

Chapter 1

Photon Scattering – Form Factors

*Und so lasset auch die Farben
Mich nach meiner Art verkünden,
Ohne Wunden, ohne Narben,
Mit der lässlichsten der Sünden.*

Goethe

Scattering experiments are the paradigm of quantum mechanical measurements. A beam of atoms, ions, electrons or photons – to mention but a few possibilities – is generally created in an accelerator. A detector is used to find the energy of the scattered particle (or the absolute value of the momentum) and the scattering angle. From this, one calculates the momentum and energy transfer to the scattering centre and thus obtains the properties of the system under investigation.

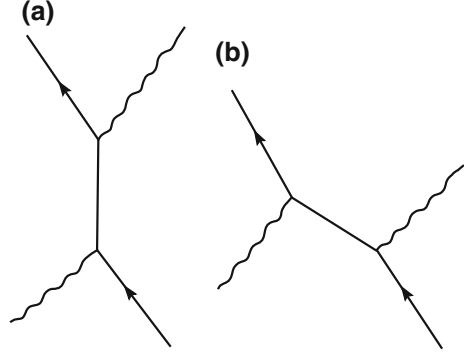
The scattering of elementary particles (photons, leptons and quarks) off each other is distinguished by these particles not displaying any excited states, and their interaction can be described via a fundamental coupling to exchange bosons. Scattering elementary particles off composite systems, such as atoms, nuclei or nucleons, offers the ideal method to explore their structure.

Photons are, of course, scattered off all charged particles. Since the scattering cross-section is proportional to the square of the acceleration, i.e., inversely proportional to the square of the mass of the particle, electromagnetic effects may most easily be seen in photon-electron scattering.

1.1 Compton Effect

The calculation of photon scattering off a free electron, Compton scattering, is a standard exercise in relativistic quantum mechanics that everyone must once endure. Here we will only treat the Klein–Nishina formula and discuss the properties of the

Fig. 1.1 Schematic representation of both the amplitudes (a) and (b) that contribute to Compton scattering at lowest order. The electrons move in the positive time direction, the positrons are represented by the negative energy electrons which move backwards in time



scattering in two interesting kinematic regimes. The two amplitudes that contribute to the scattering are symbolically represented in Fig. 1.1. The famous Klein–Nishina formula for unpolarised radiation is

$$\frac{d\sigma}{d\Omega'_{\omega}} = \frac{1}{2} r_e^2 \left(\frac{\omega'}{\omega} \right) \left(\frac{\omega'}{\omega} + \frac{\omega}{\omega'} - \sin^2 \theta \right), \quad (1.1)$$

where $\hbar\omega$ and $\hbar\omega'$ are, respectively, the energies of the incoming and outgoing photons and θ is the scattering angle. The following relation links θ and the energies:

$$\cos \theta = 1 - \frac{m_e c^2}{\hbar\omega'} + \frac{m_e c^2}{\hbar\omega}. \quad (1.2)$$

Here, r_e is the so-called classical electron radius, the picturesque interpretation of which we will discuss later:

$$r_e = \frac{e^2}{4\pi\epsilon_0 m_e c^2} = \frac{\alpha \hbar c}{m_e c^2} = \alpha \lambda_e. \quad (1.3)$$

The values of the Compton wavelength and the classical radius of the electron are $\lambda_e = \hbar/(m_e c) = 386 \text{ fm}$ and $r_e = 2.82 \text{ fm}$. For Compton scattering with highly energetic photons ($E_\gamma \gg m_e c^2$) off electrons bound in atoms, it is a good approximation to consider the electrons as free. In storage ring experiments, one can, however, observe scattering off electrons that really are free, and we will briefly treat this in Sect. 1.5.

Coherent scattering of low-energy photons off all the electrons in an atom is of particular interest. If the atoms are bound in a crystal, the coherence of the scattering can be extended to the entirety of the crystal.

At low energies, $E_\gamma \ll m_e c^2$, the recoil may be neglected and one can set $\omega = \omega'$. In this approximation, the Klein–Nishina formula gives exactly the same result as the classically calculated cross-section for Thomson scattering,

$$\frac{d\sigma}{d\Omega} = r_e^2 \frac{1 + \cos^2 \theta}{2}. \quad (1.4)$$

In the following, we will ask ourselves the following: where in the amplitudes (Fig. 1.1) is the classical picture of an oscillating electron in the field of the incoming radiation, hidden? This is, anyway, the underlying picture in the derivation of the Thomson formula (1.4).

1.2 Thomson Scattering

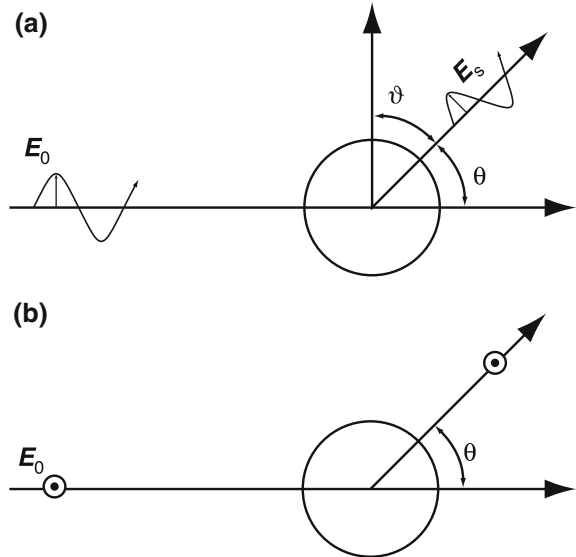
1.2.1 Classical Derivation

Let us first consider the scattering of linearly polarised light off an electron in an atom (Fig. 1.2). Neglecting the recoil, the electron moves in the electric field $\mathbf{E}_0 e^{i\omega t}$ of the incoming light wave, and its acceleration is

$$\mathbf{a} = \mathbf{E}_0 \frac{e}{m} e^{i\omega t}. \quad (1.5)$$

The accelerated charge radiates. For those waves that spread out perpendicularly to the induced dipole, the electric field strength in the radiation zone is proportional to the product of the acceleration and the charge,

Fig. 1.2 Coherent photon scattering off an atom. The polarisation vector is (a) in the plane ($\vartheta = \pi/2 - \theta$), (b) orthogonal to the plane ($\vartheta = \pi/2$)



$$\mathbf{E}_s(t, r, \vartheta = \pi/2) = \frac{1}{4\pi\epsilon_0} \frac{e^2}{mc^2} \mathbf{E}_0 \frac{e^{i(\omega t - kr)}}{r}, \quad (1.6)$$

where the factor $1/(4\pi\epsilon_0)$ ensures the correct units and the $1/r$ -dependence preserves energy conservation because $\int \mathbf{E}_s^2 r^2 d\Omega$ must be independent of r .

The amplitude of the electric field strength of the radiation in any direction where $\vartheta \neq \pi/2$ is reduced. The reduction factor is $\sin \vartheta$, where ϑ is measured from the polarisation direction of the incoming wave. This factor yields the projection of the polarisation vector of the incoming radiation with respect to the polarisation direction of the radiation field (Fig. 1.2).

The energy density,

$$\frac{1}{2}(\epsilon_0 \mathbf{E}_s^2 + \mu_0 \mathbf{B}_s^2) = \epsilon_0 \mathbf{E}_s^2, \quad (1.7)$$

multiplied by c yields the energy flux. The energy flux scattered into the solid angle $d\Omega$ is thus found to be

$$\begin{aligned} c\epsilon_0 \mathbf{E}_s^2 r^2 d\Omega &= \frac{c\epsilon_0 \mathbf{E}_0^2}{(4\pi\epsilon_0)^2} \left(\frac{e^2}{mc^2} \right)^2 \sin^2 \vartheta d\Omega \\ &= c\epsilon_0 \mathbf{E}_0^2 r_e^2 \sin^2 \vartheta d\Omega. \end{aligned} \quad (1.8)$$

The so-called classical electron radius is a measure of the acceleration of an electron in an electric field. It has nothing to do with the geometrical extension of the electron.

Its historical denotation as a radius came from the relation

$$mc^2 = \frac{e^2}{4\pi\epsilon_0 r_e}. \quad (1.9)$$

The electrostatic energy of a sphere with radius r_e and charge e is in the classical picture related to the electron mass. The appearance of the radius r_e in electrodynamics has a plausible explanation. If two electrons come together up to a separation r_e , then the potential energy is so great that an e^+e^- pair is created; the concept of a single electron thus loses its meaning. For nonpolarised light, one measures the angle θ from the beam direction (Fig. 1.2). The total intensity of the scattered light is found from incoherently averaging the contributions (1.8) of the two orthogonal polarisation states. In atoms with Z electrons and for wavelengths large in comparison with the atomic radius, the electrons oscillate with the same phase and the contributions to the scattering off the individual electrons are added coherently,

$$c\epsilon_0 \mathbf{E}_s^2 d\Omega = c\epsilon_0 \mathbf{E}_0^2 Z^2 r_e^2 \frac{1 + \cos^2 \theta}{2} d\Omega. \quad (1.10)$$

The photon flux, i.e., the number of photons that hit the target per unit area per second, is $\Phi_0 = c\varepsilon_0 E_0^2/(\hbar\omega)$. The number of photons scattered into the solid angle $d\Omega$ is found from

$$\Phi_s d\Omega = \Phi_0 Z^2 r_e^2 \frac{1 + \cos^2 \theta}{2} d\Omega, \quad (1.11)$$

from which the differential cross-section

$$\frac{d\sigma}{d\Omega} = Z^2 r_e^2 \frac{1 + \cos^2 \theta}{2} \quad (1.12)$$

may be deduced.

1.2.2 Quantum Mechanical Derivation

The same result as above can be very simply derived quantum mechanically at low energies. Because we may calculate nonrelativistically, the interaction between photons and electrons is given by the following Hamiltonian:

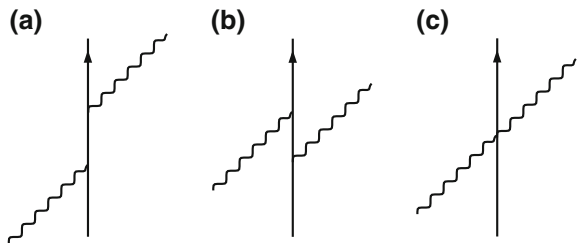
$$\frac{(\mathbf{p} - e\mathbf{A})^2}{2m_e} = \frac{\mathbf{p}^2}{2m_e} - \frac{e\mathbf{A} \cdot \mathbf{p}}{m_e} + \frac{e^2 \mathbf{A}^2}{2m_e}. \quad (1.13)$$

The first term corresponds to the kinetic energy of the electron and the rest to the perturbation. In Fig. 1.3 the amplitudes that are proportional to α are represented diagrammatically. Amplitudes (a) and (b) have the form

$$M \sim \frac{e\langle \mathbf{A} \cdot \mathbf{p} \rangle}{m_e} \frac{1}{\Delta E} \frac{e\langle \mathbf{A} \cdot \mathbf{p} \rangle}{m_e}. \quad (1.14)$$

When one explicitly writes out both amplitudes, one can easily convince oneself that they have opposite signs and cancel each other as $\omega' \rightarrow \omega$. It is easy to see that both amplitudes have opposite signs because the amplitudes have (a) $\Delta E = +\hbar\omega$ and (b) $\Delta E = -\hbar\omega$. Furthermore, for energies $\hbar\omega \ll m_e c^2$, the amplitudes (a) and (b) are anyway small compared with the amplitude (c). The first two contain two separate

Fig. 1.3 The amplitudes that contribute to Compton scattering in the nonrelativistic limit



vertices and so have a factor of m_e^2 in the denominator, while in amplitude (c), there is only one power of the electron mass.

Considered superficially, one might think that the amplitude (c) is a limiting case of (a) and (b); this is, however, not the case, as we will see in the following: If we want to calculate the amplitude (c), we have to quantise the electromagnetic field, \mathbf{A} . When a photon with polarisation ε is created or annihilated, the expectation value of \mathbf{A} is given by $(\hbar/\sqrt{2\varepsilon_0\hbar\omega})\varepsilon$. To make this “photon normalisation” plausible, we consider an electromagnetic eigenmode (with periodic boundary conditions) in a normalisation volume: $E/V = \varepsilon_0 \mathbf{E}^2/2 + \mathbf{B}^2/2\mu_0 = \varepsilon_0[d\mathbf{A}/dt]^2/2 + |\nabla \times \mathbf{A}|^2/2\mu_0 = \varepsilon_0[(\omega A)^2 + c^2(kA)^2]/2 = \varepsilon_0\omega^2 A^2 = \hbar\omega/2$. We have expressed the electric and magnetic fields in terms of A ; both fields give the same contribution. The amplitude (c) is then given as $\omega' \rightarrow \omega$ by

$$M = 2 \frac{e^2}{2m_e} \frac{\varepsilon_i}{\sqrt{\varepsilon_0}} \frac{\hbar}{\sqrt{2\hbar\omega}} \cdot \frac{\varepsilon_f}{\sqrt{\varepsilon_0}} \frac{\hbar}{\sqrt{2\hbar\omega}} = \frac{2\pi r_e (\hbar c)^2}{\hbar\omega} \varepsilon_i \cdot \varepsilon_f, \quad (1.15)$$

where ε_i and ε_f are, respectively, the polarisation vectors of the incoming and outgoing photons. Their scalar product is either 1 (Fig. 1.2b) or $\cos \theta$ (Fig. 1.2a). The cross-section obtained in this way for unpolarised radiation off Z electrons is then

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar} Z^2 \overline{|M|^2} \frac{(\hbar\omega/c)^2}{(2\pi\hbar)^3 c^2} = Z^2 r_e^2 \frac{1 + \cos^2 \theta}{2}, \quad (1.16)$$

which is identical to the classically derived equation (1.12).

1.2.3 Quantum Mechanical Interpretation of \mathbf{r}_e

Superficially considered, it sounds surprising that the Dirac equation yields the same result (1.12) in the nonrelativistic limit, despite the corresponding amplitude depicted in Fig. 1.3c not explicitly appearing. The explanation is as follows: in the relativistic case, the propagator in the amplitudes (a) and (b) of Fig. 1.1 also contains positrons. In Fig. 1.4, the positrons are explicitly shown in the two diagrams labeled by (c). While the amplitudes (a) and (b) vanish for small velocities due to the current coupling $\sqrt{\alpha} p/m_e c$, the photon coupling to the electron–positron pair is $\sqrt{\alpha}$. In the case of pair creation, the intermediate state involves two additional electron masses and the propagator is proportional to $1/2m_e$. It follows from this that the amplitudes labeled (c) in Fig. 1.4 are proportional to $\langle e^2 \mathbf{A}^2 / 2m_e \rangle$.

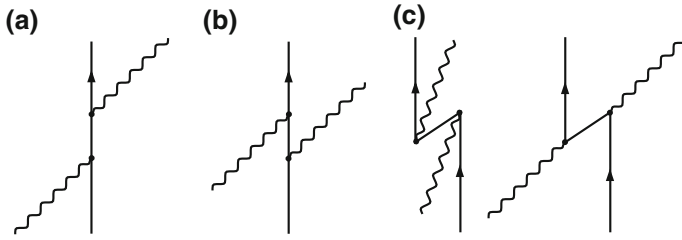


Fig. 1.4 The contribution of electron–positron pairs (c) to Compton scattering

It is well worth stressing that the classical oscillations of an electron in an electromagnetic field in the relativistic case correspond to the coupling of the photon to electron–positron pair fluctuations in the vacuum. This means that Thomson scattering in the relativistic calculation results from a sum of the contributions of the small components of the Dirac wave function.

The classical electron radius also acquires a new interpretation: Thomson scattering is proportional to

$$r_e^2 = \alpha \cdot \alpha \cdot \lambda_e^2, \quad (1.17)$$

i.e., proportional to the probability that one finds an electron–positron pair inside its range ($\propto \lambda_e^2$) and proportional to the probability that this electron–positron pair interacts with the incoming (α) and the outgoing photon (α).

1.3 Form Factor

The scattering of elementary particles off composite systems is the best method to measure their extension.

1.3.1 Geometrical Interpretation of the Form Factor

When the wavelengths of X-rays are comparable with the extension of an atom, one has to take into account the phases of the waves that are scattered off different regions of the atom. In Fig. 1.5, the planes orthogonal to the momentum transfer vector \mathbf{q} are sketched. They are denoted by dashed lines and are orthogonal to the plane of the page.

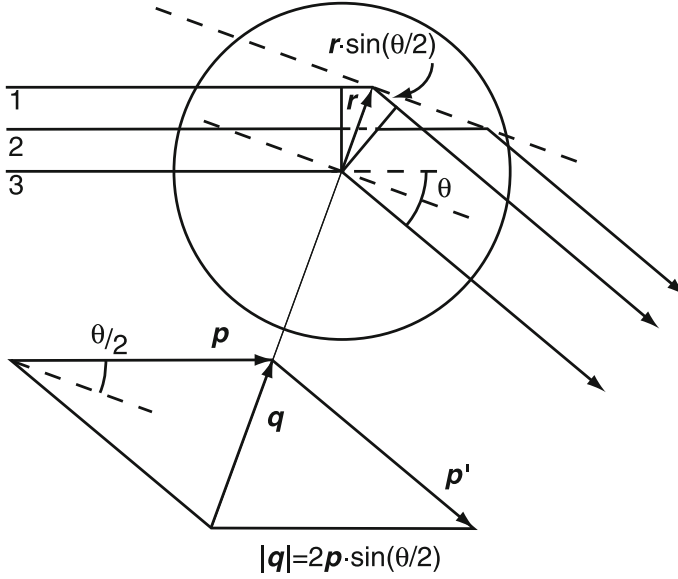


Fig. 1.5 Diffraction of X-rays off an atom

All beams that are scattered in the same plane (beams 1, 2) have the same phase and their amplitudes add together completely. It is therefore sufficient to only consider one beam in every additional plane and determine the phase differences relative to the plane that passes through the middle of the sphere (beam 3). The path length difference between beam 1 and beam 3 is $\Delta = 2r \sin(\theta/2)$ and the phase is

$$2\pi\Delta/\lambda = 2pr \sin(\theta/2)/\hbar = \mathbf{q}\mathbf{r}/\hbar, \quad (1.18)$$

where $\lambda = 2\pi\hbar/p$. The amplitude of the radiation elastically scattered through the angle θ is then reduced by the factor

$$F(q^2) = \int \rho(\mathbf{r}) e^{i\mathbf{q}\mathbf{r}/\hbar} d^3r. \quad (1.19)$$

We call this factor the form factor. It is the Fourier transform of the charge density $\rho(\mathbf{r})$ of the atom. The differential cross-section for the scattering of X-rays off atoms is thus

$$\frac{d\sigma}{d\Omega} = Z^2 r_e^2 F^2(q^2) \frac{1 + \cos^2 \theta}{2}. \quad (1.20)$$

If we write the expectation value of the square of the atomic radius as $\langle r^2 \rangle$ and expand (1.19) in q^2 around $q^2 = 0$, then we obtain

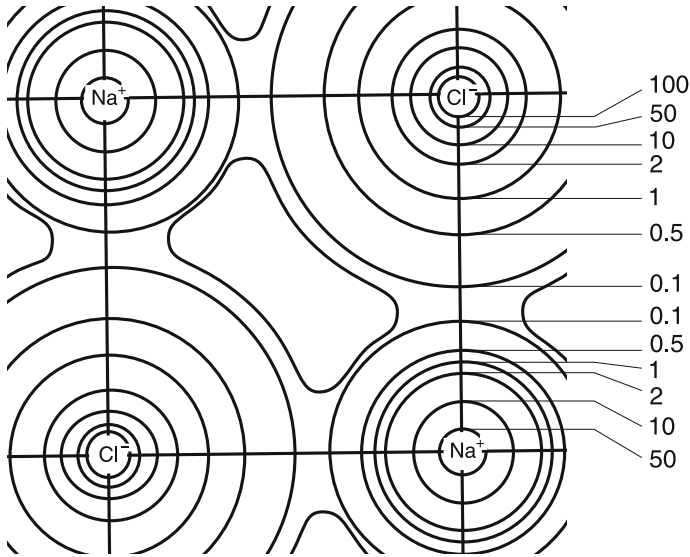


Fig. 1.6 Electron density distribution in NaCl crystal. The *numbers* show the relative electron density

$$\begin{aligned}
 F(q^2) &= 1 - \frac{q^2}{2\hbar^2} \overline{\cos^2 \theta} \int r^2 \rho(r) 4\pi r^2 dr + \dots \\
 &= 1 - \frac{\langle r^2 \rangle}{6\hbar^2} q^2 + \dots,
 \end{aligned}
 \tag{1.21}$$

where the average over $\cos^2 \theta$, as is well known, is $1/3$.

Atomic form factors have been found from X-ray diffraction off crystals. In Fig. 1.6, the experimentally determined electron densities of Na^+ and Cl^- ions in NaCl crystal are depicted. These densities roughly correspond to those of the noble gases neon and argon. To extract the form factors, one has to divide the density distributions by Z^2 for both the ions. Such normalised density distributions in noble gases have almost identical extensions and are described to a very good approximation by an exponential function (Fig. 5.3), the Fourier transform of which is

$$F(q^2) \approx \frac{1}{[1 + (qa)^2]^2},
 \tag{1.22}$$

where $a^2 = \langle r^2 \rangle / (12\hbar^2)$. The mean square radii of both ions are comparable: $\sqrt{\langle r^2 \rangle} \approx 0.13 \text{ nm}$.

In Fig. 1.6, the relative electron densities are shown and the Cl^- ion seems larger than the Na^+ ion.

1.3.2 Dynamical Interpretation of the Form Factor

Let us attempt to give a dynamical interpretation of the form factor. The extension of the atom is linked to the binding energy of the electron in the Coulomb field by the uncertainty relation. In place of the binding energy, we introduce the idea of the typical excitation of the system, which we denote by D . In the case of the oscillator potential, D is the separation of the excited states, while, for atoms, D is of the order of magnitude of the binding energy. The expectation value of $\langle r^2 \rangle$ can then be approximately replaced by D ,

$$\langle r^2 \rangle = f \frac{\hbar^2}{\langle p^2 \rangle} = f \frac{\hbar^2}{2m_e D}. \quad (1.23)$$

The value of f depends on the specific potential but is of the order of magnitude of 1. The form factor (1.21) can then be expressed in terms of the typical excitation of the system D (1.23),

$$F(q^2) = 1 - \frac{f}{12m_e D} q^2 + \dots \quad (1.24)$$

For increasing momentum transfer, the recoil energy will eventually suffice to excite the electron into a higher energy state or into the continuum. The probability that the system remains in the ground state after the scattering decreases rapidly for

$$\frac{q^2}{2m_e} \geq D. \quad (1.25)$$

1.4 Recoilless Scattering Off Crystals

Because the Nobel prize has twice been awarded (von Laue 1920, Mössbauer 1957) for the discovery of recoilless X-ray scattering off crystals and for gamma emission in crystals, we want here to derive *on the back of an envelope* the probability that the scattering takes place off the entire crystal.

Consider atoms bound in a crystal where the interatomic potential has the form of a harmonic oscillator. The typical excitation is $D = \hbar\omega$. Let us consider an atom in the ground state for which the wavefunction is

$$\psi_0(r) = \left(\frac{M\omega}{\hbar\pi} \right)^{3/4} e^{-M\omega r^2/(2\hbar)}. \quad (1.26)$$

Immediately after the recoil, the wavefunction has not had time to change its spatial form; however, the momentum received can be seen in the phase factor $\exp(iqr/\hbar)$,

$$\psi_0(r) \rightarrow \psi'(r) = e^{iqr/\hbar} \psi_0(r). \quad (1.27)$$

The probability that the atom remains in the ground state is the square of the overlap between the new wave function, ψ' , and the ground-state wave function, ψ_0 ,

$$P(0, 0) = |\langle \psi_0 | e^{iqr/\hbar} \psi_0 \rangle|^2 = \left| \int \psi_0^* e^{iqr/\hbar} \psi_0 d^3r \right|^2 = e^{-q^2/(2M\hbar\omega)}. \quad (1.28)$$

Now we must define the typical excitation of the crystal D or $\hbar\omega$. In the Debye model of the crystal, $D \approx \frac{2}{3}k\Theta$, where Θ is the Debye temperature. When we substitute this value for D into (1.28), we obtain

$$P(0, 0)_{\text{DW}} = e^{-3q^2/(4Mk\Theta)}. \quad (1.29)$$

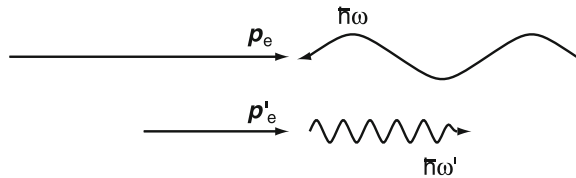
Equation (1.29) is the simplified form of the Debye–Waller factor for $T = 0\text{K}$. It gives the probability of coherent scattering off crystals and also for the recoilless emission of gamma rays from crystalline sources (the Mössbauer effect). To underline the complementarity of the dynamical and geometrical interpretations of the form factor, let us again repeat that the Debye–Waller factor is the form factor of an atom bound in a crystal.

1.5 Photon Scattering Off Free Electrons

Photon scattering (or Compton scattering) off free electrons may be easily performed at electron storage rings and has many applications in accelerator physics. At DESY, for example, a laser beam with $\hbar\omega = 2.415\text{eV}$ hits 27.570GeV electrons. The backward scattered photons are in the energy spectrum of high energy gamma rays, with an energy of 13.92GeV (Fig. 1.7).

The energy of the backward scattered photon can be easily estimated when one equates the relativistically invariant quantity s , the square of the centre of mass energy, before the scattering with its value after the scattering. Before the scattering,

Fig. 1.7 Scattering of laser light off a high energy electron



$$\begin{aligned}
s &= (E_e + E_\gamma)^2 - (p_e c - E_\gamma)^2 \\
&= m_e^2 c^4 + 2E_\gamma(E_e + p_e c) \\
&\approx m_e^2 c^4 + 4E_\gamma E_e,
\end{aligned} \tag{1.30}$$

where we assumed $E_e \approx p_e c$, and after the scattering, we have

$$\begin{aligned}
s' &= (E'_e + E'_\gamma)^2 - (p'_e c + E'_\gamma)^2 \\
&= m_e^2 c^4 + 2E'_\gamma(E'_e - p'_e c) \\
&\approx m_e^2 c^4 + E'_\gamma \frac{m_e^2 c^4}{E'_e}.
\end{aligned} \tag{1.31}$$

The final step in (1.31) is obtained when one multiplies s' by $(E'_e + p'_e c)/2E'_e$ and then assumes $E'_e \approx p'_e c$.

Making use of conservation of energy, $E'_e \approx E_e - E'_\gamma$, comparison of the two expressions for s yields

$$E'_\gamma = 4E_\gamma E_e \frac{E_e - E'_\gamma}{m_e^2 c^4}, \tag{1.32}$$

which leads to the result

$$E'_\gamma = \frac{E_e}{1 + m_e^2 c^4 / (4E_\gamma E_e)} = E_e \cdot \frac{4E_\gamma E_e}{s}. \tag{1.33}$$

For the energies mentioned above, $m_e^2 c^4 / 4E_\gamma E_e = 0.98$ and $E'_\gamma \approx E'_e \approx E_e/2$. From this, it follows that the centre of mass energy, $\sqrt{s} \approx \sqrt{2}m_e c^2$. This value contains the rest energy $m_e c^2$, so the kinetic energy is only a fraction of the total energy. Therefore, we may estimate the cross-section nonrelativistically, and we can take the Thomson value

$$\sigma = \frac{8}{3} \pi r_e^2. \tag{1.34}$$

The exact calculation of the Klein–Nishina cross-section integrated over 4π yields, for the example treated above, a result that is smaller by a factor of 0.81. For centre of mass energies below twice the electron mass, $pc \leq m_e c^2$, the Thomson cross-section is a good estimate.

Compton scattering is generally taken to refer to quasi-elastic photon scattering off an electron in an atom. For lower energy and angular resolution of the measurement, it suffices to calculate the kinematics of the scattering off a static electron. The quality of contemporary detectors is, though, sufficient to observe the influence of atomic, molecular or solid state effects on the kinematics of the scattered particle.

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Scattering and Structures

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