \) denotes the mean photon fluence (mean number of photons per area \( w^2 \)) in front of the sample, the radiant intensity (average number of photons) after propagating through the total length, \( L \), will be, according to Equation 1.12, \( N_1 = \phi_0 \cdot w^2 \cdot e^{-\mu_0 L} \cdot e^{(\mu_0 - \mu_1) w} \) behind the tumor and \( N_2 = \phi_0 \cdot w^2 \cdot e^{-\mu_1 L} \) in regions outside the detail. While we assume a spatially constant distribution, \( \phi_0(y, z) = \text{const} \), incident on the sample, the radiant photons, \( N(y, z) \), will be modulated according to the distribution of the different mass absorption coefficients. As stated earlier, we always have to think in terms of mean numbers of photons. The difference of the mean numbers of photons behind the tumors and behind the normal tissue is then given by

\[
\Delta N = \phi_0 \cdot w^2 \cdot e^{-\mu_1 L} \left( 1 - e^{-(\mu_0 - \mu_1) w} \right)
\]

or \( \Delta N = \phi_0 \cdot w^2 \cdot e^{-\mu_1 L} \Delta \mu \cdot w \), where \( \Delta \mu = \mu_0 - \mu_1 \) is the difference in the mass absorption coefficient of the detail and the environment. Recalling that the error of photon numbers is governed by Poisson statistics, and the fact that \( \Delta N \) is a function of two independent variables, \( N_1 \) and \( N_2 \), the associated error can be calculated by error propagation according to

\[
\sigma = \sqrt{\Delta N} = \sqrt{\left( \frac{\partial \Delta N}{\partial N_1} \right)^2 (\Delta N_1)^2 + \left( \frac{\partial \Delta N}{\partial N_2} \right)^2 (\Delta N_2)^2}
\]

\[
= \sqrt{\phi_0 \cdot w^2 \cdot e^{-\mu_1 L} \left( 1 + e^{-(\mu_0 - \mu_1) w} \right)}
\]

\[
= \sqrt{\phi_0 \cdot w^2 \cdot e^{-\mu_1 L} \left( 2 - (\mu_0 - \mu_1) \cdot w \right)}
\]

\[
\approx \sqrt{2 \cdot \phi_0 \cdot w^2 \cdot e^{-\mu_1 L}}
\]

FIGURE 1.18 Basic setup of absorption based imaging in parallel beam geometry with monoenergetic X-rays.
which, according to Equation 1.15 results in a signal to noise ratio (SNR) of

$$SNR^2 = \left( \frac{\Delta N}{\sigma} \right)^2 = \frac{1}{2} \cdot \varphi_0 \cdot w^4 \cdot e^{-w^L} \cdot (\mu_w - \mu_i)^2$$

Equation 1.76 represents the inherent limit of the signal to noise due to Poisson statistics, without considering the detection device. With the definition of the skin dose (Equation 1.61) and the definition of the signal to noise ratio (Equation 1.76), we get after some rearrangements

$$D_{skin} = \frac{2 \cdot SNR^2 \cdot e^{wL} \cdot E}{w^4 \cdot C_w^2 \cdot \mu_i^2} \cdot \left( \frac{\mu_i}{\rho} \right)$$

where we introduced the object contrast $C_w = (\mu_w - \mu_i)/\mu_i$, as the difference in the energy mass absorption coefficient normalized to one of the embedding tissue. Equation 1.77 is valid for all kinds of X-ray imaging methods, such as radiography and computed tomography, and represents the inherent limit of X-ray absorption imaging. Of note is that the skin dose increases quadratically with the object contrast, $C_w$, which is painful, and with the fourth power of the detail size, $w$, which is extremely painful. For instance, breast cancer: when detected and treated early the 5-year relative survival for localized breast cancer is 99%. Moreover, larger tumor size at diagnosis is also associated with decreased survival. In other words: if we want to see a breast tumor at an early stage, it should be small. If the target is to visualize a half size tumor with the same contrast and signal to noise as a full size tumor, we might kill the patient. Therefore, you might want to increase the object contrast artificially by injecting suitable materials with high atomic number, which are referred to as **contrast agents**. Such contrast agents we mentioned earlier and normally are based on iodine, barium, or gadolinium. They do their job, even diluted, since the absorption coefficient is governed by the photo effect. More recently, contrast agents based on solid metallic nanoparticles have found their way in medical imaging, which can be surface modified and designed for a specific functionality. Such contrast agents are very promising candidates in near future medical imaging with X-rays, due to their ability to cross the blood–brain barrier (Sousa et al. 2010).

If such tricks to increase contrast and sensitivity are not applicable, we have to think of something else to overcome the dose limits governed by Poisson statistics. We mentioned before that X-ray absorption imaging. Of note is that the skin dose increases quadratically with the object contrast, $C_w$, which is painful, and with the fourth power of the detail size, $w$, which is extremely painful. For instance, breast cancer: when detected and treated early the 5-year relative survival for localized breast cancer is 99%. Moreover, larger tumor size at diagnosis is also associated with decreased survival. In other words: if we want to see a breast tumor at an early stage, it should be small. If the target is to visualize a half size tumor with the same contrast and signal to noise as a full size tumor, we might kill the patient. Therefore, you might want to increase the object contrast artificially by injecting suitable materials with high atomic number, which are referred to as **contrast agents**. Such contrast agents we mentioned earlier and normally are based on iodine, barium, or gadolinium. They do their job, even diluted, since the absorption coefficient is governed by the photo effect. More recently, contrast agents based on solid metallic nanoparticles have found their way in medical imaging, which can be surface modified and designed for a specific functionality. Such contrast agents are very promising candidates in near future medical imaging with X-rays, due to their ability to cross for instance the blood–brain barrier (Sousa et al. 2010).

If such tricks to increase contrast and sensitivity are not applicable, we have to think of something else to overcome the dose limits governed by Poisson statistics. We mentioned before the extraordinary sensitivity of interferometers. Let us consider a slab of soft tissue of thickness $\Delta x = 5.4$ mm, and a photon energy of 20 keV $\lambda \sim 6.2 \cdot 10^{-4}$ m. For this photon energy, $\delta = 5.766 \cdot 10^{-2}$ and $\beta = 3.462 \cdot 10^{-10}$ and, therefore, $\Delta \varphi \sim \pi$ and $\mu = 4 \cdot \pi \cdot \beta \lambda \sim 0.7 \text{ m}^{-1}$, which translate into an absorption of 0.0034% or 0.3%. This absorption in fact is very small, while the phase shift is substantial. We should keep in mind that we cannot determine a phase shift directly by simply measuring intensities with X-ray detectors (Equation 1.67). However, using an interferometer as described above we are able to let the undisturbed wave field interfere with the wave field propagating through the slab, and we will observe destructive interference (since we have a phase shift of $\pi$). Therefore, the wave fields would add to zero and, subsequently, the photon would appear as absorbed in the slab of matter. In other words, we compare here an apparent phase driven absorption of 100% with a real absorption of 0.3%, which translates into a 333-fold increase in contrast and, according to Equation 1.77, a dose reduction by five orders of magnitude. Utilizing imaging techniques based on phase effects is referred to as phase-contrast imaging. In the optical regime, phase contrast has been exploited to distinguish between structures of similar transparency or in dark field microscopy; however, the translation of these contrast mechanisms to similar X-ray modalities is not straightforward. This is due to the fact that the index of refraction, $n$, for X-rays is very close to unity, and the wavelength in the X-ray regime is that short. To build an interferometer in the X-ray regime, for instance, it requires mirrors or optical components that are optically flat, in other words a precision of a fraction of the wavelength, which is not trivial to achieve. It, therefore, took until 1965 for the first functional X-ray interferometer to be built (Bonse and Hart 1965), and another 30 years until such a technique was applied to biomedical imaging (Momose et al. 1996). As depicted in Figure 1.1, the retarded wave will change its propagation direction by a refraction angle, $\Delta \theta_R$, which, for X-ray wavelengths, is in the order of microradians. For small phase gradients, the refraction angle can be expressed as

$$\Delta \theta_R = \frac{1}{|\mathbf{k}_R|} \frac{\partial \phi}{\partial z}$$

where $|\mathbf{k}_R|$ is the length of the wave vector of the incident radiation propagating in the x-direction and the second term on the right hand side is the first derivative of the phase in the diffraction direction z. Since the refraction angles for X-rays are in the same order as the Bragg diffraction (Equation 1.44), we can use perfect crystals to analyze the direction of the radiant radiation with great precision and in principle recover the phase information by integrating over the refraction angle, thus the differential phase (Chapman et al. 1997). Techniques using this approach are often referred to as **Analyzer Based Imaging**. If we are using wave fields with sufficient spatial coherence, the undisturbed and the refracted wave (Figure 1.1a) can interfere in the far field at intermediate distance between sample and the image receptor generating interference fringes. In contrast to crystal interferometry, the recorded interference fringes $f$ are not proportional to the phase itself, but to the second derivative of the phase, thus
Therefore, the method is most sensitive to abrupt changes in the decrement of the refractive index. This leads to stronger contrast outlining the surfaces and structural boundaries of the sample (edge enhancement) when compared with a conventional radiogram. This technique is often referred to as free propagation phase contrast (Davis et al. 1995; Snigirev et al. 1995).

Combinations of X-ray interferometry and analyzer based imaging are the so-called edge illumination technique (Olivo et al. 2001) and Talbot–Laue interferometry (David et al. 2002).

We know phase effects in the optical regime from our daily life experience, often without noticing them. For example, the water content of a storm cloud can fit into a water column of some meters high. In crystal clear water, the attenuation coefficient for a wavelength of 418 nm is about 0.0044 m⁻¹, which is an attenuation length of about 227 meters. In other words water is not a great absorber of sunlight. However, sunlight is happily refracted within the water drops that form the cloud and scatter out of the field of view of an observer at ground level. Similar to analyzer based imaging, for this observer the refracted photon was apparently absorbed. Since the scatter cross-section is that large, hardly any photons will not be refracted, and this explains why the cloud is able to entirely obscure the sun. We can exploit this effect for refraction based contrast agents, which are less toxic than absorption based contrast agents (Arfelli et al. 2010).

Regarding the free propagation phase contrast, it is sufficient to watch the ripples in a swimming pool. For the same reason, as discussed before, you do not appreciate the ripples by absorption, but due to their interference. To give a flavor of how a phase contrast or an analyzer based imaging signal looks, we can think of a simple phase object (no absorption) like a nylon wire with radius \( R \) with constant refractive index decrement \( \delta \) measured against a constant background. The phase shift is then, according to Equation 1.72, given by \( \Delta \phi \sim \delta \cdot \Delta x = \delta \cdot \sqrt{R^2 - z^2} \). With such a phase shift we can calculate the signal derived from analyzer based imaging and free propagation phase contrast according to Equations 1.78 and 1.79. The situation is shown in Figure 1.19, where we can appreciate the contrarian refraction angles on the opposing boundaries of the wire and the associated interference fringes from free propagation phase contrast.

We will stop reviewing different phase-contrast techniques here, since they will be discussed in detail in the subsequent chapters. However, we should still point out that the phase shift, \( \phi \), and subsequently the scattering angle, \( \Delta \theta_p \), are proportional to \( n_0 \) (the number of atoms of per unit volume) and, hence, to the nuclear charge \( Z \) (Equation 1.68). This dependency is similar to that of the Compton cross-section (Equation 1.36). The latter, however, is well known to produce little contrast in radiographic images when compared to photoelectric absorption imaging, since here the cross-section is proportional to \( Z^2 \). However, the expectation of faint images in phase-contrast imaging is not justified for the following reasons: both Compton and photo effect cross-sections are proportional to \( r_0^2 \) instead of the much larger factor \( n_0 \cdot \lambda^2 \) appearing in Equation 1.68. Moreover, the phase shift at a given energy is only weakly coupled to absorption through the Kramer Kronig dispersion relations (Equation 1.71) and last the interference with the primary wave gives a strong enhancement on boundaries of materials featuring different indices of refraction. Although phase contrast techniques were mostly developed and fine-tuned at synchrotron radiation sources, their final success depends on their transfer to compact X-ray sources and exploitation in the clinical environment.

Up to now we have mentioned but not drawn too much attention to the fact that we hardly find X-ray sources providing sufficient monoenergetic X-rays for medical imaging. In most of the cases we will be confronted with a continuous and wide distribution of photon energies delivered by an X-ray generator such as an X-ray tube, which we denoted previously with \( P(E) \). In the following, we will discuss some characteristics of the latter and will explore which sort of energy spectra we can expect from X-ray tubes.

### 1.4.11 Generation of X-rays

Although X-ray tubes will be discussed in the following chapters, we should have a brief discussion of their basic setup. An X-ray tube converts electrical input power into X-rays, and consists basically of a heated cathode and an anode, which are connected across a high voltage (15–150 kV) power supply. Both electrodes are accommodated into a vacuum tube. The cathode, which is normally a metal wire, is heated by an electric current generated by a second power supply, and emits electrons by the thermionic effect. The latter is a thermally induced flow of charge carriers from a surface, which we know from old fashioned style light bulbs. The emission current density, \( J \), of electrons at a temperature, \( T \), is given by (Richardson 1901):

\[
J = A \cdot T^2 \cdot e^{-\frac{w_{\text{m}}}{kT}},
\]

where \( w_{\text{m}} = 4.5 \text{ eV} \) is the material specific work function, and \( A = 60 \text{A/(cm}^2\cdot K^2) \) is a material dependent constant. The values quoted here are given for tungsten. As a result of the potential difference, \( U \), between the cathode and the anode, the emitted electrons will be accelerated towards the anode gaining a maximum kinetic energy of \( E_{\text{kin}} = e \cdot U \). If we consider an acceleration voltage, \( U = 150 \text{ kV} \), the electrons gained a kinetic energy
of $E_{\text{kin}} = 150$ keV before they crashed into the anode. As we discussed in Section 1.4.5, energetic electrons or in general moving charges are losing energy when traveling through matter. Similar to the earlier discussion regarding photoelectrons also here we will observe two mechanisms of energy loss, through ionization (thus, impact ionization, see Bethe–Bloch [Equation A.107]) and through radiative processes (bremsstrahlung [Equation A.113]). The latter is providing us our X-rays, while the former essentially heats up the anode. Therefore, we should use anode materials possessing high fusion temperatures. For tungsten (W, $Z = 74$, $\rho = 19.25$ g/cm$^3$) this would be 3370°C, and for molybdenum (Mo, $Z = 42$, $\rho = 10.28$ g/cm$^2$) 2620°C. Both materials are good heat conductors to dissipate the heat produced by the energy loss.

Knowing the densities, we can estimate the penetration depths of 150 keV electrons in Mo (range = 0.047) and W (range = 0.057 g/cm$^2$) from Figure 1.20, as 0.05 mm and 0.03 mm, respectively. The ratio between collision and the radiative stopping power gives us the X-ray yield, which is approximately 2% for W and 1.3% for Mo, which is not a great deal. In other words, most of the electric power we put into our X-ray tube is just used to heat the thing up. In Section A.3, we see that electron-induced bremsstrahlung is given by

\[
\frac{dE}{dx} \propto Z^2 \cdot \frac{E}{m^2}.
\]  

(1.81)

The energy loss and, subsequently, the emission of bremsstrahlung scales with the square of the atomic number of the target material. Moreover, it scales with the square of the inverse mass of the projectile. For this reason, only light particles such as electrons are accelerated in X-ray tubes and heavy materials, such as W, are used as anode material in order to have a good radiation yield.

We still have not solved the remaining question of how the spectral distribution, $P(E_{\gamma})$, looks in the case of an X-ray tube. In Section A.3, we use classical electrodynamics to elucidate the differential number of photons per energy and solid angle unit emitted during impact, and we come up with

\[
\frac{d^2N}{d\Omega \cdot dE_{\gamma}} = \frac{\alpha \cdot Z^2}{32 \cdot \pi^2 \cdot c \cdot E_{\gamma}} \left( \frac{\hat{n} \times (\hat{n} \times \hat{v})}{1 - \hat{n} \cdot \hat{v} / c} \frac{\hat{n} \times (\hat{n} \times \hat{v})}{1 - \hat{n} \cdot \hat{v} / c} \right)^2,
\]  

(1.82)

recalling that the fine structure constant is given by $\alpha = e^2 / (\hbar \cdot c) = 1/137$. We see that the number of photons emitted during the bremsstrahlung process decreases with increasing photon energy, $E_{\gamma} = \hbar \cdot \omega$. However, in this approach we face two problems: first, we have to deal with the pole for $E_{\gamma} \to 0$ and, second, we have to introduce a cutoff for higher photon energies. For the latter, we can use the argument of energy conservation. Since the electron possesses a given kinetic energy, $E_{\text{kin}}$, the maximum energy transmitted to a single photon cannot exceed $E_{\text{kin}}$ in other words $E_{\max} = \hbar \cdot \omega_{\max} = E_{\text{kin}}$. This situation is given when the entire kinetic energy of the electron is transmitted to the photon and eventually the electron remains at rest. Therefore, the kinetic energy of the accelerated electron in an X-ray tube is $E_{\text{kin}} = e \cdot U_{\max} = \hbar \cdot \omega_{\max}$, when $U_{\max}$ is the maximum electric potential (or voltage) between the emitting cathode and the anode material. Regarding the pole for $E_{\gamma} \to 0$ we note that the number of emitted photons will become very large once their energy tends to zero. However, since also the energy of each photon tends to zero, the emitted energy, thus the number of photons multiplied by their energy, remains finite.

Therefore, we would expect, for the spectrum of an X-ray tube, a $P(E_{\gamma}) \sim 1/E_{\gamma}$, dependency possessing a maximum photon energy of $E_{\gamma} = e \cdot U_{\max}$.

As we estimated before, the electrons penetrate the anode material up to a certain depth, which was some tenths of a millimeter. Subsequently, the bremsstrahlung generated within the material is prone to the interaction mechanism we discussed before, and predominately to photoelectric absorption with the subsequent emission of characteristic lines or Auger electrons. For tungsten possessing a K-edge energy of $E_{\text{K}} = 69.52$ keV, we will have two fluorescence transitions in the hard X-ray regime, at $K_{\alpha} = 59.3$ keV line and at $K_{\beta} = 67.2$ keV line. As shown in Figure 1.4, the name K line indicates that the transition is ending on the K-shell. The suffix $\alpha$ is used for a transition between adjacent levels (from L to K, from M to L, etc.) and a suffix $\beta$ for a transition between non-adjacent levels (e.g., from M to K). We basically can neglect the Auger yield of 4.2% with respect to the substantially higher fluorescence yield of 95.8% (see Figure 1.11) and, therefore, we expect the appearance of these characteristic lines in the energy spectrum once $e \cdot U_{\max} \geq E_{\text{K}}$ on top of the $1/E_{\gamma}$ dependency. Since our X-rays are generated within a vacuum tube, but we want them for use outside in air, they have to exit through a suitable window and, in doing so, they will interact with matter again, predominately through photoelectrical absorption. Due to the dominant $E_{\gamma}^{-1/2}$ dependency in the absorption coefficient, low energy photons will be preferentially absorbed within the X-ray spectrum. Moreover, we should remember that, also, the radiation dose or KERMA (Equation 1.61) is vulnerable to low energy X-rays. Following the rule to keep the radiation dose as low as reasonably possible, we should try to cut away most of the low frequency X-rays that are absorbed within the patient and not contribute to increase the SNR (see Equation 1.77) in the radiography. We can manage this by utilizing appropriate filters that we introduce between the tube’s exit window and the patient. As a result, we can expect, for the spectral density incident on the patient, an intensity cutoff at a low photon energy cutoff. Aluminum possesses a low atomic number ($Z = 13$), and a relative low density of 2.7 g/cm$^3$ is frequently used as filter material. Due to its relatively low K-edge at 1.56 keV, the transmission of X-ray energies above 15 keV is dominated by the

**FIGURE 1.20** Stopping power and range of electrons versus the kinetic energy of electrons for W and Mo.
Basic Physics of X-ray Interactions in Matter

Compton effect and, subsequently, varies slowly with the energy. Shown in Figure 1.21 is the flux of an X-ray tube with tungsten anode versus the X-ray energy or, in other words, the non-normalized spectral density function, $P(E)$, which has been calculated using the X-ray Oriented Programs (XOP) (Sánchez del Río and Dejus 2004). The flux is given here in photons per second and per mm², which you can measure in one meter distance from the source for a normalized tube current of 1 mA. Since the number of X-rays is proportional to the tube current $I$, you have to multiply with $I$ to obtain the real photon numbers. Moreover, the spectral density shows the integral numbers of photons in an energy band (or bandwidth [BW]) of 1 keV. The sum of all energy bands gives us eventually the total number of photons generated by the X-ray tube. As a parameter, we used the maximum acceleration voltage $U_{\text{max}}$. As expected beyond the energy cutoff, the spectra follow the $1/E$ dependency with the appearance of characteristic lines once $e^{-U_{\text{max}}/E} \geq E_{\beta}$.

When we increase the filter thickness we move the energy cutoff towards higher energies (Figure 1.22). However, we also realize that the relative proportion of low energy to high energy photons decreases with increasing absorber thickness. For instance, at 30 keV without absorber, we obtain a flux of about 50,000, while we measure 30,000 in the $K_{\alpha}$ line resulting in a ratio (high to low) of about 0.6. Adding 5 mm of Al ($Z = 13$) we end up with a flux of $\sim 10,000$ at 30 keV against 23,000 in the $K_{\beta}$ line, thus a ratio of 2.3. This phenomenon is called beam hardening, which also has the effect of increasing the relative proportion of the $K_{\beta}$ line as compared to the $K_{\alpha}$ line. Again, due to the photoelectric absorption, the effect is more pronounced for high Z materials. As with Al, the beam will also be hardened due to the presence of a patient, especially when bones ($Z_{\text{eff}} = 13.8$) but also muscles ($Z_{\text{eff}} = 7.46$) are the target or even worse, when metallic components such as pacemakers or metallic joint prostheses are present. Since most of the detectors used in medical imaging rather integrate over the entire energy spectrum than measuring the energy distribution, such beam hardening is a painful issue in computed tomography, because it generates hardly correctable artifacts in the final image reconstruction.

The Compton contribution in the cross-section for light elements is an issue in soft tissue imaging such as mammography. To increase the object contrast between adipose, glandular, and tumor tissue, we need to employ low energy photons in the energy range between 18 and 22 keV. Therefore, we should use in this application anode materials possessing characteristic emission lines in this energy range. Mo with $K_{\alpha} = 17.48$ keV, $K_{\beta} = 19.61$ keV and

![Figure 1.21](image-url) Typical spectra $P(E)$ of an X-ray tube with a tungsten anode for different acceleration voltages.

![Figure 1.22](image-url) Calculated energy spectra for a tungsten X-ray tube with a maximum acceleration voltage of 150 kV and different Al filters. Due to the increasing filter thickness, beam hardening can be observed.

![Figure 1.23](image-url) Energy spectrum for Mo/Ro X-ray tubes.

![Figure 1.24](image-url) Spectra for an X-ray tube with Mo anode for an acceleration voltage of 30 kV without filter, a 50 µm Mo filter, and after 5 cm of breast tissue.
TABLE 1.2
Effective Energy and HVL for Al, Bone, and Muscle

<table>
<thead>
<tr>
<th>Effective Energy (keV)</th>
<th>HVL Al (mm)</th>
<th>HVL Bone (mm)</th>
<th>HVL Tissue (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>2.27</td>
<td>4</td>
<td>18</td>
</tr>
<tr>
<td>50</td>
<td>6.97</td>
<td>12</td>
<td>30</td>
</tr>
<tr>
<td>100</td>
<td>15.06</td>
<td>23</td>
<td>39</td>
</tr>
<tr>
<td>150</td>
<td>18.02</td>
<td>28</td>
<td>45</td>
</tr>
</tbody>
</table>

Rh (Z = 45, ρ = 12.41 g/cm³) Kα = 20.22 keV, Kβ = 22.07 keV are excellent candidates here. As we can note from Figure 1.23, characteristic lines dominate the unfiltered energy spectra at least for elevated acceleration when utilizing Mo and Rh anodes, resulting in a narrow energy distribution. With a clever choice of appropriate filters, we can further reduce the bremsstrahlung background.

This is shown in Figure 1.24, where we filtered the spectrum of a Mo anode with a 50 μm Mo filter, that effectively cuts off the high and low energy background. Note we are using a log scale in the ordinate and normalized on the absorption. After filtering, we basically are left with an energy band of about 5 keV, which comprises the Mo Kα and Kβ lines. As we also notice using such filtered radiation in mammography, we will observe the previously discussed beam hardening effect once we pass 5 cm of breast tissue. Common anode filter combinations that are used in mammography are Mo/Mo, Mo/Rh, and Rh/Rh. A Mo target in combination with a Rh filter is common for imaging thicker and denser breasts. A Rh/Rh combination will result in the lowest average dose, followed by Mo/Rh, and Mo/Mo.

We can calculate the X-ray spectrum, $P(E, \gamma)$, of X-ray tubes and associated filters, but it is not that trivial to really measure it, even when employing state of the art, high rate energy dispersive detectors such as silicon drift detectors (Gatti and Rehak 1984; Lechner et al. 2004). The knowledge of the energy spectrum is important in the quality control of X-ray tubes. If we are not able to determine it through a direct measurement, we can at least use the HVL (Section 1.3) to elucidate something like an effective X-ray energy of a polychromatic beam. An effective energy is equivalent to the energy of a monochromatic beam that would produce the same HVL. We can think of it as a sort of average beam energy whose numerical value is typically between one third and one half of the maximum energy. For instance, for an applied potential of 150 kV and a tungsten anode, the effective energy is about 68 keV. Some examples for effective energies as a function of the HVL in millimeters of Al, soft tissue, and bone are given in Table 1.2.

Due to the relativistic correction factor in the denominator of Equation A.112, the donut shape of the emission pattern will be deformed (Figure A.9). At low electron energy $\sqrt{\frac{E}{1 - \gamma}} \ll c$, bremsstrahlung is emitted preferentially between 60° and 90°, while for higher electron energies photons tend to be emitted in the forward direction with respect to the acceleration (Figure 1.25).

It is shown in Section A.1.4 and especially in Figure A.2 that, in circular particle accelerators, the emitted power of X-ray scales with the 4th power of the Lorentz factor, $\gamma$, which is substantially larger than the relativistic correction factor for bremsstrahlung. This explains why synchrotron radiation sources deliver abundant photon flux. As we notice, the spectrum of a bending magnet radiation in a synchrotron source delivers 3 to 4 orders of magnitude more photons than a high power X-ray tube with a tungsten anode. Therefore, we can employ crystal diffraction (Bragg’s Law; Equation 1.44) to select very narrow energy bands (0.1% bandwidth) for imaging, yielding substantially more flux than you find in the characteristic lines. Moreover, bending magnet radiation possesses a high degree of spatial and temporal coherence, meaning that all photons are emitted from a small source point and their relative phases are very similar, which allows the exploitation of the phase effects described in Section 1.4.10. The energy selectivity in combination with the delivered high photon flux allowed single, dual, and multi energy, or in general spectral imaging modalities, which were exploited first at synchrotron radiation source (see Arfelli 2000, and the references therein). In contrast to the limitation in the choice of the energy spectrum of mammographic X-ray tubes (Figure 1.23) with synchrotron radiation, we can find for each breast thickness and composition the appropriate energy to obtain the best SNR for a given radiation dose (Equation 1.77). In addition, the geometry of synchrotron radiation inherently reduces scattering and subsequently image blur.

We discussed before, in order to increase the image contrast, for instance of the coronary arteries in clinical routine, iodine based contrast agents are utilized, which are power injected for example into the lumen of each of the coronary arteries. For this (unpleasant) procedure, it is necessary to introduce a catheter into a peripheral artery and thread it into the ostium of one of the two coronary arteries. During and after the power injection, transmission radiographs of the upper torso are recorded either in a static fashion or in a time sequence (so-called cines). In this fashion, the coronary arteries are imaged with excellent SNR; however, hazards associated with the catheter placement are numerous, spanning from arterial perforation to embolic obstructions in various distal arteries, including those of the heart and brain.

As early as 1953 (Jacobson 1953), efforts were reported to avoid the arterial catheter and image the coronary arteries after an intravenous injection of contrast agent. Since in this modality the
Interesting for the enhancement of contrast agents are narrow energy bands bracketing the K-edge of a contrast agent.

Possible energy bands that can be used for spectral imaging. The iodine bolus is substantially diluted before it arrives in the coronary arteries (factor 20 or more), the iodine contrast is in the order of 1%, and is hooded by higher absorbing structures like bones and muscles. The aim of Jacobson was to use dichromatic absorption radiography, that is to say two images are recorded one after the other, with two different energies bracketing somehow the iodine absorption edge (Figure 1.26). The image which is taken with energy beyond the K-edge of the iodine (33.18 keV)—in the following called “high image”—comprises absorption effects from iodine, bones, fat, and muscles, while the image taken at lower energy (“low image”) has a sixfold less iodine contrast and serves as a mask. In order to increase the iodine contrast, one simply has to perform a logarithm subtraction of the high image and the low image. In the image attained in this fashion, only iodine should contribute to the signal. Even though the idea was advanced, this modality was never really utilized, since the sources available at that time would not deliver a sufficient flux. Nor were appropriate detection systems available. Moreover, high and low images were taken in a time sequence, that is to say one after the other. Since the heart is a rapidly moving organ and the patient could move at the time, the subtraction never really worked out, and moving artifacts destroyed the image contrast.

We could make use of two different X-ray energies in which different physical effects predominate. Thus, we can use low energy bands, high energy bands, plus small energy bands bracketing the absorption edges of materials (Menk et al. 1997a). The translation of spectral imaging from synchrotrons to clinical environment is not straightforward. However, it would help, for example, to dramatically reduce beam hardening artifacts in clinical computed tomography. We could make use of two different X-ray sources (or anode materials) or try to switch rapidly the high voltage in the X-ray source. This would provide the two (or more) different X-ray energies required for spectral imaging that are used by Siemens Healthcare and GE Healthcare. The third method (Philips Medical Systems) is to use beam hardening in a double layer X-ray detector. The first upstream detector would see mainly the low energy photons, while the second downstream layer would record the beam hardened high energy band. This brings us to a brief discussion of X-ray detectors. Up to now most of the detectors used in medical imaging are so-called integrating detectors that measure the total charge, $Q$, released in the detector volume by integration over the photo current, $i(t)$, in the time interval, $dt$.

$$Q = \int i(t) \cdot dt = \int \int \varepsilon(E_i) \cdot \varepsilon_{CC} \cdot \frac{E_i}{W_{\text{ion}}} \cdot P(E_i, t) \cdot dE_i \cdot dt$$  

(1.85)

where $\varepsilon(E_i)$ denotes the quantum efficiency and $\varepsilon_{CC}$ the charge collection efficiency of the detector. The former, in the sense of Equation 1.5, tells us how many photons on average are absorbed in the detector, and the latter tells us how many charges released by the X-rays (Equation 1.52) are eventually collected to generate a measurable current. It is clear that X-ray detectors are subject to the absorption processes and charge transport we discussed above. If the integration time, $dt$, is long...
in comparison to the waiting time, \( \tau \), between two consecutive hits (Equation 1.16), such a detector cannot discriminate the energy of the photons. For example, 5 photons of 10 keV arriving during the integration time, \( dt \), would generate the same charge as a single photon of 50 keV in such a time interval. If \( \tau_p \ll dt \ll \tau \), where \( \tau_p \) is the inherent dead time to process a photon detection event, then we can count single photons once the charge is above a certain threshold. Detectors working in this modality are called single photon counters. They count X-rays, but we just know that the energy of the photon was above a certain threshold. If we spend even more money we can measure the charge released by each X-ray and, subsequently, we know not only that a photon was detected but we are also able to elucidate the energy that this photon carried. Detectors possessing such capability are called spectroscopic detectors. The latter are those that are very interesting for spectral imaging because the energy discrimination does not rely on sources or optical components, but is just done in the detector. In recent years there was notable progress in highly segmented spectroscopic detectors where each cell (pixel) comprises multi-thresholding, pulse height analysis, and storage circuits. These devices can be tiled up to larger active areas, which are required in medical imaging. Originally, they were fabricated in 300 \( \mu \)m thick silicon (\( Z = 14 \), \( \rho = 2.33 \) g/cm\(^2\)), which is a great material, but, due to the low atomic number, not a great absorber. Very recently, stable room temperature semiconductors (CdTe, GaAs) have been developed that can be used to assemble pixel detectors, providing high quantum efficiency for high energy X-rays.

In Section 1.4.10, and especially in Equation 1.77, we saw that the radiation dose scales with the square of the SNR governed by Poisson statistics. What we calculated there was the pre-detection image, which has to be recorded with our imaging detector. Whatever imaging detector we use, we end up with a digitized version of the pre-detection image and the detector will mess it up: it will sample the pre-detection image in discrete spatial points (pixels), it will sample it in well-defined time intervals (image frames), it will spatially and temporally distort the image, it will sample the intensity in discrete steps, and it will add noise. Moreover, depending on its quantum efficiency, it will not stop all the photons escaping the patient. However, it should conserve to a certain extent the SNR of the pre-detection image. If we measure the \( \text{SNR}_{\text{sat}} \) in the digital image it will be coupled to the SNR by

\[
\text{SNR}_{\text{sat}}^2 = \text{DQE} \cdot \text{SNR}^2 \tag{1.86}
\]

The DQE is called the detective quantum efficiency (Menk et al. 1997b), and thoroughly characterizes the detectors. Its numerical value ranges from zero to unity. If we insert Equation 1.86 into Equation 1.77, we get

\[
D_{\text{sat}} = \frac{2 \cdot \text{SNR}_{\text{sat}}^2 \cdot e^{\mu t} \cdot E_z}{w^2 \cdot C_\mu \cdot \mu_2^2 \cdot \text{DQE}} \left( \frac{\mu_1}{\rho} \right) . \tag{1.87}
\]

We should note that the radiation dose now scales with the inverse of the DQE, which is not a good thing because \((1 - \text{DQE})\) is the additional dose we put into the patient that does not contribute to increase the SNR. We should be, therefore, be very careful with the selection of our imaging detector and make sure that it is very close to unity.

### Appendix A

#### A.1 Radiation and Scattered Fields

##### A.1.1 Maxwell Equations and Wave Equation

As stated before, we can solve most of the phenomena using classical electrodynamics, which implies finding solutions for Maxwell’s equations. According to the correspondence principle, the result of quantum mechanics and electrodynamics should be similar in the low energy limit. Since the rest mass of the photon is zero, we can approach the limit of null energy, tweaking the frequency of the electromagnetic waves of the photons toward zero. However, in the high energy limit of the bremsstrahlung spectrum and the Compton effect kinematics, we should not forget that the energy of the photon is given by \( h \cdot \omega \), which we then have to take into account for correction.

To calculate scattered fields we start with the Faraday–Maxwell equation, which we can write in the MKS system (that is based on units on measuring lengths in meters, mass in kilograms, and time in seconds) as

\[
\nabla \times \overrightarrow{E}(r,t) = \frac{-\partial \overrightarrow{B}(r,t)}{\partial t} \tag{A.1}
\]

where \( \overrightarrow{E}(r,t) \) is the electric field vector, and \( \overrightarrow{B}(r,t) \) is the magnetic induction.

We note that, in free space or vacuum, the magnetic field vector \( \overrightarrow{H}(r,t) \) and the electric displacement \( \overrightarrow{D}(r,t) \) are linearly coupled to the electric field and magnetic induction

\[
\overrightarrow{D}(r,t) = \varepsilon_0 \cdot \overrightarrow{E}(r,t), \quad \overrightarrow{B}(r,t) = \mu_0 \cdot \overrightarrow{H}(r,t) \tag{A.2}
\]

through the permittivity, \( \varepsilon_0 \), and the magnetic permeability, \( \mu_0 \).

The physical interpretation of the Faraday–Maxwell equation in the static case, in which the time derivation of the magnetic induction disappears, is that field lines of the electric field are open. Together with the Coulomb Maxwell equation,

\[
\nabla \cdot \overrightarrow{D}(r,t) = \rho(r,t), \tag{A.3}
\]

we note that it requires a source or a sink or in general an arbitrary charge density distribution, \( \rho(r,t) \), at which the open field lines have their origin or end, respectively.

Applying the curl on the Faraday–Maxwell equation and utilizing the vector identity \( \nabla \times (\nabla \times \overrightarrow{E}) = \nabla \left( \nabla \cdot \overrightarrow{E} \right) - \nabla^2 \overrightarrow{E} \), we get

\[
\nabla \times (\nabla \times \overrightarrow{E}) = \nabla \times \left( -\frac{\partial \overrightarrow{B}}{\partial t} \right), \tag{A.4}
\]

\[
\nabla \cdot (\nabla \cdot \overrightarrow{E}) - \nabla^2 \overrightarrow{E} = \mu_0 \cdot \frac{\partial}{\partial t} \left( \nabla \times \overrightarrow{H} \right)
\]
To simplify this further we need the Ampere Maxwell equation

\[ \nabla \times \vec{H}(\vec{r}, t) = \frac{\partial \vec{D}(\vec{r}, t)}{\partial t} + \vec{j}(\vec{r}, t) \quad (A.5) \]

which couples the electric and magnetic field through the current density \( \vec{j}(\vec{r}, t) \). As before in the static case and for a constant current density in time, Equation A.5 tells us that magnetic field lines are closed.

Using Equations A.2 to A.4 and rearranging terms we get

\[ \left( \frac{\partial^2}{\partial t^2} - c^2 \cdot \nabla^2 \right) \vec{E}(\vec{r}, t) = -\frac{1}{\varepsilon_0} \left[ \frac{\partial j(\vec{r}, t)}{\partial t} + c^2 \cdot \nabla \cdot \rho(\vec{r}, t) \right], \]

\[ (A.6) \]

which is the general form of the wave equation. Mathematically, this equation is an inhomogeneous differential equation of second order, which is far beyond being easily solvable. The mixing between the charge density and the current density on the right hand side of Equation A.6 makes it solving very difficult. We will see, further on, how to avoid this, by utilizing what is known as the Lorentz gauge.

Due to the non-existence of magnetic monopoles, thus magnetic sources or sinks, the gradient on the magnetic field must disappear, according to Equation A.3, thus

\[ \nabla \cdot \vec{B}(\vec{r}, t) = 0. \quad (A.7) \]

Since the gradient is perpendicular to the curl on the vector field \( \vec{A}(\vec{r}, t) \) or \( \nabla \perp \nabla \times \vec{A}(\vec{r}, t) \), we could automatically satisfy Equation A.7 by writing

\[ \vec{B}(\vec{r}, t) = \nabla \times \vec{A}(\vec{r}, t), \quad (A.8) \]

where \( \vec{A}(\vec{r}, t) \) is termed a vector potential. Moreover, we could also automatically satisfy Equation A.1 by introducing

\[ \vec{E}(\vec{r}, t) = -\nabla \cdot \varphi(\vec{r}, t) + \frac{\partial \vec{A}(\vec{r}, t)}{\partial t}, \quad (A.9) \]

where \( \varphi(\vec{r}, t) \) is called a scalar potential. The problem is that expressing electric and magnetic fields in terms of the scalar and vector potentials does not uniquely define the potentials. We can show that, if \( \vec{A}(\vec{r}, t) \rightarrow \vec{A}(\vec{r}, t) + \nabla \cdot \psi(\vec{r}, t) \) and \( \varphi(\vec{r}, t) \rightarrow \varphi(\vec{r}, t) + \partial \psi(\vec{r}, t)/\partial t \), where \( \partial \psi(\vec{r}, t)/\partial t \) is an arbitrary scalar field, then the associated electric and magnetic fields are unaffected. The root of the problem lies in the fact that Equation 1.11 specifies the curl of the vector potential, but leaves the divergence of this vector field completely unspecified. We can avoid this by adopting a convention that specifies the divergence of the vector potential. Such a convention is usually called a gauge condition. Since Maxwell’s equations are Lorentz invariant, thus they take the same form in all inertial frames, it makes a lot of sense to adopt such a gauge condition that is also Lorentz invariant. This leads us to the so-called Lorentz gauge condition

\[ \varepsilon_0 \cdot \mu_0 \cdot \frac{\partial \varphi(\vec{r}, t)}{\partial t} + \nabla \cdot \vec{A}(\vec{r}, t) = 0 \quad (A.10) \]

Equations A.8 to A.10 can be combined with Equations A.3 and A.5 to give

\[ \frac{1}{c^2} \cdot \frac{\partial^2 \varphi(\vec{r}, t)}{\partial t^2} - \nabla^2 \cdot \varphi(\vec{r}, t) = \frac{\rho(\vec{r}, t)}{\varepsilon_0} \quad (A.11) \]

and

\[ \frac{1}{c^2} \cdot \frac{\partial^2 \vec{A}(\vec{r}, t)}{\partial t^2} - \nabla^2 \cdot \vec{A}(\vec{r}, t) = \mu_0 \cdot \vec{j}(\vec{r}, t), \quad (A.12) \]

where \( c^2 = 1/(\varepsilon_0 \cdot \mu_0) \) is the square of the phase velocity of the wave in vacuum. The beauty here is that the fields are now given exclusively in terms of the charge density and current density. We should note that the four Maxwell equations are reduced to Equations A.11 and A.12, which are referred to as the wave equations, and in which particles contribute to and are affected by the potentials. Mathematically, they represent inhomogeneous differential equations of second order. In the absence of particles or currents, the right hand sides are zero, and we can solve the now homogenous wave equation, for instance Equation A.11, by utilizing the generic ansatz of separation of variables.

\[ \varphi(\vec{r}, t) = R(\vec{r}) \cdot T(t) \quad (A.13) \]

Substituting this form into the Equation A.12 wave equation we obtain:

\[ \frac{(\nabla^2 + k^2) \cdot \varphi(\vec{r}, t)}{R(\vec{r})} \frac{1}{c^2 \cdot T(t)} \frac{\partial^2 T(t)}{\partial t^2} = -k^2, \quad (A.14) \]

where we have chosen, without loss of generality, the expression \(-k^2\) for the value of the constant. Rearranging the first equation, we obtain the Helmholtz equation (von Helmholtz 1894):

\[ (\nabla^2 + k^2) \cdot \varphi(\vec{r}, t) = 0. \quad (A.15) \]

To specifically solve, for instance Equation A.12, we choose

\[ \vec{A}(\vec{r}, t) = \vec{A}_0 \cdot e^{-i(k \cdot \vec{r} - \omega t)} \quad (A.16) \]

Inserting Equation A.16 into Equation A.12 and executing the second derivatives in space and time results in

\[ \vec{A}_0 \cdot (-\omega^2 + c^2 \cdot |k|^2) = 0 \quad (A.17) \]

or \( k = \pm \omega/c \), which couples the wave number \( k \) with the frequency of the free propagating wave in vacuum. The two solutions of Equation A.17 represent two waves propagating in opposite directions. In a conventional dielectric medium possessing a real
dielectric constant, \( \varepsilon \), which is greater than unity, an electromagnetic wave propagates with a phase velocity

\[
v = \pm \frac{c}{n} = \pm \frac{\omega}{k}
\]  

(A.18)

that is slower than the velocity of light in vacuum. In this case, \( n = \sqrt{\varepsilon} \).

We can substitute in Equations A.11 and A.12 the current density in terms of the charge density and vice-versa. For that we release the gradient (\( \nabla \)) on the Ampere Maxwell (Equation A.5) and we get

\[
\nabla \cdot \nabla \times \mathbf{H}(r, t) = \nabla \cdot \frac{\partial \mathbf{D}(r, t)}{\partial t} + \nabla \cdot \mathbf{j}(r, t).
\]  

(A.19)

Since the angle between gradient and curl on the vector field is 90 degrees (in other words \( \nabla \times \nabla = 0 \)), the left hand side equals zero. Additionally, since time derivation and gradient are commutative operations, we can rewrite the first term on the right hand side as

\[
\frac{\partial}{\partial t} \nabla \cdot \mathbf{D}(r, t) = \frac{\partial \rho(r, t)}{\partial t},
\]  

(A.20)

resulting in the equation of charge continuity:

\[
\nabla \cdot \mathbf{j}(r, t) = -\frac{\partial \rho(r, t)}{\partial t}.
\]  

(A.21)

We can think of the current density as a charge density, \( q \cdot \eta(r, t) \), moving with the respective velocity, \( \mathbf{v}(r, t) \), thus

\[
\mathbf{j}(r, t) = q \cdot \eta(r, t) \cdot \mathbf{v}(r, t),
\]  

(A.22)

with \( \eta(r, t) \) being the charge distribution function. The interpretation of the continuity equation is the following: if charge is moving out of a differential volume (i.e., divergence of current density is positive), then the amount of charge within that volume is going to decrease, so the rate of change of charge density is negative. With other words the continuity equation amounts to the conservation of charge. Whatever charge moves out of the volume has flow through the surface, which encapsulates the charge. Equation A.21 is somewhat a common sense concept that can be applied to all fields of science, including economics. Unfortunately, the continuity equation possesses only modest consideration on the stock market, where the money flow on the market is not necessary coupled to the encapsulated capital, which explains hyped markets and bubbles.

### A.1.2 Fields from Accelerated Charges

Obviously, as soon as charges and currents are involved, the right hand side, for instance of Equation A.12, differs from zero, and things become trickier, since we have to solve the inhomogeneous partial vector differential equation, which is not trivial at all. We have to find a particular integral for \( \overrightarrow{A}(\overrightarrow{r}, t) \). The general solution to the linear differential equation is the sum of the general solution of the related homogeneous equation and the particular integral. Or, when the initial conditions are set, we can use a guess to obtain the particular solution directly. Such a guess that would solve Equation A.12 is Green’s function, which is given by

\[
G(\mathbf{r}, \mathbf{r}', t, t') = \frac{\delta\left(t - t' - \frac{\mathbf{r} - \mathbf{r}'}{c}\right)}{4\cdot \pi \cdot \left|\mathbf{r} - \mathbf{r}'\right|},
\]  

(A.23)

and which would invert Equation A.12 to obtain

\[
\overrightarrow{A}(\mathbf{r}, t) = \frac{\mu_0}{4 \cdot \pi} \int \frac{G(\mathbf{r}, \mathbf{r}', t, t') \cdot \delta\left(t - t' - \frac{\mathbf{r} - \mathbf{r}'}{c}\right)}{\left|\mathbf{r} - \mathbf{r}'\right|} \cdot d^3r',
\]  

(A.24)

where \( \mathbf{r}' \) denotes the position of the charge density, and \( \mathbf{r} \) is the position where the vector potential is observed. We note Green’s function satisfies the boundary conditions that the fields have to disappear for \( |\mathbf{r} - \mathbf{r}'| \to \infty \) and that it requires the time \( |\mathbf{r} - \mathbf{r}'|/c \) to observe fields at \( \mathbf{r} \) which have been generated by a charge at the position \( \mathbf{r}' \). Using the Maxwell Ampere equations (Equations A.5 and A.8) we get for the field, in the source free region

\[
\overrightarrow{E}(\mathbf{r}, t) = \frac{\mu_0}{k} \nabla \times \mathbf{B}(\mathbf{r}, t).
\]  

(A.25)

Let us define a unit vector, \( \hat{n} = \mathbf{r}/|\mathbf{r}| \), and let us assume that \( |\mathbf{r}'| \ll |\mathbf{r}| \), then we can approximate the denominator in Equation A.24 as \( r \), provided that the distance from the accelerated charge is much greater than its extension, \( r' \). Thus, Equation A.24 reduces to

\[
\overrightarrow{A}(\mathbf{r}, t) = \frac{\mu_0}{4 \cdot \pi} \int G(\mathbf{r}, \mathbf{r}', t, t') \cdot \delta\left(t - t' - \frac{\mathbf{r} - \mathbf{r}'}{c}\right) \cdot d^3r',
\]  

(A.26)

Let us now consider a constant accelerated single electron moving along the z-axis with the velocity \( \mathbf{v}(\mathbf{z}, t) = \mathbf{v}(z, t) \cdot \hat{z} \). In this case, we can write the charge distribution function \( \eta(\mathbf{r}, t) \equiv 1 \) and, according to Equation A.22, we obtain

\[
\mathbf{j}(\mathbf{r}, t) = e \cdot \mathbf{v}(z, t) \cdot \hat{z},
\]  

(A.27)

And, subsequently, using Equations A.26 and A.27,

\[
\overrightarrow{A}(\mathbf{r}, t) = \frac{\mu_0}{4 \cdot \pi \cdot |\mathbf{r}|} \cdot \int e \cdot \mathbf{v}(z, t) \cdot \hat{z} \cdot \delta\left(t - t' - \frac{\mathbf{r} - \mathbf{r}'}{c}\right) \cdot d^3r',
\]  

(A.28)
where $\delta$ denotes Dirac’s delta function. Executing the integration, we get for the magnetic vector potential:

$$\vec{A}(\vec{r},t) = \frac{\mu_0}{4 \pi} \cdot \vec{e} \cdot e \left( t - \frac{|\vec{r}|}{c} \right) \vec{e}. \quad (A.29)$$

Furthermore, corresponding to the figure, we imagine an electron oscillating around the origin with maximum amplitude, $r_0$, that is small in comparison the position of the observer (far field). We identify

$$e \cdot \left( t - \frac{|\vec{r}|}{c} \right) \cdot \vec{e} = \frac{\partial \vec{d}_s(t)}{\partial t}$$

as the time derivation of the dipole moment with $\vec{d}_s(t) = e \cdot r_0 \cdot \vec{e}$. Substituting the vector potential into the Lorentz gauge (Equation A.10) we get for the scalar potential

$$\varphi(\vec{r},t) = -\frac{\mu_0}{4 \pi} \cdot \vec{e} \cdot \nabla \cdot \int \frac{\partial \vec{d}_s(t - \frac{|\vec{r}|}{c})}{\partial t} \cdot \vec{e} \cdot \frac{\vec{r}}{c \cdot |\vec{r}|} \cdot \vec{e} dt = -\frac{\mu_0}{4 \pi} \cdot \vec{e} \cdot \frac{d_0(t - \frac{|\vec{r}|}{c})}{|\vec{r}|}. \quad (A.30)$$

Performing now the differentiation the scalar potential is

$$\varphi(\vec{r},t) = \frac{\mu_0}{4 \pi} \cdot \left( \frac{\partial \vec{d}_s(t - \frac{|\vec{r}|}{c})}{\partial t} \cdot \vec{e} \cdot \frac{\vec{r}}{c \cdot |\vec{r}|} \right) \approx \frac{\mu_0}{4 \pi} \cdot \frac{\partial d_0(t - \frac{|\vec{r}|}{c})}{\partial t} \cdot \vec{e} \cdot \frac{\vec{r}}{c \cdot |\vec{r}|} \cdot \vec{e}. \quad (A.31)$$

where the second summand tends to zero more rapidly and can be neglected if we are interested in radiated fields in the far zone. Substituting this into Equations A.8 and A.9, we get, for the electric field,

$$\vec{E}(\vec{r},t) = \frac{\mu_0}{4 \pi} \cdot \left( \frac{\partial^2 d_0(t - \frac{|\vec{r}|}{c})}{\partial t^2} \cdot \vec{e} \cdot \frac{1}{c^2 \cdot |\vec{r}|^2} \right) + \frac{\partial^2 d_0(t - \frac{|\vec{r}|}{c})}{\partial t^2} \cdot \vec{e} \cdot \frac{\vec{r}}{c^2 \cdot |\vec{r}|^2} \cdot \vec{r} \right)$$

and, for the magnetic field,

$$\vec{H}(\vec{r},t) = \frac{\mu_0}{4 \pi} \cdot \left( \frac{\partial^2 d_0(t - \frac{|\vec{r}|}{c})}{\partial t^2} \cdot \vec{e} \times \frac{\vec{r}}{c^2 \cdot |\vec{r}|^2} \right) = \frac{\mu_0}{4 \pi} \cdot \frac{e \cdot (\vec{a} \times \vec{r})}{c^2 \cdot |\vec{r}|^2}. \quad (A.34)$$

neglecting higher terms in $|\vec{r}|$ in the far zone. The radiated electric field is, therefore, dependent only on the velocity/acceleration, which can be observed at the position $|\vec{r}|$ with a time delay of $t - \frac{|\vec{r}|}{c}$. Furthermore, it follows directly that, in the far zone, $\vec{E}(\vec{r},t)$ and $\vec{H}(\vec{r},t)$ are mutually orthogonal, propagating in the $\vec{r}$ direction.

$$\vec{E}(\vec{r},t) = \vec{H}(\vec{r},t) \times \frac{\vec{r}}{|\vec{r}|} \quad \text{and} \quad \vec{H}(\vec{r},t) = -\vec{E}(\vec{r},t) \times \frac{\vec{r}}{|\vec{r}|} \quad (A.35)$$

Using the conservation of energy for the electromagnetic field, Poynting (1884) showed that the Poynting vector represents a vector flow of an energy density in an direction orthogonal to $\vec{E}(\vec{r},t)$ and $\vec{H}(\vec{r},t)$ or

$$\vec{S}(\vec{r},t) = \vec{E}(\vec{r},t) \times \vec{H}(\vec{r},t) \quad (A.36)$$

Using Equations A.33 and A.34, we can show that the Poynting vector is given by

$$\vec{S}(\vec{r},t) = \frac{e_0}{\mu_0} \cdot \left( \frac{\vec{E}(\vec{r},t)}{|\vec{r}|} \cdot \frac{\vec{r}}{|\vec{r}|} \right) = \frac{e^2 \cdot |\vec{a}|^2 \cdot \sin^2(\theta)}{16 \cdot \pi^2 \cdot |\vec{e} \cdot e^1 \cdot \vec{a}^2 | \cdot \vec{n}. \quad (A.37)$$

where $\theta$ is the angle with the propagation direction $\vec{r}/|\vec{r}| = \vec{n}$. For an oscillating charge, where the acceleration is parallel to the velocity of the electron, we deal with Hertzian dipole, where the flow of the energy density is proportional to $|\vec{a}|^2$. In the far field, the energy density drops with the square of the distance $|\vec{r}|^2$ and follows a donut shaped emission pattern (Figure A.1a and b).

We ask ourselves now what is the radiated power density (in other words the power per solid angle, $dP/d\Omega$) of the electromagnetic fields generated by the accelerated charge. The power radiated per unit solid angle $r^2 \cdot d\sin(\theta) \cdot d\varphi$ is

$$dP/d\Omega = r^2 \cdot d\sin(\theta) \cdot d\varphi = r^2 \cdot d\Omega$$

FIGURE A.1 Donut-shaped emission pattern for dipole radiation. (a and b) For linear acceleration and (c) for circular acceleration.
\[ \frac{dP}{d\Omega} = \left| \frac{\vec{v} \cdot \vec{p}}{m} \right| = \frac{e^2 \cdot |\vec{v}|^2 \cdot \sin^2(\theta)}{16 \cdot \pi^2 \cdot \varepsilon_0 \cdot c^3}, \tag{A.38} \]

Which, integrated over the solid angle, gives

\[ P = \frac{8 \cdot \pi}{3} \cdot \left( \frac{e^2 \cdot |\vec{v}|^4}{16 \cdot \pi^2 \cdot \varepsilon_0 \cdot c^3 \cdot R^2} \right). \tag{A.39} \]

the total power emitted by the accelerated charge.

For a circular movement of the electron where the angular velocity \( |\vec{v}| \) is small in comparison to \( c \) (Figure A.1c) we can substitute the acceleration by the centripetal acceleration \( |\vec{v}|^2/R \), where \( R \) is the radius of the orbit, thus we would get for the total power emitted:

\[ P = \frac{8 \cdot \pi}{3} \cdot \left( \frac{e^2 \cdot |\vec{v}|^4}{16 \cdot \pi^2 \cdot \varepsilon_0 \cdot c^3 \cdot R^2} \right). \tag{A.40} \]

For increasing circular velocity of the electron, as we can find in particle accelerators and synchrotron radiation sources, we need to substitute the centripetal acceleration with the relativistic acceleration, which we can get in a less rigorous fashion as follows:

\[ |\vec{v}| = \frac{1}{m} \cdot \frac{d}{d\tau} |\vec{p}| = \frac{1}{m} \cdot \gamma \cdot \frac{d(\gamma \cdot v \cdot |\vec{v}|)}{d\tau} = \gamma^2 \cdot \frac{|\vec{v}|^2}{R}. \tag{A.41} \]

where \( \tau = t/\gamma \) is the time in the moving reference frame of the electron, \( \gamma = 1/\sqrt{1 - \beta^2} \) is the Lorentz factor (Lorentz 1882), and \( \beta = v/c \). Inserted into Equation A.39, we then get

\[ P = \frac{8 \cdot \pi}{3} \cdot \left( \frac{e^2 \cdot \gamma^4 \cdot |\vec{v}|^4}{16 \cdot \pi^2 \cdot \varepsilon_0 \cdot c^3 \cdot R^2} \right). \tag{A.42} \]

In circular particle accelerators, the velocity of the particles is almost the speed of light in vacuum—let us say in the order of 0.99999995c to be very prudent. This means \( \beta \sim 1 \), which boosts the Lorentz factor and subsequently the emitted power with the 4th power of \( \gamma \). For a small sized electron accelerator, such as a synchrotron source with \( R = 200 \) m, the total power radiated per electron is then around \( 2 \cdot 10^{-11} \) W, which sounds not that great but, multiplied with the number of electrons in the accelerator (for instance at 300 mA around \( 2 \cdot 10^3 \)), this results in some thousands of watts (~38 kW). In the reference frame that travels with the particle within the accelerator, the emission pattern in the far zone is still donut shaped; however, seen from an observer in the laboratory reference frame, the donut is contracted by the Lorentz factor \( \gamma \) in the direction of the velocity vector (Figure A.2).

This means the radiation is folded into a narrow forward cone possessing an opening angle, which is proportional to \( 1/(2 \cdot \gamma) \) and which is called synchrotron radiation. Due to the small opening angle and other characteristics, such spatial and temporal coherence of the emitted wavefield’s synchrotron radiation is very similar to lasers in the optical wavelength regime, and belong to the brightest X-ray sources.

### A.1.3 Rutherford’s Atom Model Failure

After the short excursion into the relativistic world we can try to estimate the lifetime of a Rutherford hydrogen atom, where the electron is moving around the nucleus in a circular orbit with the radius \( R \), using the arguments developed above. From Newton’s second law for circular motion we get (classical and non-relativistic)

\[ m \cdot \omega^2 \cdot R = \frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot R^2} \Rightarrow \omega^2 \cdot R^2 = \frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot R \cdot m}. \tag{A.43} \]

The energy of the non-relativistic electron is

\[ E = \frac{1}{2} \cdot m \cdot v^2 - \frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot R} = -\frac{1}{2} \cdot \frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot R}. \tag{A.44} \]

Since the energy loss \( dE/dt = -P \) and using Equation A.40, we find

\[ \frac{1}{2} \cdot \frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot R^2} \cdot \frac{dR}{dt} = -\frac{8 \cdot \pi}{3} \cdot \left( \frac{e^2 \cdot \omega^4}{16 \cdot \pi^2 \cdot \varepsilon_0 \cdot c^3 \cdot R^3} \right) = -\frac{2}{3} \cdot \frac{e^2 \cdot e^4}{4 \cdot \pi \cdot \varepsilon_0 \cdot m^2 \cdot c^3 \cdot R^3} \Rightarrow \frac{dR}{dt} = -\frac{4}{3} \cdot \frac{e^4}{m^2 \cdot c^3 \cdot R^2}. \tag{A.45} \]
With the frame condition that $R(t_0) = a_o$, the Bohr radius, and $R(t) = R$, we can solve the integral by separation of the variables and we get

$$t - t_0 = -\frac{1}{4} \frac{m^2 \cdot c^3}{e^2} \cdot (R^3 - a_o^3).$$  \hspace{1cm} (A.46)

With the frame conditions $t_0 = 0$ and $R(T) = 0$, the decay time $T$ is

$$T = t - t_0 = -\frac{1}{4} \frac{m^2 \cdot c^3 \cdot a_o^5}{e^2} = 3.2 \cdot 10^{-13} \text{s}. \hspace{1cm} (A.47)$$

### A.1.4 Scattering of Radiation on Free Electrons

We now try to understand the effect of a plane wave field (Equation A.16) propagating in the $\vec{k}_0$ direction with well-defined frequency, $\omega_0$, impinging on an electron of mass $m$ and charge $e$. We include in the discussion that this electron can also be weakly bound, for instance in the outer shells of atoms.

In accordance with Equation A.16, we denote the external plane wave as

$$\vec{E}_{\text{ext}}(\vec{r}, t) = \vec{E}_0 \cdot e^{-i(\vec{k}_0 \cdot \vec{r} - \omega_0 t)}.$$  \hspace{1cm} (A.48)

where we write the amplitude $\vec{E}_0 = \vec{E}_0 \cdot E_0$ in terms of a polarization unit vector $\vec{\Pi}_0$ with $|\vec{\Pi}_0| = 1$ and the scalar $E_0$, which describes the magnitude of the oscillation.

The flux of incident energy is given by the time average of the Poynting vector (left hand side of Equation A.37) of the incident wave and, therefore,

$$\vec{S} = \frac{\varepsilon_0}{\mu_0} \frac{|E_0|^2}{2},$$ \hspace{1cm} (A.49)

where the process of averaging over time of a periodic wave produces the factor 1/2. We also note that the average is

$$\bar{T} = |\vec{S}| = \frac{\varepsilon_0}{\mu_0} \frac{|E_0|^2}{2}. \hspace{1cm} (A.50)$$

Similar to a cork bouncing on water waves, this external field would accelerate the electron along the polarization of the wave in the z-direction, $\vec{\Pi}_0 = \vec{\Pi}_0 \cdot \hat{e}_z$, as long as the wavelength, $\lambda$, is large enough. What this means we will see in a second. For simplification, we will treat everything in a classical way, thus the involved processes are neither quantum mechanic nor relativistic. This allows us to neglect magnetic fields, which are proportional to $v/c$. We, therefore, can use Newton’s second law of motion

$$\vec{F}(\vec{r}, t) = m \cdot \vec{a}(\vec{r}, t) = e \cdot \vec{E}_{\text{ext}}(\vec{r}, t)$$

$$\Rightarrow \vec{a}(\vec{r}, t) = \frac{e}{m} \vec{\Pi}_0 \cdot \vec{E}_0 \cdot e^{-i(\vec{k}_0 \cdot \vec{r} - \omega_0 t)}.$$  \hspace{1cm} (A.51)

instead of the Lorentz force, $\vec{F} = e \cdot (\vec{E} + (\vec{v} \times \vec{B}))$. As described in the previous section, and using the acceleration found in Equation A.51, the average radiated energy per solid angle unit is then

$$\frac{dP}{d\Omega} = \frac{e^4 \cdot E_0^2 \cdot \sin^2(\theta)}{m^2 \cdot 16 \cdot \pi^2 \cdot \varepsilon_0 \cdot c^2}.$$  \hspace{1cm} (A.52)

It now makes a lot of sense to compare the energy radiated per time unit and solid angle, thus $dP(\Omega)$, with the flux of incident energy per unit surface and time which we found previously (Equation A.49), which gives us the so-called differential cross-section, and which is given by

$$\frac{d\sigma_{\text{th}}}{d\Omega} = \frac{dP}{d\Omega} \left/ \vec{S} = \left( \frac{\varepsilon_0}{4 \cdot \pi \cdot \varepsilon_0 \cdot m \cdot c^2} \right)^2 \cdot \sin^2(\theta). \right.$$  \hspace{1cm} (A.53)

Integrating over the solid angle, $d\Omega$, we will get the scattering cross-section as the equivalent area of the incident wavefront that delivers the same power as that re-radiated by the particle: that is

$$\sigma_{\text{th}} = \int d\sigma \frac{d\Omega}{d\Omega} = \frac{8 \cdot \pi \cdot m \cdot c^2}{3} \cdot \left( \frac{\varepsilon_0}{4 \cdot \pi \cdot \varepsilon_0 \cdot m \cdot c^2} \right)^2$$

$$= \frac{8 \cdot \pi \cdot (2.8 \cdot 10^{-15} m)^2}{3} \cdot \frac{8 \cdot \pi \cdot r_0^2}. \hspace{1cm} (A.54)$$

Equation A.54 is the well-known Thomson scattering cross-section. The quantity $2.8 \times 10^{-15} \text{ m}$ is the value of the so-called classical electron radius, $r_0$, which can be understood as the radius of a spherical shell of total charge $e$, whose electrostatic energy equals the rest mass energy of the electron. We can, therefore, consider an electron, when scattering radiation, as a solid sphere whose radius is of the order of the classical electron radius.

Up to now we assumed an acceleration that is parallel to the polarization, $\vec{a} \parallel \vec{\Pi}_0 \rightarrow \vec{a} \parallel \vec{\Pi} = \cos(\vec{\theta})$. For the general case of randomly polarized incident radiation, we can express $\vec{n}$ in terms of the polarization vectors $\vec{\Pi}_1, \vec{\Pi}_2, \vec{\Pi}_3$ (see Figure A.3) as

$$\vec{n} = \sin(\phi) \cdot \cos(\theta)\vec{\Pi}_1 + \sin(\phi) \cdot \sin(\theta) \cdot \vec{\Pi}_2 + \cos(\phi) \cdot \vec{\Pi}_3. \hspace{1cm} (A.55)$$

Averaging over all possible polarizations of the incident wave we obtain

![FIGURE A.3 Model for scattering of radiation on free electrons.](image-url)
It is clear that the differential scattering cross-section is independent of the frequency of the incident wave, and is also symmetric with respect to forward and backward scattering. Moreover, the frequency of the scattered radiation is the same as that of the incident radiation. For the sake of completeness, we should note that Thomson scattering occurs when the wavelength \( \lambda \gg a_0 \).

\[ \sigma = \frac{n_e \left( 1 + \cos^2(\varphi) \right)}{2} \quad \text{(A.56)} \]

### A.1.5 Bohr’s Atom Model

In order to calculate the energy levels in Bohr’s atom model, we start, as in Section A.1.3, with Newton’s second law of a circular movement of an electron orbiting the nucleus, with the total charge \( Z \cdot e \) at a distance \( R \). Noting that the Coulomb force is equal to the centripetal force (Equation A.43), we get

\[ m \cdot \frac{v^2}{R} = \frac{e^2}{4 \cdot \pi \cdot \varepsilon_0 \cdot R^2}, \quad \text{(A.57)} \]

now in terms of the angular velocity \( v \). Using the conservation of the angular (quantum mechanical) momentum

\[ m \cdot v \cdot R = n \cdot \hbar \Rightarrow v = \frac{n \cdot \hbar}{m \cdot R}, \quad \text{(A.58)} \]

we get an expression for the angular velocity in terms of \( \hbar \), which we then insert into Equation A.57. Solving for \( R \), we obtain

\[ R = \frac{n^2}{Z} \cdot \frac{4 \cdot \pi \cdot \varepsilon_0 \cdot \hbar^2}{m \cdot e^2} = a_0 \cdot \frac{n^2}{Z}. \quad \text{(A.59)} \]

In order to calculate the energy levels in the atom in terms of the quantum number, \( n \), we use the electrostatic potential and the radius found in Equation A.59, which gives

\[ E_n = -\frac{Z \cdot e^2}{8 \cdot \pi \cdot \varepsilon_0 \cdot R} = -\frac{m \cdot Z^2 \cdot e^2}{32 \cdot \pi^2 \cdot \varepsilon_0^2 \cdot h^2} \cdot \frac{1}{n^2}. \quad \text{(A.60)} \]

For a transition from the initial energy state of the atom, \( n_i \), to a final state, \( n_f \), the difference in energy is then given by

\[ E_i - E_f = \hbar \cdot \omega = \frac{m \cdot e^4}{32 \cdot \pi^2 \cdot \varepsilon_0^2 \cdot h^2} \cdot \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \cdot Z^2. \quad \text{(A.61)} \]

The energy difference can be positive or negative, which corresponds to an emission or absorption of a photon.

### A.1.6 Scattering on Bound Electrons

We now explore the interaction of electromagnetic radiation on a harmonically bound electron orbiting an atomic nucleus (see Figure 1.9a). This implies a sort of Bohr atom, but we try to avoid quantum mechanics and solve the equations classically, in which the electron is viewed as being bound to the nucleus via a spring with a natural, angular frequency, \( \omega_n \). If the electron is perturbed, it will oscillate at this natural frequency, which will result in the emission of photons of energy \( E_i = \hbar \cdot \omega_n \). Hence, the bound electron is an example of a damped, harmonic oscillator. We also assume that the damping rate, \( \gamma_a \), of this oscillation is much smaller than \( \omega_n \) (thus, \( \gamma_a \ll \omega_n \)), and we treat everything non-relativistic as in the previous sections. Applying again Newton’s second law of motion we get

\[ m \cdot \frac{d^2 \vec{r}}{dt^2} + m \cdot \gamma_a \frac{d \vec{r}}{dt} + m \cdot \omega_n^2 \cdot \vec{r} = -e \cdot \vec{E} \quad \text{(A.62)} \]

For ease of discussion, we just assume a time dependency of \( e^{-i \omega_n t} \) for \( \vec{r} \) and \( \vec{E} = E_0 \cdot \vec{\Pi}_0 \), and we find, by executing the time derivatives and rearranging terms, that a steady solution is given by

\[ \vec{r} = \frac{1}{\omega_n^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_n^2} \cdot \frac{e}{m} \cdot E_0 \cdot \vec{\Pi}_0 \cdot e^{-i \omega_n t}, \quad \text{(A.63)} \]

and, subsequently,

\[ \vec{a} = \frac{d^2 \vec{r}}{dt^2} = \frac{\omega_n^2}{\omega_n^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_n^2} \cdot \frac{e}{m} \cdot E_0 \cdot \vec{\Pi}_0 \cdot e^{-i \omega_n t}. \quad \text{(A.64)} \]

Having found the acceleration, we follow the same steps as in the previous sections, thus calculating the fields and the pointing vector according to Equations A.33 to A.37, normalizing this to the incident power density, and eventually we find

\[ \sigma = \sigma_{\text{Th}} \cdot \frac{\omega_a^4}{(\omega_n^2 - \omega_a^2)^2 + (\gamma_a \cdot \omega_n^2)^2}. \quad \text{(A.65)} \]

We notice that the angular distribution of the radiation is the same as we found previously for the free electron. Furthermore, we realize for the resonant case when \( \omega_a = \omega_n \) the value of the cross-section maximizes at \( \sigma = \sigma_{\text{Th}} \cdot \omega_n^2 / \gamma_a^2 \) and outstrips the value of Thomson scattering cross-section easily, since we assumed \( \omega_n \gg \gamma_a \).

For a strong binding, which means \( \omega_a \ll \omega_n \), we can neglect all terms in \( \omega_a \) in the denominator, and Equation A.65 reduces to

\[ \sigma_{\text{res}} = \sigma_{\text{Th}} \cdot \left( \frac{\omega_n}{\omega_a} \right)^4 \quad \text{(A.66)} \]

This cross-section is known as the Rayleigh scattering cross-section, and depends on the inverse fourth power of the wavelength of the incident radiation.

We try now to extend this to \( Z \) bound electrons in hydrogen like atoms. We assume the nucleus is positioned in the origin of the coordinate system, and the distance of each of the electrons is given by \( \Delta a_e \). Finally, we are observing the scenery from a distant point at \( \vec{r} \). Since all electrons will be involved in the scatter process, we have to extend Equation A.64 to
\[\vec{a} = \frac{e}{m} \sum_{a=1}^{Z} \frac{\omega_a^2 - \omega_0^2 + i \cdot \gamma_a \cdot \omega_0}{\omega_a^2 - \omega_0^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \vec{E}_0 \cdot \vec{k}_b \cdot e^{-i(\omega_0 t)}, \]

where the expression \(\Delta \vec{k} \cdot \Delta \vec{E}_r\) gives the phase variation of the scattered fields due to the different electron positions as seen by the observer. \(f(\Delta \vec{k}, \omega_0)\) is called the complex atomic scattering factor, which is rather complicated to determine due to the phase variation factor \(e^{-i(\Delta \vec{k} \cdot \Delta \vec{E}_r)}\) in Equation A.67.

Following the steps in the previous sections we get, for the differential cross-section,

\[\frac{d\sigma_{\text{coh}}}{d\Omega} = r_0^2 \cdot |f(\Delta \vec{k}, \omega_0)|^2 \cdot \sin^2(\theta), \quad (A.68)\]

and for the total cross-section,

\[\sigma_{\text{coh}} = \frac{8 \cdot \pi}{3} \cdot r_0^2 \cdot |f(\Delta \vec{k}, \omega_0)|^2 \cdot Z^2. \quad (A.69)\]

We should keep in mind that \(f(\Delta \vec{k}, \omega_0) \approx Z\), which, together with Equation A.54, yields

\[\sigma_{\text{coh}} \sim \frac{8 \cdot \pi}{3} \cdot r_0^2 \cdot Z^2 = \sigma_{\text{th}} \cdot Z^2. \quad (A.70)\]

For \(\Delta \vec{k} \cdot \Delta \vec{E}_r \to 0\), which is given for forward scattering or in the long wavelength limit \((r_d \lambda \ll 1)\), the atomic scattering factor reduces to

\[f(0, \omega_0) = f^0(\omega_0) = \sum_{a=1}^{Z} \frac{\omega_a^2}{\omega_a^2 - \omega_0^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \omega_a^2 \cdot \omega_0^2 \quad \text{ (A.71)}\]

where we introduced the oscillator strength, \(\omega_a\), which gives us the number of electrons that contribute to a certain resonance frequency, \(\omega_a\), in the scattered fields. Since we have \(Z\) electrons involved in the scattering process, this should be reflected in the sum of all the oscillator strengths, thus \(\sum_{a=1}^{Z} \omega_a = Z\).

Since \(f^0(\omega_0)\) is a complex function of the frequency, we can rewrite it in terms of its real part and imaginary part, respectively, as

\[f^0(\omega_0) = f_r^0(\omega_0) - i \cdot f_i^0(\omega_0). \quad (A.72)\]

In the following, we want to show that the atomic scattering factors in the forward direction can be associated with a complex index of refraction, \(n(\omega_0)\). In doing so, we are going back to the wave equation, as defined in Equation A.12. In order to solve the wave equation, we need to have a reasonable expression for the current density, \(j(\vec{r}, t)\) (Equation A.22), for atoms in a poly electron configuration. Therefore, we need to know the velocity of the electrons that are involved in the process and which have been accelerated in the external electromagnetic field, \(\vec{E}(\vec{r}, t)\). Moreover, we know from Equation A.63 that

\[\vec{r}_a = \frac{1}{\omega_0^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \frac{e}{m} \cdot \vec{E}(\vec{r}, t) \quad \Rightarrow \vec{v}_a = \frac{1}{\omega_0^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \frac{e}{m} \cdot \frac{\partial \vec{E}(\vec{r}, t)}{\partial t}. \quad (A.73)\]

is a steady solution to solve the equation of motion (Equation A.62), which, after the time derivative, yields the velocity we need to insert into the current density. The total current density must be the sum of all bound electrons in an atom and in principle summed over all atoms involved. In the special case of forward scattering, similar atoms contribute identically; therefore, we just have to sum over identical resonances, \(\omega_a\), and multiply with the average density of atoms, \(n_a\). We, therefore, get

\[\vec{j}(\vec{r}, t) = e \cdot n_a \cdot \sum_{a=1}^{Z} \frac{o_a \cdot \vec{v}_a(\vec{r}, t)}{\omega_0^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \frac{\partial \vec{E}(\vec{r}, t)}{\partial t}. \quad (A.74)\]

Inserting this into Equation A.12 yields

\[\frac{1}{c^2} \cdot \frac{\partial^2 \vec{A}(\vec{r}, t)}{\partial t^2} - \vec{\nabla}^2 \cdot \vec{A}(\vec{r}, t) = \mu_0 \cdot \frac{e^2 \cdot n_a}{m} \cdot \sum_{a=1}^{Z} \frac{o_a}{\omega_0^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \frac{\partial \vec{E}(\vec{r}, t)}{\partial t}. \quad (A.75)\]

In order to express the electric field, \(\vec{E}(\vec{r}, t)\), on the right hand side in terms of the vector potential, \(\vec{A}(\vec{r}, t)\), we use the time derivative of Equation A.9. For the propagation of transverse waves, the time derivative on \(\vec{\nabla} \cdot \varphi(\vec{r}, t)\) does not contribute; thus, we get

\[\frac{\partial^2 \vec{A}(\vec{r}, t)}{\partial t^2} - c^2 \cdot \vec{\nabla}^2 \cdot \vec{A}(\vec{r}, t) = \frac{e^2 \cdot n_a}{\varepsilon_0 \cdot m} \cdot \sum_{a=1}^{Z} \frac{o_a}{\omega_0^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \frac{\partial^2 \vec{A}(\vec{r}, t)}{\partial t^2} \quad (A.76)\]

Rearranging terms with similar differential operators we get

\[\left| \frac{\partial^2 \vec{A}(\vec{r}, t)}{\partial t^2} - c^2 \cdot \vec{\nabla}^2 \cdot \vec{A}(\vec{r}, t) \right| = \frac{1}{\varepsilon_0 \cdot m} \sum_{a=1}^{Z} \frac{e^2 \cdot n_a}{\omega_0^2 - \omega_a^2 + i \cdot \gamma_a \cdot \omega_0} \cdot \frac{\partial^2 \vec{A}(\vec{r}, t)}{\partial t^2} \quad (A.77)\]
This is the standard form of the wave equation for

\[ n(\omega_0) = \sqrt{1 - \frac{e^2 \cdot n_a}{\varepsilon_0 \cdot m} \cdot \sum_{a=1}^{Z} \omega_a^2 - \omega_0^2 + i \cdot \frac{\gamma_a \cdot \omega_0}{\omega_a}} \]  

(A.78)

If \( \omega_0 \) is large compared to the coefficient in front of the sum we can expand the square root yielding

\[ n(\omega_0) = 1 - \frac{e^2 \cdot n_a \cdot \lambda^2}{2 \cdot \pi} \cdot \left( f_i^0(\omega_0) - if_i^0(\omega_0) \right) = 1 - \delta + i \cdot \beta \]  

(A.79)

Using Equation A.72 and our previous definition of \( r_a \) we can express the (complex) index of refraction in terms of the atomic (forward) scattering factors as

\[ n(\omega_0) = 1 - \frac{r_a \cdot n_a \cdot \lambda^2}{2 \cdot \pi} \cdot \left( f_i^0(\omega_0) - if_i^0(\omega_0) \right) = 1 - \delta + i \cdot \beta \]  

(A.80)

The refractive index can be greater or smaller than unity. In the former case this is called normal dispersion, and in the latter anomalous dispersion.

### A.1.7 Compton Scattering on Free Electrons

When the wavelength is in the order of the Bohr radius, \( \lambda \sim a_o \) or smaller, the electron with the mass \( m \) will not just bounce up and down anymore, as assumed previously, but, as shown in Figure 1.6b, will receive a momentum transfer of the incident wave field, which is given by \( P^i_\gamma = \omega^i \cdot h/c. \) We saw before that the frequency of the incident and radiated fields are the same, which means that the energies of incident and radiated photons are equal. Therefore, no energy transfer on the electron took place. Now, when the photon momentum is in the order of \( m \cdot c \), we have to correct the classical Thomson cross-section accordingly. Such corrections for scattering on electrons are needed for photon energies of the order of tens or hundreds of keV. In this case our photon-electron scattering can be considered as a two-body process obeying momentum and energy conservations. Before the scattering event, we consider the electron at rest that its total energy, \( E_e = m \cdot c^2 \), is given by its rest mass \( m \) only. Consequently, also its momentum, \( \vec{P}_e \), prior to impact is effectively zero. Therefore, we get for the energies

\[ h \cdot \omega^i + m \cdot c^2 = h \cdot \omega^f + \sqrt{\left(P^i_\gamma \cdot c\right)^2 + \left(m \cdot c^2\right)^2} \]

\[ \Rightarrow \left(P^i_\gamma \cdot c\right)^2 = \frac{(h \cdot \omega^i + m \cdot c^2 - h \cdot \omega^f)^2}{(m \cdot c^2)^2} \]  

(A.81)

where the indices \( i \) and \( f \) indicate the initial energy (or state) prior and the final state after the scatter process. We cannot exclude that the electron after the scatter process might be accelerated to a significant fraction of the speed of light. Therefore, we should use for the energy of the electron in the final state the relativistic energy–momentum relation. Regarding the conservation of momentum, we get

\[ \vec{P}_e = \vec{P}^i_\gamma + \vec{P}^f_\gamma \]  

(A.82)

We will now use Equation A.82 to calculate \( \vec{P}^f_\gamma \) in Equation A.81:

\[ P^i_\gamma = \vec{P}^f_\gamma \cdot \vec{P}^i_\gamma \cdot \left(P^i_\gamma - \vec{P}^f_\gamma \right) = \left(P^i_\gamma \right)^2 + \left(P^f_\gamma \right)^2 \]

\[ -2 \cdot \left(P^i_\gamma \right) \cdot \left(P^f_\gamma \right) \cdot \cos(\theta), \]  

(A.83)

which gives us then

\[ \left(P^f_\gamma \cdot c\right)^2 = h \cdot \omega^f + h \cdot \omega^i = 2 \cdot c^2 \cdot h^2 \cdot \omega^f \cdot \omega^i, \]  

(A.84)

and, by rearranging terms,

\[ 2 \cdot m \cdot c^2 \cdot h \cdot (\omega^f - \omega^i) = 2 \cdot h^2 \cdot c^2 \cdot \omega^f \cdot \omega^i (1 - \cos(\theta)) \]

\[ \Rightarrow \frac{1}{\omega^f} - \frac{1}{\omega^i} = \frac{h}{m \cdot c^2} \cdot (1 - \cos(\theta)). \]  

(A.85)

More commonly you will find Equation A.85 written in terms of the incident photon energy, \( E^i_\gamma \), and that of the scattered photon, \( E^f_\gamma \), that we can write

\[
\frac{E^f_\gamma}{E^i_\gamma} = \frac{1}{1 + \left( \frac{E^f_\gamma}{m \cdot c^2} \cdot (1 + \cos(\theta)) \right)} \Leftrightarrow \frac{k^f_\gamma}{k^i_\gamma} = \frac{1}{1 + \left( \frac{h \cdot \omega^f}{m \cdot c^2} \cdot (1 + \cos(\theta)) \right)}. \]  

(A.86)

The right hand side of Equation A.86, thus \( \left[k^f_\gamma / k^i_\gamma \right]^2 \), is the quantum mechanical correction for the unpolarized differential Thomson cross-section (Equation A.56) in the high energy limit. Therefore, we obtain

\[
\frac{d\sigma}{d\Omega} = \frac{k^i_\gamma}{2} \cdot \left( \frac{1 + \cos^2(\theta)}{2} \right) \cdot \left( \frac{k^f_\gamma}{k^i_\gamma} \right)^2 \]

\[= \frac{n_a^2}{2} \cdot \left( \frac{1 + \cos^2(\theta)}{2} \right) \cdot \left( \frac{1}{1 + \left( \frac{h \cdot \omega^f}{m \cdot c^2} \cdot (1 - \cos(\theta)) \right)} \right)^2. \]  

(A.87)

When the electron spin is also taken into account, the Compton differential cross-section is modified into the so-called Klein–Nishina differential cross-section, which is given by

\[
\frac{d\sigma}{d\Omega} = \frac{n_a^2}{2} \cdot \left( \frac{1 + \cos^2(\theta)}{2} \right) \cdot \left( \frac{1 + \left( \frac{h \cdot \omega^f}{m \cdot c^2} \cdot (1 - \cos(\theta)) \right)^2}{1 + \left( \frac{h \cdot \omega^f}{m \cdot c^2} \cdot (1 - \cos(\theta)) \right)} \right)^2. \]  

(A.88)
with \( \Theta = h \cdot \omega_i / (m \cdot c^2) \) (Figure A.4).

Again, we see that, for the low energy limit, thus \( \omega_i \to 0 \), we obtain the differential Thomson cross-section for unpolarized radiation, as previously shown in Equation A.56. We can express Equation A.81 in terms of the kinetic energy, \( E_{\text{kin}} \) of the outgoing electron, which is given as

\[
E_{\text{kin}} = \frac{\Theta (1 - \cos(\theta))}{1 + 2 \cdot \Theta (1 - \cos(\theta))}
\]  

(A.89)

and whose value is maximized for \( \theta = 180^\circ \), thus for backscattering. In this case we will have the maximum energy transfer on the electron, \( E_{\text{kin}} \), and on the backscattered photon, \( E_{\gamma} \),

\[
E_{\text{kin}} = \frac{E_{\gamma}^2}{1 + m \cdot c^2} \wedge E_{\gamma} = \frac{m \cdot c^2}{2} \cdot \left( 1 - \frac{m \cdot c^2}{2 \cdot E_{\gamma}} \right)
\]  

(A.90)

noting that the difference is given by \( \Delta E = E_{\text{kin}} - E_{\gamma} = E_{\gamma} \cdot \left( 1 + 2 \cdot E_{\gamma}/(m \cdot c^2) \right)^{-1} \). This is important to know for single photon detection. If the photon is not completely absorbed, a minimal amount of energy is always missing. In this view, we might be interested to know the probability of measuring electrons with a given kinetic energy \( E_{\text{kin}} = E_{\gamma} - m \cdot c^2 \). We can readily get this expression by substituting for the angle \( \theta \) in Equation A.88 via Equations A.81 and A.85 and noting that:

\[
\frac{d\sigma}{dE_{\text{kin}}} = \frac{d\sigma}{d\Omega} \cdot d\Omega = \frac{d\sigma}{d\Omega} \cdot \frac{2 \cdot \pi}{(\Theta - E_{\text{kin}})^2}
\]  

(A.91)

The differential cross-sections associated with Equation A.91 are depicted in Figure A.5 for different incident photon energies and show rises with increasing kinetic energy (which is also referred to as Compton plateau) up to the kinematic limit, where it abruptly falls to zero (Compton edge/shoulder). If we are measuring the energy of incident X-rays on an energy dispersive detector via the charge release in the detector volume, then we will see such energy distribution.

Executing the integration of Equation A.91 we obtain the Compton cross-section on a single electron

\[
\sigma_{\text{C}} = 2 \cdot \pi \cdot n \cdot \left[ \left( \frac{1 + \Theta}{\Theta^2} \right) \cdot \left( \frac{1 + 2 \cdot \Theta}{\Theta} \right) - \frac{\ln(1 + 2 \cdot \Theta)}{\Theta} \right] + \frac{\ln(1 + 2 \cdot \Theta)}{2 \cdot \Theta} - \frac{1 + 3 \cdot \Theta}{(1 + 2 \cdot \Theta)^2}
\]  

(A.92)

For a Compton event on an atom we can assume that the cross-section is increased by the factor \( Z \) (i.e., \( \sigma_{\text{C}}^{\text{em}} = Z \cdot \sigma_{\text{C}} \)), since in an atom we have \( Z \) electrons as potential scatters available. For the low energy limit \( E_{\gamma} \gg m \cdot c^2 \) and the high energy limit \( E_{\gamma} \ll m \cdot c^2 \), we can approximate the Compton cross-section with

\[
\sigma_{\text{C}}^{\text{low}} = \sigma_{\text{C}} \cdot (1 - 2 \cdot \Theta) \wedge \sigma_{\text{C}}^{\text{high}} \propto \ln(E_{\gamma}) / E_{\gamma}
\]  

(A.93)

The angular distribution of secondary radiation can be described using the concept of a probability density function (PDF). The latter is the normalized probability of scattering a photon or an electron into an angle, and is given by the ratio of the differential cross-section per unit angle and the total cross-section. Doing this and rearranging terms we obtain

\[
PDF(\theta) = \frac{1}{\sigma_{\text{C}}} \cdot \left( \frac{\pi}{2} \cdot (1 + \cos^2(\theta)) \cdot \frac{d\sigma}{d\Omega} \right) \cdot 2 \cdot \pi \cdot \sin(\theta)
\]  

(A.94)

which describes the directional distribution of secondary radiation from a Compton scatter process, and depends on the energy of the incident X-ray and the type of material.
A.2 Energy Loss by Ionization

We saw that the Compton electron or in general a charged particle after a Compton process may have substantial kinetic energy in matter and subsequently will produce further ionization while traveling through the material. Therefore, the charged particle will have a certain range until it is thermalized, thus it loses almost all its kinetic energy.

Let us assume a particle of mass $M$ with charge $z\cdot e$ that travels with the velocity $\vec{v} = \vec{v} \cdot \hat{e}$, through a medium with electron density, $n_e$. The other electrons in the medium are considered free and initially at rest. What we want to calculate now is the momentum transfer of the moving particle on a single electron in the medium. We start with the integral form of the Gauss theorem (Equation A.3), which gives us

$$\int \vec{E}(\vec{r},t) \cdot d\vec{a} = \frac{4\pi}{\varepsilon_0} \int \rho(\vec{r},t) \cdot d\vec{r}. \tag{A.95}$$

If we imagine the particle traveling along the $x$-axis of an infinitely long cylinder and the electron is situated in the distance $b$ (which is also referred to as the impact parameter) from the center of the cylinder (Figure A.6b) then only the transversal contribution of the electric field, $\vec{E}_\perp(\vec{r},t) = \vec{E}_\perp \cdot e \hat{\vec{e}}_\perp$, should contribute and Equation A.95 can be rewritten as

$$2\cdot\pi\cdot b \cdot \int E_\perp \cdot dx' = \frac{4\pi}{\varepsilon_0} \cdot z \cdot e \rightarrow \int E_\perp \cdot dx = \frac{2\cdot z \cdot e}{\varepsilon_0 \cdot b}. \tag{A.96}$$

Knowing the force, $F_\perp = e \cdot E_\perp$, and recalling that the momentum transfer is given by

$$\Delta p_\perp = \int F_\perp \cdot dt = \int F_\perp \cdot \frac{dx}{v} \cdot dx = \int F_\perp \cdot \frac{dx}{v}, \tag{A.97}$$

we get, by inserting Equation A.96 into Equation A.97,

$$\Delta p_\perp = e \cdot \int \frac{E_\perp \cdot dx}{v} = \frac{2\cdot z \cdot e^2}{\varepsilon_0 \cdot b \cdot v}. \tag{A.98}$$

Now, the energy transfer of a single electron is given by $\Delta E = \Delta P^2/2m$. For a given electron density, $n_e$,

$$n_e = \frac{N_A \cdot \rho \cdot Z}{A}, \tag{A.99}$$

we will find $n_e \cdot 2\cdot \pi \cdot b \cdot db \cdot dz$ in a cylindrical barrel between $b$ and $b + db$. Therefore, the energy loss, $-dE$, per path length, $dz$, for distances between $b$ and $b + db$ in medium with electron density, $n_e$, is given by

$$-dE = \frac{4\cdot \pi \cdot n_e \cdot z^2 \cdot e^4}{\varepsilon_0 \cdot m \cdot v^2} \cdot \frac{db}{b} \cdot dx. \tag{A.100}$$

The energy loss diverges for $b \rightarrow 0$ and tends to zero for large distances. Therefore, it makes a lot of sense to define cutoff parameters $b_{\text{max}}$ and $b_{\text{min}}$ when executing the integral over the impact parameter, thus we will have

$$\frac{dE}{dx} = \frac{4\cdot \pi \cdot n_e \cdot z^2 \cdot e^4}{\varepsilon_0 \cdot m \cdot v^2} \cdot \int_{b_{\text{min}}}^{b_{\text{max}}} \frac{db}{b} = \frac{4\cdot \pi \cdot n_e \cdot z^2 \cdot e^4}{\varepsilon_0 \cdot m \cdot v^2} \cdot \ln\left(\frac{b_{\text{max}}}{b_{\text{min}}}\right). \tag{A.101}$$

To solve the problem of the cutoff parameters, Bohr suggested using the Heisenberg uncertainty principle or the argument that the electron is located within de Broglie wavelength for the lower cutoff; thus, $b_{\text{min}} = (2\cdot \pi \cdot h)/(\gamma \cdot m \cdot v)$. For the higher cutoff the argument is that the interaction time $(b/v)$ must be much shorter than the period of the electron $(\gamma / \omega_\text{e})$ to guarantee a relevant energy transfer. Using this cutoff parameter, we get for the energy loss:

$$\frac{dE}{dx} = \frac{4\cdot \pi \cdot n_e \cdot z^2 \cdot e^4}{\varepsilon_0 \cdot m \cdot c^2 \cdot \beta^2 \cdot \gamma^2} \cdot \ln\left[\frac{m \cdot c^2 \cdot \beta^2 \cdot \gamma^2}{2\cdot \pi \cdot \omega_\text{e} \cdot w_\text{ion}}\right]. \tag{A.102}$$

where $w_\text{ion} = h \cdot \langle \omega_\text{e} \rangle$ is the effective ionization potential averaged over the oscillator strengths for the absorbing material. Using the Avogadro number, $N_a$, we can express the electron density of the

FIGURE A.6 Schematic models for energy loss by ionization (a) and radiation (b).
Basic Physics of X-ray Interactions in Matter

Absorber material with density, \( \rho \), atomic number, \( Z \), and atomic weight, \( A \), as

\[
\frac{dE}{dx} = 4 \cdot \pi \cdot N_a \cdot \rho \cdot z^2 \cdot e^4 \cdot \frac{Z}{A} \cdot \ln \left( \frac{m \cdot c^2 \cdot \beta^2 \cdot \gamma^2}{2 \cdot \pi \cdot w_{ion}} \right)
\]

\[(A.103)\]

This differs only by a factor of two from the Bethe–Bloch (Bloch 1933; Bethe and Ashkin 1953) equation, which derives from rigorous quantum mechanical calculations and is given by

\[
\frac{dE}{dx} = 4 \cdot \pi \cdot N_a \cdot r_0^2 \cdot c^2 \cdot m \cdot z^2 \cdot \frac{1}{\beta^2 \cdot \gamma^2} \cdot \frac{Z}{A} \cdot \ln \left( \frac{m \cdot c^2 \cdot \beta^2 \cdot \gamma^2}{2 \cdot \pi \cdot w_{ion}} \right) \left( \beta^2 - \frac{\delta}{2} \right)
\]

\[(A.104)\]

where \( \delta \) is a factor that accounts for the shielding effect of the atomic electrons of the absorber material. Using the definition of the classical electron radius, \( r_0 \), in Equation A.54 we notice that the factors in front of the brackets in Equations A.103 and A.104 are identical. A useful constant is

\[
\kappa = 4 \cdot \pi \cdot N_a \cdot r_0^2 \cdot m \cdot c^2 = 0.307 \text{MeV/(g/cm}^2\text{)} (\text{Figure A.7})
\]

The expression in the nominator of the logarithmic term is the maximal kinetic energy transfer on the electron. With \( I = 2 \cdot \pi \cdot w_{ion} \) we can write the Bethe–Bloch equation in compact form

\[
\frac{dE}{dx} = \kappa \cdot z^2 \cdot \frac{1}{\beta^2} \cdot \frac{Z}{A} \left[ \ln \left( \frac{E_{\text{kin}}}{I} \right) - \beta^2 - \frac{\delta}{2} \right].
\]

\[(A.105)\]

The effective ionization potential for a specific material with atomic number \( Z \) is given by \( I = 16 \cdot Z^{0.6} \text{eV} \), but depends on the molecular binding of the absorber atoms.

Initially, the energy loss drops with \( \beta^{-2} \), which is due to the fact that slower particles feel the electric forces of the atomic electron for a longer time.

After running through a broad minimum at about \( \beta \cdot \gamma \approx 4 \) we observe a relativistic rise, which is due to the Lorentz transform of the transversal electric field. Thus, the interaction cross-section increases. Relativistic particles (\( \beta \approx 1 \)), which possess an energy loss in the minimum, are called minimum ionizing particles (MIPs). In light absorbers where \( Z/A \approx 0.5 \), the energy loss of single charged MIPs can be approximated by

\[
\frac{dE}{dx} \approx 2 \cdot \frac{\text{MeV}}{\text{g/cm}^2}.
\]

\[(A.106)\]

The energy loss for relativistic electrons (\( z = 1 \)) is acquired by substituting the maximum energy transfer in Equation A.105 with \( E_{\text{kin}} = \gamma \cdot m \cdot c^2/2 \), thus

\[
\frac{dE}{dx} = \kappa \cdot \frac{1}{\beta^2} \cdot \frac{Z}{A} \left[ \ln \left( \frac{\gamma \cdot m \cdot c^2}{2 \cdot I} \right) - \beta^2 - \frac{\delta}{2} \right].
\]

\[(A.107)\]

We should note that the moving charged particle releases energy and, according to Equation 1.61, deposits dose along its path. Since the energy lost is inversely proportional to the square of their velocity, the interaction cross-section increases as the energy of the charge decreases. As a result, we expect the highest dose deposition just before the particle comes to a complete stop, which is known as the so-called Bragg peak, which should not be confused with the Bragg peaks in X-ray diffraction. Such a dose deposition of protons is shown as a function of water (patient) thickness in Figure A.8 for three different energies. We note the well-pronounced Bragg peaks, which are exploited in particle therapy of cancer. Due to the Bragg peaks, we can concentrate the dose delivery on the tumor while minimizing the effect on the surrounding healthy tissue.

This is much more efficient than using X-rays or \( \gamma \)-rays, where we basically have the highest dose deposition in the first layers of the patient.

### A.3 Bremsstrahlung

A second mechanism of energy loss of a charged particle traveling through matter is the emission of radiation. We now try

---

**FIGURE A.7** Energy loss by ionization for protons in water versus the proton energy.

**FIGURE A.8** Dose released by protons, X-rays, and \( \gamma \)-rays versus the thickness of matter.
to understand the energy distribution of the emitted radiation, which is in the following referred to as energy spectra, applied to the case in which a charged particle of charge $e$ is accelerated in the Coulomb field of a massive nucleus with charge $Z\cdot e$ of a target material. This effect is referred to as bremsstrahlung. When the impact parameter, $b$, between the moving electron and the nucleus is small (in about 0.5% of the events), the electron becomes subject to a very strong attraction and gets accelerated. We assume the interaction lasts only for a short time interval, $\Delta \tau$, and results in a sudden change of the particle velocity from a value $v$ to a value $v'$. However, the associated velocities are small in comparison to $c$. The intensity of the radiated field will depend on the difference in the velocity after and prior to impact from $\Delta v = v' - v$. As before, we will consider here the low frequency spectrum, thus $\omega \to 0$ only. The total emitted electromagnetic energy, $dW$, in a solid angle element, $d\Omega$, is the time integral over the emitted power, $dP/d\Omega = |\mathbf{A}(\vec{r}, t)|^2$; thus

$$
\frac{dW}{d\Omega} = \int \frac{dP}{d\Omega} \cdot dt = \int |\mathbf{A}(\vec{n}, t)|^2 \cdot dt
$$

where $|\mathbf{A}(\vec{n}, \omega)|^2$ is the Fourier transform of the vector potential $\mathbf{A}(\vec{n}, t)$, and $\vec{n}$ is the unit vector connecting the charge and the acceleration (Figure A.9). We use here Parseval’s theorem, telling us that the integral of the square of a function is equal to the integral of the square of its Fourier transform. The radiated field will depend on the atomic number, $Z$, of the target material and on $\Delta v = v' - v$. Using Equation A.33 we get then, for the electric field,

$$
\vec{E}(\vec{r}, t) = \frac{Z \cdot \mu_0}{4 \cdot \pi} \cdot \frac{e \cdot (\vec{n} \times \vec{n}) \times \vec{n}}{c^2 \cdot |\vec{r}|}
$$

$$
= \frac{Z \cdot \mu_0 \cdot e}{4 \cdot \pi} \cdot \int \frac{d\vec{n} \times (\Delta \vec{v} \times \vec{n}) \cdot dt}{c^2 \cdot |\vec{r}|}.
$$

Inserting this into Equation A.50, we get, for the bremsstrahlung spectrum,

$$
\frac{d^2 I}{d\Omega \cdot d\omega} \sim \frac{e^2 \cdot Z^2}{32 \cdot \pi^2 \cdot c^2} \cdot |\vec{n} \times (\vec{n} \times \vec{v}) - \vec{n} \times (\vec{n} \times \vec{v})|^2
$$

(A.110)

under the frame condition that $\Delta \tau \to 0$.

Dividing both sides by $h^2 \cdot \omega$ and recalling that the fine structure constant is given by $\alpha = e^2(h \cdot c) = 1/137$, we can rewrite Equation A.110 in terms of the differential number of photons per energy and solid angle unit emitted during impact.

$$
\frac{d^2 I}{d\Omega \cdot h^2 \cdot \omega \cdot d\omega} \sim \frac{\alpha \cdot Z^2}{32 \cdot \pi^2 \cdot e \cdot h \cdot \omega} \cdot |\vec{n} \times (\vec{n} \times \vec{v}) - \vec{n} \times (\vec{n} \times \vec{v})|^2.
$$

(A.111)

We realize that the number of photons emitted increases with the square of the atomic number, which means we need to have heavy materials in order to generate intense radiation. Since the photon energy is given by $E_p = h \cdot \omega$, we can rewrite Equation A.111 in terms of energy and, with some relativistic corrections,

$$
\frac{d^2 N}{d\Omega \cdot dE_p} \sim \frac{\alpha \cdot Z^2}{32 \cdot \pi^2 \cdot c \cdot E_p} \cdot \left[\frac{\vec{n} \times (\vec{n} \times \vec{v}) - \vec{n} \times (\vec{n} \times \vec{v})}{1 - \frac{n^2}{c^2}}\right]^2.
$$

(A.112)

Instead of using classical electrodynamics, we can calculate electron-induced bremsstrahlung also using a modified Bethe–Bloch equation (Equation A.105), which is given by

$$
\frac{dE}{dx} = 4 \cdot \alpha \cdot N_A \cdot Z^2 \cdot \frac{1}{A} \cdot \left(\frac{1}{4 \cdot \pi \cdot \epsilon_0} \cdot \frac{c^2}{m \cdot c^2}\right) \cdot E \cdot \ln\left(\frac{183}{Z^2}\right) \sim \frac{E}{m^2}.
$$

(A.113)

The radiated energy loss and, therefore, the emission of bremsstrahlung scales with the inverse mass of the projectile. For this reason, only light particles such as electrons are accelerated in X-ray tubes. Due to the relativistic correction in Equation A.112, the mission pattern of bremsstrahlung in modulated, and depends on the electron velocity. At low electron energy, $l/\vec{v} \ll c$, bremsstrahlung is emitted preferentially between 60° and 90°, while for higher electron energies photons tend to be emitted in the forward direction with respect to the acceleration (Figure A.9).

The factor $x_0 = A/(4 \cdot \alpha \cdot N_A \cdot Z^2 \cdot \mu_0^2 \cdot \ln(183/Z^2))$ has the dimensions $[g/cm^2]$ and is called radiation length. We can use this radiation length to simplify Equation A.113 further, and we get a homogeneous differential equation very similar to Lambert–Beer (Equation 1.1):

$$
\frac{dE}{dx} = \frac{E}{x_0}.
$$

(A.114)

which we can solve by separating the variables and the subsequent integration to get

$$
E = E_0 \cdot e^{-x/x_0}.
$$

(A.115)

This means that, after the passage of one $x_0$, the electron has lost all but $(1/e)$th; thus, 63% of its initial energy, $E_0$. The radiation length in a mixture of $n$ elements can be calculated using the weight fractions, $f_i$, of the materials using

$$
x_0 = \sum_{i=1}^{n} \frac{1}{f_i x_0^i}.
$$

(A.116)
We saw up to now that energy losses due to bremsstrahlung are proportional to the energy of the projectile, while losses due to ionization beyond the ionization minimum scale with the logarithm of the energy. The energy, $E_c$, for which the energy losses of these two mechanisms are equal, is called critical energy, which can be calculated by equalizing Equation A.113 and Equation A.104. For heavier elements ($Z > 13$), we can determine the critical energy through

$$E_c = \frac{550 \text{MeV}}{Z}. \quad (A.117)$$

Dividing Equation A.113 by Equation A.104, we obtain the ratio of the two effects, which is given by

$$\frac{dE/dx}{dE/dx} = \frac{E \cdot Z}{820}. \quad (A.118)$$

where $E$ is the incident particle energy in MeV. For a typical acceleration voltage of 100 keV for electrons and a tungsten target ($Z = 74$) the ratio is about 1%, thus not that great yield for X-rays.

### A.4 Range of Charged Particles

Because of the different energy loss mechanisms, it is virtually impossible to find a holistic solution for the range of charged particles in matter. In general, we get the range by integrating over the energy loss as it slows down to rest ($E = 0$); thus

$$R = \int_0^E \frac{dE}{dE/dx}. \quad (A.119)$$

However, we see the energy loss is a quite complicated function of the energy. Therefore, normally we will use a mostly empirical approximation of the integral. For instance, the range, in centimeters, in air for $\alpha$ particles with energies $2.5 \text{ MeV} \leq E_{kin} \leq 20 \text{ MeV}$ is given by the empirical formula

$$R_\alpha = 0.31 \cdot E_{kin}^{1/2}. \quad \text{For a coarse estimation of the range of } \alpha \text{ particles in other materials, we can use } R_\alpha = 3.2 \cdot 10^{-4} \sqrt{A/\rho} \cdot R_\alpha^\text{air}. \quad \text{If we neglect fluctuation in energy loss, and we assume the rate of energy loss at every point along the track to be equal to the total stopping power, then we can calculate the average path length traveled by a charged particle by the so-called continuous-slowing-down approximation (CSDA) (Bichsel 1988). Fortunately, we do not have to accomplish this sort of calculation by hand, since others already did it. There are several databases that allow one to calculate the range of charged particles in arbitrary materials for electrons, protons, and $\alpha$ particles, in particular a very convenient one provided by the National Institute of Standards and Technology (NIST) (Berger 1992).}

### A.5 Schrödinger Equation and Hydrogen Atom

In quantum mechanics, typical particle parameters such as energy, $E$, or momentum, $\vec{P}$, are associated with differential operators:

$$E \rightarrow i \cdot h \frac{\partial}{\partial t} \text{ and } \vec{P} \rightarrow -i \cdot h \cdot \vec{\nabla}. \quad (A.120)$$

Due to the wave–particle dualism, we can describe the particle’s motion by its complex wave function, $\varphi(\vec{r}, t)$. The probability $P(\vec{r}, t)$ to find the particle at a position $d\vec{r}$ is given by

$$P(\vec{r}, t) \cdot d\vec{r} = \varphi^*(\vec{r}, t) \cdot \varphi(\vec{r}, t) \cdot d\vec{r}, \quad (A.121)$$

where $\varphi^*(\vec{r}, t)$ is the complex conjugate of the wave function $\varphi(\vec{r}, t)$, which generally is normalized to unity, thus...
\[
\int |\psi(\vec{r},t)|^2 \cdot d\vec{r} = 1. \tag{A.122}
\]

The expectation values for particle parameters such as to find it at a position \( \vec{r} \), in an energy state of \( E \), to find it in its momentum \( \vec{P} \), or in general in a state \( \Sigma \), are given by
\[
\langle \Sigma \rangle = \int \phi^*(\vec{r},t) \cdot \Sigma \cdot \phi(\vec{r},t) \cdot d\vec{r}. \tag{A.123}
\]

To solve the motion of a particle with charge \( e \) and mass \( m \) described by its wave function, \( \psi(\vec{r},t) \), in an external potential, \( V(\vec{r},t) \), we start with the ansatz of the conservation of energy:
\[
\frac{\hbar^2}{2m} \cdot \phi(\vec{r},t) + V(\vec{r},t) \cdot \phi(\vec{r},t) = H(\vec{r},t) \cdot \phi(\vec{r},t) = E \cdot \phi(\vec{r},t), \tag{A.124}
\]
where \( H \) is the so-called Hamiltonian. Now, substituting the operators (Equation A.120) into Equation A.124, we get the Schrödinger equation
\[
\left( -\frac{\hbar^2}{2\mu} \cdot \nabla^2 + V(\vec{r},t) \right) \cdot \phi(\vec{r},t) = i \cdot \hbar \cdot \frac{\partial \phi(\vec{r},t)}{\partial t}. \tag{A.125}
\]

To fill the Schrödinger equation with a bit of life, we need to add the specifics for the system of interest into the Hamiltonian. We are interested in a hydrogen like atom, which consists of a nucleus with mass \( M \) and with the charge \( Z \cdot e \) and just one electron. As before, in Section A.1.5, the electrostatic potential \( V(\vec{r},t) \) between the electron and the nucleus is described by the Coulomb term, as defined in Equation A.60, and we obtain,
\[
\left( -\frac{\hbar^2}{2\mu} \cdot \nabla^2 + \frac{Z \cdot e^2}{4\pi \varepsilon_0 |\vec{r}|} \right) \cdot \phi(\vec{r},t) = i \cdot \hbar \cdot \frac{\partial \phi(\vec{r},t)}{\partial t} \tag{A.126}
\]
where \( \mu \) is now the reduced mass for the electron nucleus system, thus \( \mu = m \cdot M/(m + M) \). Using the same argument as in Section A.1.1 and, more specifically, in Equation A.13, we try to solve this differential equation by separating the variables according to their time and space dependencies
\[
\phi(\vec{r},t) = R(\vec{r}) \cdot T(t) = R(\vec{r}) \cdot e^{-iEt/\hbar}. \tag{A.127}
\]

Inserting this into Equation A.126 and using the differential operator in polar coodinated \( (\vec{r},\theta,\phi) \) we get
\[
-\frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{r^2} \sin(\theta) \frac{\partial}{\partial \theta} \left( \sin(\theta) \frac{\partial R}{\partial \theta} \right) + \frac{1}{r^2} \sin^2(\theta) \frac{\partial^2 R}{\partial \phi^2} \right] - \frac{Z \cdot e^2}{4\pi \varepsilon_0 |\vec{r}|} \cdot R = E \cdot R. \tag{A.128}
\]

This looks even more complicated, but has the advantage that we can solve Equation A.128 again using the method of separating variables into a radial, a polar, and azimuthal component, respectively, and, therefore, \( R(\vec{r}) = \rho(\vec{r}) \cdot \theta(\theta) \cdot \phi(\phi) \). With this approach, we get three now independent differential equations, which are all solvable. The calculation is lengthy, but straightforward; therefore, we will just give the final solution, which is given by
\[
R(\vec{r}) = N_l \cdot e^{\xi_x} \cdot R_{lm}^n (\cos(\phi)) \cdot e^{i\omega_\phi}, \tag{A.129}
\]
where \( E_n \) are the energy levels we have calculated previously in Section A.1.5 and, more specifically, in Equation A.60, \( R_{lm}^n \) are Legendre’s polynomials that solve the polar equation, and the last factor is the solution of the azimuthal equation. The wave function, for instance for electrons in the 1s state in a hydrogen like atom with atomic number \( Z \), is then given by
\[
\phi(\vec{r},t) = \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} \cdot e^{-\frac{Zr^*}{a_0}}, \tag{A.130}
\]

We should add here the probability that a given system changes its initial to a final state \( \psi_1(\vec{r},t) \rightarrow \psi_f(\vec{r},t) \) is given by
\[
\langle M_{lf} \rangle = \int \phi_1^*(\vec{r},t) \cdot M_{lf} \cdot \phi_f(\vec{r},t) \cdot d\vec{r}, \tag{A.131}
\]
where \( M_{lj} \) is the transition matrix element.

### A.6 The Photoelectric Effect

We assume the photoelectric effect takes place on an isolated hydrogen like atom occupying a volume, \( V \), and its electron is found in the 1s state (Figure 1.9b). From the previous section, we know that the wave function of the bound electron is then given by
\[
\phi_b(\vec{r},t) = \frac{1}{\sqrt{V}} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} \cdot e^{-\frac{Zr^*}{a_0}} \tag{A.132}
\]

In the final state, we will approximate the electron wave function with a plane wave with wave vector \( \vec{k}_f \). If the energy of the emitted electron is lower than 150 keV we can apply a good approximation in non-relativistic kinematics and we can write the wave function of the electron in the continuum as
\[
\phi_f(\vec{k}_f) = \frac{1}{\sqrt{V}} \cdot e^{i\vec{k}_f \cdot \vec{r}}. \tag{A.133}
\]

The wave function of the incident photon in the initial state is given by the wave function of the ejected electron
\[
\phi_\gamma(\vec{k}) = \frac{2 \cdot \pi \cdot \hbar \cdot e^2}{V \cdot \omega} \cdot e^{i\vec{k} \cdot \vec{r}}. \tag{A.134}
\]
In order calculate the probability of a transition from a bound electron and an incident photon described by its vector potential \( \vec{A}(\vec{r}, t) \) and scalar potential \( \varphi(\vec{r}, t) \) into a moving electron in the continuum, we need to find the Hamiltonian of the system and apply it to Equation A.131. For this, we start from Equation A.126 and add the vector potential \( \vec{A}(\vec{r}, t) \) and the scalar potential \( \varphi(\vec{r}, t) \) in the Hamiltonian. Therefore, we will obtain

\[
H = \frac{1}{2\cdot m} \left( \vec{P}(\vec{r}, t) - \frac{e}{c} \cdot \vec{A}(\vec{r}, t) \right)^2 + e \cdot \varphi(\vec{r}, t) - \frac{Z \cdot e^2}{4 \cdot \pi \cdot \varepsilon_0 |\vec{r}|} \approx \frac{i \cdot e}{m \cdot c} \cdot \vec{A}(\omega) \cdot \vec{v}.
\] (A.135)

To obtain the right hand side we used the differential operator representation of the momentum, we employed the Coulomb gauge to get rid of the scalar potential, and we neglect quadratic terms in the vector potential—an approximation that is valid for weak fields. Finally, we made use of Equation A.108 to express the vector potential in the frequency domain. Applying Equation A.106 to get rid of the scalar potential, and we neglect quadratic \( \omega \cdot \varphi \) which leads to

\[
\langle M_{if} \rangle^2 = \left\{ \frac{2 \cdot \pi \cdot e}{m \cdot c} \cdot \vec{A}(\omega) \right\}^2 \cdot \int \left[ \varphi^*_f(\vec{r}, t) \cdot e^{i \vec{k} \cdot \vec{r}} \cdot \vec{P}_0 \cdot \vec{v} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r} \right]^2 \cdot \delta(\omega - \omega_f).
\] (A.136)

As in Section A.1.4, we consider the incident electromagnetic radiation polarized along the z-axis of a Cartesian reference frame, thus \( \vec{P}_0 = \vec{P}_0 \cdot \hat{e}_z \). What we are interested in is the cross-section for the photoelectric effect, thus the transition probability normalized to the energy density per time (see Section A.1.6) of the incident photon:

\[
\frac{d\sigma_{pe}}{d\Omega} = \omega \cdot \langle M_{if} \rangle^2 \cdot \frac{2 \cdot \pi \cdot e}{m \cdot c} \cdot \vec{A}(\omega)
\]

\[
= \int \left[ \varphi^*_f(\vec{r}, t) \cdot e^{i \vec{k} \cdot \vec{r}} \cdot \vec{P}_0 \cdot \vec{v} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r} \right]^2 \cdot \delta(\omega - \omega_f) \cdot \frac{\omega^2}{2 \cdot \pi \cdot c} \cdot \left| \vec{A}(\omega) \right|^2
\]

\] (A.137)

where we made use of Equations A.50 and A.108. We can simplify this by using the fine structure constant and expressing the Dirac function in terms of the energy

\[
\frac{d\sigma_{pe}}{d\Omega} = \frac{4 \cdot \pi \cdot \alpha^3}{m^2 \cdot \omega} \cdot \int \left[ \varphi^*_f(\vec{r}, t) \cdot e^{i \vec{k} \cdot \vec{r}} \cdot \vec{P}_0 \cdot \vec{v} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r} \right]^2 \cdot \delta(E - E_f).
\] (A.138)

We keep in mind that transitions to a number of \( n \) states are possible, and we need to estimate how many states can be populated in a given volume, \( V \). If we assume a cube with an edge length of \( \sqrt[3]{V} \), we can fit \( n \cdot \lambda = \sqrt[3]{V} \) wavelengths per axis \( (i = 1,2,3) \) or expressed in the components of the wave vector, \( k = 2 \cdot \pi \cdot n_i / \sqrt[3]{V} \). Subsequently, we get, for the energy states,

\[
E = \frac{\hbar^2 \cdot k^2}{2 \cdot m} = \frac{2 \cdot \pi \cdot \hbar^2}{m \cdot \sqrt[3]{V^2}} \cdot n^2.
\] (A.139)

Using this definition of the energy, the number of states in a volume element is the given by

\[
n^2 \cdot d\mathbf{n} \cdot d\Omega = n^2 \cdot \frac{dE}{d\mathbf{n}} \cdot d\Omega = m \cdot k \cdot \frac{V}{16 \cdot \pi^3} \cdot dE \cdot d\Omega.
\] (A.140)

Now we integrate over all possible energy states

\[
\frac{d\sigma_{pe}}{d\Omega} = m \cdot k \cdot \frac{V}{16 \cdot \pi^3} \cdot \frac{4 \cdot \pi^2 \cdot \alpha^3}{m^2 \cdot \omega_f} \cdot \int \left[ \varphi^*_f(\vec{r}, t) \cdot e^{i \vec{k} \cdot \vec{r}} \cdot \vec{P}_0 \cdot \vec{v} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r} \right]^2 \cdot \frac{dE}{d\mathbf{n}}.
\] (A.141)

which leads to

\[
\frac{d\sigma_{pe}}{d\Omega} = m \cdot k \cdot \frac{V}{16 \cdot \pi^3} \cdot \frac{4 \cdot \pi^2 \cdot \alpha^3}{m^2 \cdot \omega_f} \cdot \int \left[ \varphi^*_f(\vec{r}, t) \cdot e^{i \vec{k} \cdot \vec{r}} \cdot \vec{P}_0 \cdot \vec{v} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r} \right]^2.
\] (A.142)

It remains now to solve the integral, thus the matrix transition element, by inserting Equation A.133:

\[
M_{if} = \int \left[ \frac{1}{\sqrt{V}} \cdot e^{i(\vec{k} - \vec{k}_f) \cdot \vec{r}} \cdot \vec{P}_0 \cdot \vec{v} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r} \right]^2.
\] (A.143)

The momentum operator acts on the function \( e^{i(\vec{k} - \vec{k}_f) \cdot \vec{r}} \), which is an eigenfunction of the momentum, and is producing a factor \( 1 - k_f k \). Since the polarization is parallel to \( \vec{k} \), we remain with

\[
M_{if} = \frac{-i}{\sqrt{V}} \cdot \vec{P}_0 \cdot \vec{k}_f \cdot \int e^{i(\vec{k} - \vec{k}_f) \cdot \vec{r}} \cdot \varphi_i(\vec{r}, t) \cdot d\vec{r}.
\] (A.144)

where \( \varphi \) is the angle between the polarization and the direction of the emission of the electron. Inserting the wave function of the initial state (Equation A.134) and integrating over the volume, we get

\[
M_{if} = \frac{8 \cdot \pi}{\sqrt{\pi}} \cdot \left( \frac{Z}{a_0} \right)^2 \cdot \frac{1}{\left( \left| Z^2 + a_0^2 \cdot 1 \cdot k - k_f \cdot \mathbf{P} \right| \cdot a_0^2 \right)^2}.
\] (A.145)

Inserting this into Equation A.142, we get for the differential cross-section

...
\[
\frac{d\sigma_{PE}}{d\Omega} = \frac{32 \cdot \alpha \cdot k_f^5}{m \cdot \omega_f^5} \left( \frac{Z^5 + a_0^2 \cdot \cos^2(\vartheta)}{\left( Z^2 + a_0^2 \cdot \left| k - k_f \right|^2 \right)^2} \right). \tag{A.146}
\]

If the photon energy, \( \hbar \cdot c \cdot k \), is substantially greater than the binding energy, \( E_p \), but the ejected electron is still non-relativistic, then the kinetic energy of the photoelectron corresponds in practice to the incident photon energy, and we can approximate \( |k - \tilde{k}_f| \) with

\[
|\tilde{k}_f|^2 = \left| \frac{\hbar \cdot k^0 \cdot \sin(\vartheta)}{m \cdot c \cdot \cos(\vartheta)} \right|^2 \approx \left| \frac{\hbar \cdot k^0}{m \cdot c} \right|^2 . \tag{A.147}
\]

where \( \tilde{v}_f \) is the velocity of the electron and \( \theta \) is the angle between \( \tilde{k} \) and \( \tilde{k}_f \). To simplify further (Equation A.146), we try to find a reasonable approximation of the denominator. For a non-relativistic photoelectron, we find

\[
|k - \tilde{k}_f| \approx \sqrt{\frac{2 \cdot m \cdot E}{\hbar}} = \left( 0.51 \cdot 10^3 \right) \cdot \left( \sqrt{\frac{\hbar}{E}} \right) \cdot \text{cm}. \tag{A.148}
\]

Inserting this into Equation A.146, we eventually get for the differential cross-section for unpolarized photons,

\[
\sigma_{\text{PE}} = \frac{16 \cdot \alpha \cdot \left| k^0 \right|^2 \cdot a_0^2 \cdot Z^5 \cdot \sin^2(\vartheta)}{m \cdot \omega_f \cdot k_f^5 \cdot \left( 1 - \frac{\tilde{v}_f}{c} \cdot \cos(\vartheta) \right)^2}. \tag{A.149}
\]

For non-relativistic velocities of the photoelectron, the denominator \( 1 - \frac{\tilde{v}_f}{c} \cdot \cos(\vartheta) \approx 1 \) is close to unity. Utilizing the relation \( k_f = \sqrt{\frac{2 \cdot m \cdot \omega_f}{\hbar}} \), we obtain the total photoionization cross-section by integrating the differential cross-section over the solid angle

\[
\sigma_{\text{PE}} = \frac{16 \cdot \alpha \cdot \left| k^0 \right|^2 \cdot \sin(\vartheta) \cdot d\theta \cdot d\varphi = \frac{16}{3} \cdot \sqrt{\frac{2 \cdot \pi \cdot \alpha^3 \cdot Z^5 \cdot \left( \frac{m \cdot c^2}{\hbar \cdot \omega} \right)^2 \cdot a_0^2 \cdot \vartheta}}. \tag{A.150}
\]

A.7 Cherenkov Effect

As a charged particle is traveling through a medium of refractive index, \( n \), with a velocity, \( v > c/n \), it radiates characteristic electromagnetic wave fields, which is the so-called Cherenkov radiation.

We can employ a very simple model to explain this effect. While traveling through matter, the charged particle shortly polarizes the atoms in the vicinity of its track, which then become electrical dipoles. Due to the temporal change in the dipole field, electromagnetic wave fields are radiated. As long as the particle velocity is small in comparison to \( c/n \), we can assume a symmetrical distribution of dipoles along the track, as indicated in Figure A.10a, and the superposition of all individual dipole fields sums up to zero in the far field. In other words, we would not measure any radiation. The situation changes when the particle velocity is greater than \( c/n \). In this case, the generation of dipoles is retarded, and the resulting dipole field is asymmetric (Figure A.10b). The temporal change of the remaining dipole moment then causes the emission of Cherenkov radiation. The relative contribution of Cherenkov radiation is small in comparison to the energy loss by ionization (Equation A.105). For light gases, it is in the order of 5%, while for gases with \( Z > 7 \) it is around 1%. The angle between the emitted Cherenkov photons and the particle track we get through a simple geometrical consideration: while the particle travels the distance \( AB = t \cdot \beta \cdot c \), the photon just made it to \( AC = t \cdot c/n \). Therefore, we get

\[
\cos(\vartheta) = \frac{c}{n \cdot \beta \cdot c} = \frac{1}{n \cdot \beta}. \tag{A.152}
\]

In principle, we should correct the recoil effect of the photon momentum (\( \hbar \cdot k \)) onto the particle momentum, \( p \). However, since \( \hbar \cdot k \ll p \), Equation A.152 represents a decent approximation, which is good enough for most purposes. Cherenkov radiation is only emitted when the particle velocity exceeds the threshold \( \beta > 1/n \). From this threshold on the photons will be emitted in a forward direction up to a maximum angle of

\[
\theta_{\text{max}} = \arccos \left( \frac{1}{n} \right). \tag{A.153}
\]

The number of emitted Cherenkov photons in the wavelength range of \( \lambda_i \) and \( \lambda_f \) per path length, \( dx \), is given by
\[
\frac{dN}{dx} = 2 \cdot \pi \cdot z^2 \cdot \int_{\lambda}^{\infty} \left[ 1 - \frac{1}{n^2 \cdot r^2} \right] \cdot d\lambda
\]

\[
= 2 \cdot \pi \cdot z^2 \cdot \sin^2(\theta) \cdot \frac{\lambda_2 - \lambda_1}{\lambda_2^2 - \lambda_1^2},
\]  

(A.154)

where \( z \) is the charge of the particle. For a single charged particle \( (z = 1) \) we will get something like 490 \( \cdot \sin^2(\theta) \) photons per centimeter radiator material length in the optical wavelength range from 400 to 700 nm.

### A.8 Photonuclear Interactions

As we discussed earlier, when the wavelength becomes much smaller than the Bohr radius, \( \lambda \ll \alpha_0 \), the incident wave field will start to work on the nucleus. As seen in Section 1.4.7, we can imagine the nucleus as a drop of incompressible nuclear proton/neutron fluid of very high density, which is held together by the strong nuclear force. This strong nuclear force is visible only on the baryon level, and vanishes at the boundary of the nucleus. From the distance, \( \vec{r} \), we therefore see only the Coulomb force of the charge density of the protons, \( \rho(\vec{r}) \). The resulting potential we can denote as

\[
\varphi(\vec{r}) = \int \rho(\vec{r}) \cdot d\vec{r}' = \int \frac{\rho(\vec{r}) \cdot d\vec{r}'}{r \cdot \rho(\vec{r})} = \frac{1}{r} \cdot \int \sum_{l=0}^{\infty} \left( \frac{\rho(\vec{r}) \cdot d\vec{r}'}{r} \right) \cdot P_l(\cos(\theta)) \cdot \rho(\vec{r}) \cdot d\vec{r}',
\]

(A.155)

where \( P_l(\cos(\theta)) \) are Legendre’s polynomials for \( m = 1 \) that we introduced earlier when discussing in Section A.5. For \( 1 \cdot \vec{r} / \vec{r} \neq \vec{r} \) the series converges rapidly, and we just have to take care of the first order terms of the expansion

\[
\varphi(\vec{r}) = \frac{Z \cdot e}{1 \cdot \vec{r}} + \frac{|q_0|}{1 \cdot \vec{r}^2} + \frac{Q_0}{2 \cdot 1 \cdot \vec{r}^3} + \ldots,
\]

(A.156)

where the first term of the series is the monopole \( \int \rho(\vec{r}) \cdot d\vec{r}'' = Z \cdot e \), which is due to the charge of the nucleus, the second term is the dipole moment in the sense of Equation A.30, thus \( \vec{d}_0(\vec{r}) = \int \rho(\vec{r}) \cdot z_0 \cdot \vec{e}_r \cdot d\vec{r}'' \), and \( Q_0 = \int \rho(\vec{r}) \cdot \{ 3 \cdot \vec{z}_0^2 - |\vec{r}|^2 \} \cdot d\vec{r}'' \) is the quadrupole when we assume that the symmetry axis of the nucleus is parallel to the z-axis of a coordinate system with origin in the center of the liquid drop. Higher terms are dropping rapidly with the distance and can be neglected. We can imagine these electric (but also magnetic) multipoles in the nucleus according to the simplified sketch depicted in Figure A.11. Now it is clear that an incident wave field on the nucleus can generate low and high order oscillations and work pretty much the same way as we saw before in the case of bound electrons. Similarly to the scattering of X-rays on bound electrons, the dipole moment of the nucleus for instance can act as an effective antenna for the absorption of the incident \( \gamma \)-rays or emitting the latter. In addition, we will find monopole modes, thus the swelling and shrinking of the nucleus and the activation of quadrupole moments, which as a side remark are the sources of gravitational waves.

These three modes of oscillation (monopole, dipole, and quadrupole) are known as the giant nuclear resonances (GNR) and are associated to the giant electric monopole resonance (E0 or GMR), the giant electric dipole resonance (E1 or GDR), and, eventually, the giant electric quadrupole resonance (E2 or GQR).
Historically, the oldest and best-studied GNR is the E1/GDR. This resonance occurs in medium and heavy nuclei at an energy of about $E_{\gamma} = 78 \cdot A^{-1/3}$ MeV, where $A$ is the atomic mass number. In spherical nuclei, the width of the resonance is more or less $4$ MeV in a wide range of atoms, which broadens up the $8$ MeV in deformed nuclei, since here lateral and longitudinal components and their linear combinations will contribute. Sometimes these contributions can be experimentally resolved. E0 and E2 resonances are lying energetically very close to the GDR, but they are strongly released in forward direction. To get an idea about the cross-sections, we take the example of the GDR and use the same ansatz as in Equation A.62, where we now use the mass, $M$, of the nucleus and the charge, $Z \cdot e$. Moreover, we consider the protons bound in the nucleus via a spring with a natural, angular frequency, $\omega_{\text{GDR}}$ to obtain Newton’s second equation of motion

$$M \cdot \frac{d^2 \vec{r}}{dt^2} + M \cdot \Gamma_{\text{GDR}} \frac{d\vec{r}}{dt} + M \cdot \omega_{\text{GDR}}^2 \cdot \vec{r} = -Z \cdot e \cdot E_0 \cdot e^{-i \omega_{\gamma} t} \cdot \hat{e}_z,$$  

(A.157)

where $\Gamma_{\text{GDR}}$ is the damping rate. As discussed previously, we consider the incident wave field polarized in the $z$-direction. Executing exactly the same steps as in Section A.1.6, we yield

$$\sigma_{\text{GDR}}(\omega_{\gamma}) = \frac{\left(\sigma'_{\text{GDR}} \cdot \omega_{\gamma}^2\right)}{\left(\omega_{\gamma}^2 - \omega_{\text{GDR}}^2\right)^2 + \omega_{\gamma}^2 \cdot \Gamma_{\text{GDR}}^2}$$  

(A.158)

which is nothing else but a Lorentzian shape with an amplitude of $\sigma'_{\text{GDR}}$. Equation A.158 can be expressed in terms of energy, which gives us

$$\sigma_{\text{GDR}}(E_{\gamma}) = \frac{\left(\sigma_{\text{GDR}} \cdot E_{\gamma}^2\right)}{\left(E_{\gamma}^2 - E_{\text{GDR}}^2\right)^2 + E_{\gamma}^2 \cdot \hbar^2 \cdot \Gamma_{\text{GDR}}^2}$$  

(A.159)

Appendix B

FIGURE B.1 Summary of elementary photon interactions on atomic electrons.
Appendix C

TABLE C.1
Physical Constants Used

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Speed of light in vacuum</td>
<td>c</td>
<td>299,792,458</td>
<td>m/s</td>
</tr>
<tr>
<td>Planck’s reduced constant</td>
<td>ħ</td>
<td>6.582 · 10⁻¹⁶</td>
<td>eV·s</td>
</tr>
<tr>
<td>Electron charge</td>
<td>E</td>
<td>1.602 · 10⁻¹⁶</td>
<td>C</td>
</tr>
<tr>
<td>Electron mass</td>
<td>M</td>
<td>9.109 · 10⁻³¹</td>
<td>kg</td>
</tr>
<tr>
<td>Electron rest mass</td>
<td>m·c²</td>
<td>0.511</td>
<td>MeV</td>
</tr>
<tr>
<td>Classical electron radius</td>
<td>r₀</td>
<td>2.817 · 10⁻¹⁵</td>
<td>m</td>
</tr>
<tr>
<td>Bohr radius</td>
<td>a₀</td>
<td>0.529 · 10⁻¹⁰</td>
<td>m</td>
</tr>
<tr>
<td>Permeability of vacuum</td>
<td>μ₀</td>
<td>4 · π · 10⁻⁷</td>
<td>N/A²</td>
</tr>
<tr>
<td>Permittivity of vacuum</td>
<td>ε₀</td>
<td>8.854 · 10⁻¹²</td>
<td>F/m</td>
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<tr>
<td>Fine structure constant</td>
<td>α</td>
<td>7.297 · 10⁻³</td>
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</tr>
<tr>
<td>Avogadro’s number</td>
<td>Nₐ</td>
<td>6.022 · 10⁻²³</td>
<td>1/mol</td>
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<tr>
<td>Boltzmann constant</td>
<td>K</td>
<td>8.617 · 10⁻⁵</td>
<td>eV/K</td>
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<tr>
<td>Atomic mass unit</td>
<td>mₑ</td>
<td>1.660 · 10⁻²⁷</td>
<td>kg</td>
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<tr>
<td>Thomson cross-section</td>
<td>σₜₖ</td>
<td>0.665 · 10⁻¹⁸</td>
<td>m²</td>
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<tr>
<td>Rydberg constant</td>
<td>R</td>
<td>13.605</td>
<td>eV</td>
</tr>
<tr>
<td>Proton diameter</td>
<td>π</td>
<td>0.8418 · 10⁻¹⁵</td>
<td>m</td>
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</table>

Appendix D

<table>
<thead>
<tr>
<th>Energy Range (eV)</th>
<th>Wavelength Range</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;10⁻⁷</td>
<td>cm to km</td>
<td>Radio Waves (short, medium, long waves)</td>
</tr>
<tr>
<td>&lt;10⁻³</td>
<td>mm to cm</td>
<td>Microwave</td>
</tr>
<tr>
<td>&lt;10⁻³</td>
<td>mm to mm</td>
<td>Infra Red</td>
</tr>
<tr>
<td>0.0017–0.0033</td>
<td>380–750 nm</td>
<td>Visible Light</td>
</tr>
<tr>
<td>0.033–0.1</td>
<td>10–380 nm</td>
<td>Ultra Violet</td>
</tr>
<tr>
<td>0.11–100</td>
<td>0.01–12 nm</td>
<td>X-rays</td>
</tr>
<tr>
<td>10–5000</td>
<td>0.0002–0.012 nm</td>
<td>Gamma Radiation</td>
</tr>
</tbody>
</table>

Appendix E

TABLE E.1
URLs of Useful Databases

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<thead>
<tr>
<th>Name</th>
<th>Type</th>
<th>URL</th>
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<tbody>
<tr>
<td>Center of X-ray Optics</td>
<td>X-ray Interactions With Matter</td>
<td><a href="http://henke.lbl.gov/optical_constants/">http://henke.lbl.gov/optical_constants/</a></td>
</tr>
<tr>
<td>NIST ESTAR</td>
<td>Stopping power electrons</td>
<td><a href="http://physics.nist.gov/PhysRefData/Star/Text/ESTAR.htm">http://physics.nist.gov/PhysRefData/Star/Text/ESTAR.htm</a></td>
</tr>
<tr>
<td>NIST PSTAR</td>
<td>Stopping power protons</td>
<td><a href="http://physics.nist.gov/PhysRefData/Star/Text/PSTAR.html">http://physics.nist.gov/PhysRefData/Star/Text/PSTAR.html</a></td>
</tr>
<tr>
<td>XOP</td>
<td>X-ray Oriented Programs</td>
<td><a href="http://www.esrf.eu/Instrumentation/software/data-analysis/xop2.4">http://www.esrf.eu/Instrumentation/software/data-analysis/xop2.4</a></td>
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</table>
REFERENCES


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Basic Physics of X-ray Interactions in Matter


von Bortkiewicz, L. 1898. *Das Gesetz der kleinen Zahlen (The law of small numbers)*. B.G. Teubner Leipzig, Germany.


