Theoretical Resumé
2.1 Interaction of γ rays with matter.

γ rays are photons produced during nuclear transitions. The interaction of these photons with matter is characterized by the fact that each photon is removed individually from the incident beam in a single event. Therefore, a well-collimated beam of monochromatic γ rays shows a truly exponential absorption in matter.

In general, γ rays interact with matter in twelve different processes (Fano, 1953). These processes are illustrated in Table 2.1. In the energy region 50 keV to 50 MeV, four major processes contribute to the interaction, viz., incoherent scattering, Coherent (Rayleigh) scattering from atomic electrons, Photoelectric effect and Pair production. However, for the sake of completeness, a brief description of all the twelve processes is outlined here.

2.1.a Photoelectric effect

In this process the incident photons are absorbed by the atom and this energy is transferred to the bound atomic electron which uses part of this energy to overcome its binding energy to the atom and carries the rest as kinetic energy. It is the dominant process at low energies and in high Z materials. When energy increases the Z dependence also increases approximately from $Z^4$ to $Z^5$.

2.1.b Rayleigh scattering

It is the elastic scattering of photons from bound electrons of the atom, where the atom as a whole is considered to absorb the transferred momentum. It follows that the energies of the incident and scattered photons are the same and there is a definite phase relationship between the scattering amplitudes for different electrons of the same atom. The total scattered intensity is accordingly a coherent sum of the individual contributions i.e. the amplitude of the radiation scattered by each electron must be added together and the sum acquired to obtain the resultant intensity. It is significant at low energies and confined to very small angles because the recoil imparted to the atom must not produce atomic excitation or ionization. Rayleigh scattering is significant for low $h\nu$ and large $Z$ and is negligible for high $h\nu$ and small $Z$. At small and large angles Rayleigh scattering varies respectively as $Z^2$ and $Z^3$.

2.1.c Thomson scattering with free electrons

It is the coherent scattering of γ rays by free electrons. This is energy dependent and varies linearly with atomic number. Thomson scattering is regarded as the low energy limit of Compton effect.
### Table 2.1. Gamma ray interaction with matter

<table>
<thead>
<tr>
<th>Process</th>
<th>Kind of interaction and approximate energy range</th>
<th>Other name and (Z)-dependence</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Absorption with atomic electrons</strong></td>
<td>Complete absorption by bound atomic electrons. Dominaates at low energy (1 keV to 500 keV). Decreases as (E) increases.</td>
<td>Photoeffect proportional to (Z^4) to (Z^2).</td>
</tr>
<tr>
<td><strong>Scattering from electrons</strong></td>
<td>Coherent With bound atomic electrons. (&lt;1) MeV — greatest at small scattering angles</td>
<td>Rayleigh scattering. Electron resonance scattering. Proportional to (Z^2) (small angles) to (Z^3) (large angles).</td>
</tr>
<tr>
<td></td>
<td>Incoherent With bound atomic electrons. (&lt;1) MeV — least at small scattering angles</td>
<td>Thomson scattering. Proportional to (Z).</td>
</tr>
<tr>
<td></td>
<td>With free electrons. Independent of energy</td>
<td>Proportional to (Z).</td>
</tr>
<tr>
<td><strong>Absorption by the nucleus</strong></td>
<td>Complete absorption by the nucleus. Emits photon or nucleons. Dominaates in the energy range 10 to 30 MeV.</td>
<td>Nuclear photoeffect. Nuclear photodisintegration.</td>
</tr>
<tr>
<td><strong>Scattering with nucleons</strong></td>
<td>Coherent With the material as a whole. Dependent on nuclear energy levels. Important only in very narrow resonance range.</td>
<td>Mössbauer effect. Nuclear resonance scattering.</td>
</tr>
<tr>
<td></td>
<td>With nucleus as a whole. Dependent on nuclear energy levels. Narrow resonance maxima at low energies. Broad maximum in the range of 10 to 30 MeV.</td>
<td>Nuclear resonance scattering proportional to (Z^2/A^2).</td>
</tr>
<tr>
<td></td>
<td>Incoherent With nucleus as a whole. Independent of nuclear energy levels.</td>
<td>Nuclear Thomson scattering. Proportional to (Z^2/A^2).</td>
</tr>
<tr>
<td><strong>Interaction with coulomb field</strong></td>
<td>Pair production In Coulomb field of the nucleus. Threshold about 1 MeV. Dominates at high (E). ((E &gt; 5) or 10 MeV) Increases as (E) increases.</td>
<td>Elastic pair production. Proportional to (Z^2).</td>
</tr>
<tr>
<td></td>
<td>In Coulomb field of the electron. Threshold at 2 MeV. Increases with (E).</td>
<td>Triplet production. Inelastic pair production. Proportional to (Z).</td>
</tr>
<tr>
<td><strong>Nuclear potential scattering</strong></td>
<td>In Coulomb field of the nucleus Increases with (E).</td>
<td>Dolbrick scattering. proportional to (Z^4).</td>
</tr>
<tr>
<td><strong>Interaction with mesons</strong></td>
<td>With the meson field of the nucleus (E \geq 150) MeV</td>
<td>Photomeson production.</td>
</tr>
</tbody>
</table>
2.1.d Nuclear Thomson scattering

It is the Coherent scattering of $\gamma$ rays by the nucleus. The process is independent of nuclear energy levels and incident energy. The effects though small appear to have been detected.

2.1.e Compton Scattering

It is the incoherent scattering of incident $\gamma$ rays by quasifree electrons. At energies much greater than the binding energies of the atomic electrons, the $\gamma$ rays are scattered as if from a free electron, since the binding effects are negligible. The Compton scattering cross section decreases as incident energy increases and it varies linearly with atomic number. It is the dominant mode of interaction around 1 MeV.

2.1.f Nuclear Compton scattering

It takes place when the incident $\gamma$ energy is greater than 100 MeV. The process is similar to the Compton scattering from electrons excepting that it is the interaction with protons and neutrons.

2.1.g Nuclear photoeffect

The process is energetically possible whenever the photon energy exceeds the separation energy of protons and neutrons. This is characterized by a broad resonance ie the cross section is very small for low energy $\gamma$ rays (even if the energy is greater than the binding energy, of a nucleon) increases to a maximum for a certain energy value and than becomes very small again for higher energies.

2.1.h Nuclear resonance scattering

It involves the resonant absorption of $\gamma$ rays. The energy levels of the nucleus are excited by the absorbed energy and this excitation is followed by emission of $\gamma$ rays during de-excitation. It has been detected and depends on $Z^2/A^2$.

2.1.i Mössbauer effect

It is called as the recoil-less emission and absorption of resonance radiation by nuclei embedded in crystal lattice. The energy that can be transferred to the lattice during nuclear transition is very small compared to the $\gamma$ ray energy. The probability of recoil-less transition is, in most cases, small and is governed by the Debye-Waller factor, familiar in the theory of x-ray and neutron scattering. The cross sections for these processes show energy dependence and vary as the full width of the absorption line.
2.1.j Pair production

It is the photon interaction at high energies. A photon disappears in the field of a charged particle (nucleus) and an electron-positron pair appears. The total kinetic energy of the resultant particles is equal to the photon energy minus the rest energy. The cross section for pair creation varies as $Z^2$.

2.1.k Delbrück scattering

It is also called as “nuclear potential scattering” is due to virtual electron pair formation in the coulomb field of the nucleus. The effect is extremely small and it can not be experimentally distinguished as it combines coherently with other types of elastic scattering like Rayleigh scattering, nuclear resonance scattering and nuclear Thomson scattering. It is predicted by quantum electrodynamics as a second order interaction.

2.1.l Inelastic pair production

It is in the field of an electron (or triplet production) is basically pair production with an atom where one of the atomic electron absorbs all the recoil energy and leaves the atom. The threshold energy of the photon for this reaction is about 2.04 MeV.

2.2 Outlines of the theoretical calculations of coherent scattering

$\gamma$ rays may be scattered coherently, in which case the energy of the incident and scattered photon is the same. The electron returns to its initial state after the interaction. Alternatively, the photon may be scattered incoherently, in which case the energy of the scattered photon is less than that of the incident photon. Some of the momentum of the incident photon is transferred to the bound electron, which is then raised to an excited state or may even be ejected from the atom altogether.

The total elastic scattering amplitude $A$ can be written as the coherent sum of each of the elastic scattering amplitudes,

$$A = A_R + A_{NT} + A_{NR} + A_D$$

(2.1)

Where $A_R$, $A_{NT}$, $A_{NR}$ and $A_D$ represent respectively the Rayleigh, nuclear Thomson, nuclear resonance and Delbrück scattering amplitudes. Each of the scattering processes may be described in terms of linearly or circularly polarized photons. The corresponding amplitudes are represented by $A^{||}$ and $A^{\perp}$ for the case of linear polarization parallel and perpendicular respectively to the scattering plane, and $A^{NSF}$ (no spin flip) and $A^{SF}$ (spin flip) for the case of no change, and change respectively in the state of circular polarization.
The differential scattering cross section for the elastic scattering of initially unpolarized photons in the linear polarization description is given by

\[ \frac{d\sigma}{d\Omega} = \frac{1}{2} \left[ |A_R| + |A_{NT}| + |A_{NR}| + |A_D|^2 \right]^2 + |A^*_{NT} + A^*_{NR} + A_{D}|^2 \]  

(2.2)

The expression for the elastic differential cross section in the circular polarization description is

\[ \frac{d\sigma}{d\Omega} = \left[ |A^\text{NSF}_R + A^\text{NSF}_{NT} + A^\text{NSF}_{NR} + A^\text{NSF}_D|^2 \right]^2 + |A^\text{SF}_R + A^\text{SF}_{NT} + A^\text{SF}_{NR} + A^\text{SF}_D|^2 \]  

(2.3)

The theory of scattering of γ rays by electrons is most complete and satisfactory for photon energies large compared with the electron binding energies. In the more general case, the effects of the binding of electrons to the atom and their motions and distributions within the atom must be considered. Theoretically, the scattering of γ rays by bound electrons is described as a second order process where one photon is absorbed and another one is emitted, the process involving initial intermediate and final states of the electron. An accurate theory must include all possible intermediate states and must take into account the two cases of the absorption of the incident photon first, emission of the scattered photon second, and vice-versa. It should also take into account the two possible spin orientations of the scattering electron and the two possible polarizations of the incident photon as well as the two of the outgoing photon. A few such exact calculations (Brown et al 1954, 1956, 1957; Johnson et al 1968, 1969, 1975, 1976, Kissel et al 1978, 1980) have been made in recent years. These accurate calculations would have to be carried out separately for each electron shell of the atom. This is difficult enough for coherent scattering where the final state is the same as the initial one, but is much more difficult for incoherent scattering where the final state can be any one of the discrete states or the continuum. Thus, most of the presently available theories for coherent and incoherent scattering are based on approximate models of the charge distribution within the atom (Davisson 1968). We now describe below the theory of various coherent photon scattering processes with special attention given to the calculation of Rayleigh scattering cross sections as they will be of particular interest in the energy region considered here.

2.3 Calculations of Rayleigh scattering cross section

Rayleigh scattering is an atomic process in which the incident photon is absorbed by a bound atomic electron. This electron is raised to a higher energy state, and a second photon of the same energy as the incident photon is then emitted, and the excited electron returns to its original state. It is also called elastic (coherent) scattering, or electron resonance scattering. This process predominates at energies below 1 MeV and at small
scattering angles. Then the recoil momentum imparted to the atom does not produce any excitation or ionization.

In the lowest non-vanishing order of perturbation theory, Rayleigh scattering is a two vertex process described by the two Feynman diagrams displayed in Fig. 2.1a and 2.1b. The double lines indicate that the electron in the initial, intermediate, and final states is within the influence of the atomic field. Therefore bound state wave functions must be used to describe the electron in the initial and final states, whereas in the intermediate states, bound state and Coulomb continuum state wave functions must be used. As a result the treatment of Rayleigh scattering is difficult.

![Feynman diagram](image)

(a) (b)

Fig. 2.1. Feynman diagram. (a) absorption of the incoming photon first and (b) emission of the incoming photon first.

Rayleigh scattering can also be formulated in terms of conventional second order, three dimensional perturbation theory, which predicts a transition amplitude given by the expression

\[
M = \sum_n \frac{\langle f | \delta H | n \rangle \langle n | \delta H | i \rangle}{E_f - E_n \pm \hbar \omega}
\]

Because the scattering is elastic, the final state \(|f\rangle\) is equal to the initial state \(|i\rangle\). The summation is over all intermediate states \(|n\rangle\) and integration over intermediate states in the continuum. The (+ ve) sign refers to absorption of the incoming photon first (Fig. 2.1a) and the (− ve) sign refers to emission of the outgoing photon first (Fig. 2.1b). The perturbation Hamiltonian is given by

\[
\delta H = e \alpha A(x),
\]
where \( A \) is the vector potential, \( \alpha \) is the Dirac matrix, which is expressed in terms of the 2 \( \times \) 2 Pauli matrices as

\[
\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}
\]  

(2.6)

In the non-relativistic limit,

\[
\delta H = \frac{e}{mc} (p \cdot A) 
\]  

(2.7)

\[
\delta H = -i \frac{e\hbar}{mc} (\nabla \cdot A). 
\]  

(2.8)

In addition to the difficulties of using bound state wave functions and of summing over an infinite number of intermediate states, an accurate treatment of Rayleigh scattering must take into account: (i) The two cases of absorption first or emission first represented by the two diagrams in Figs. 2.1a and 2.1b. (ii) Two possible spin orientations of the scattering electron. (iii) The two possible polarizations of the incident photon and the two polarization of the out going photon, leading to four possible cases. It is usually assumed that the incident radiation is unpolarized and ignoring the polarization of the out going photon the transition probability is averaged over incident polarizations and summed over final polarizations. (iv) The scattering from each atomic sub-shell takes place separately. Because, the bound state wave functions describing electrons in different sub-shells are not the same, a separate calculation must be performed for each sub-shell.

The first calculation of the photon elastic scattering cross sections by a free electron was made by J J Thomson in 1906. These cross sections are called the “Thomson scattering cross sections”. However as the incident energy increases the atomic electrons are no longer free because their motion is so rapid that they must be characterized by a stationary charge distribution. The photon scattering by such bound electrons is called “coherent scattering”. In the energy region of current interest, this is only due to “Rayleigh scattering”.

### 2.3.1 Scattering by a free electron

We consider an electron of mass \( m \) and charge \( e \) in the path of a plane polarized monochromatic electromagnetic wave in vacuum. Considering only the action of the electric field \( E \) and assuming that this force \( F \) is balanced by the Newtonian force on the charge, we can write,

\[
m \frac{d^2 r}{dt^2} = eE
\]  

(2.9)

Since in a plane wave,
\[ E = E_0 \exp[-i(\omega t - k \cdot r)] \] (2.10)

This equation becomes
\[
\frac{d^2 r}{dt^2} = \frac{eE_0}{m} \exp[-i(\omega t - k \cdot r)]
\] (2.11)

This implies that the acceleration, velocity and displacement of the charge are all in the same direction as \( E_0 \) which itself is constant and that the charge is oscillating sinusoidally.

Now if the incident electromagnetic wave in which the electric vector is along the X-axis (as it is plane polarized) is moving along the Z-axis, then the acceleration in the X-direction is given by
\[
\frac{d^2 x}{dt^2} = \frac{eE_0}{m} \exp[-i(\omega t - kz)]
\] (2.12)

so that the displacement \( x \) at time \( t \) will be given by
\[
x = \frac{eE_0}{m\omega^2} \exp[-i(\omega t - kz)]
\] (2.13)

Now since an oscillating electric charge behaves like an oscillating electric dipole with dipole moment
\[ p = ex \] (2.14)

it follows that
\[
p = -\frac{e^2 E_0}{m\omega^2} \exp[-i(\omega t - kZ)]
\] (2.15)

or
\[
p_0 = \frac{e^2 E_0}{m\omega^2}
\] (2.16)

But as the average energy radiated per sec. per unit area in a normal direction by an oscillating dipole is given by
\[
S = \frac{1}{4\pi\varepsilon_0} \frac{\omega^4 P_0^2}{8\pi c^3 r^2} \sin^2 \theta
\] (2.17)

In terms of \( P_0 \) this becomes
\[
S = \frac{1}{4\pi\varepsilon_0} \frac{q^4 E_0^2}{8\pi m^2 c^3 r^2} \sin^2 \theta
\] (2.18)

Since the average value of the Poynting vector is given by
The differential scattering cross section is given by
\[
\frac{d\sigma}{d\Omega} = \frac{S^2}{\langle S \rangle} = \left( \frac{e^2}{4\pi \epsilon_0 mc^2} \right)^2 \sin^2 \theta
\]
(2.20)

where \( r_0 \) is called the classical electron radius.

The total scattering cross section will be
\[
\sigma_T = \int \frac{d\sigma}{d\Omega} d\Omega
\]
(2.22)

After suitable integration this yields
\[
\sigma_T = \frac{8\pi}{3} r_0^2
\]
(2.23)

This result was first derived by Thomson and so after his name it is called Thomson scattering cross section.

### 2.3.2 Scattering by a bound electron (Form factor approximation)

The form factor approximation, which was originally derived classically to correct the Thomson formula for scattering by a distribution rather than a point charge, is still used extensively today to predict Rayleigh scattering amplitudes in the x-ray and \( \gamma \) ray region (Kissel et al 1980). In fact, all the present tabulations of elastic scattering cross sections (Hubbell et al 1975, Hubbell and Overbo 1979) use this approximation to estimate the contribution made by Rayleigh scattering. It is particularly attractive due to its relative ease of calculation, requiring simply the evaluation of a radial integral over the atomic charge density.

The form factor was also derived using non-relativistic quantum mechanics (Sommerfeld 1939) followed by relativistic derivations due to Franz (1935,1936) and Bethe (1952). The form factor for an atom of atomic number \( Z \), \( F(q, Z) \) is defined (see e.g. Nelms and Oppenheim 1955) as the matrix element
\[
F(q, Z) = \sum_{j=1}^{Z} \langle \psi_0 | \exp(iq \cdot r_j) | \psi_0 \rangle
\]
(2.24)
Where $\psi_0$ is the ground state wave function of the atom, $q$ is the moment transfer vector with magnitude $q = \frac{2K}{\hbar} \sin \theta / 2$. $K$ is the photon energy in units of electron rest energy and is the radius vector from the nucleus to the $j$th electron. The matrix element in equation (2.24) can be evaluated in the position representation

$$\sum_{j=1}^{Z} \langle \psi_0 | \exp(iq \cdot r_j) | \psi_0 \rangle = \sum_{j=1}^{Z} \exp(iq \cdot r_j) \left[ \int | \psi_0 \rangle^2 \prod_{i \neq j} d^3 r_i \right] d^3 r_j$$

(2.25)

the quantity in the curly brackets is the probability density of the $j$th electron. Defining

$$\rho(r_j) = Z \int | \psi_0 \rangle^2 \prod_{i \neq j} d^3 r_i$$

(2.26)

$F(q, Z)$ then becomes

$$F(q, Z) = \frac{1}{Z} \sum_{j=1}^{Z} \rho(r_j) \exp(iq \cdot r_j) d^3 r_j$$

$$= \int \rho(r) \exp(iq \cdot r) d^3 r$$

(2.27)

Where $\rho(r)$ is the total electron-density at $r$. It may be noticed that the form factor is essentially the Fourier transform of the electron-density. Hence, by performing the inverse Fourier transformation, the electron-density can be expressed in terms of the integral over the form factor, i.e.,

$$\rho(r) = 2\pi^{-3} F(q, Z) \exp(iq \cdot r) d^3 q$$

(2.28)

For a spherically symmetric atom the angular integration in equation (2.27) can be performed resulting in (see e.g. Debye 1930, and Pirenne 1946),

$$F(q, Z) = 4\pi \int_{0}^{z} \rho(r) \frac{\sin qr}{qr} r^2 dr$$

(2.29)

The variable $x$, which is proportional to the momentum transfer $q$, is often used in place of $q$ in recent tabulations (Hubbell et al 1975; Hubbell and Øverbø 1979) and is defined by

$$x = \sin(\theta / 2) / \lambda (\text{Å})$$

(2.30)

The momentum transfer variable $x$ may be converted from the $q$-argument in mc units by multiplying by the factor 20.60744. In terms of the $x$-argument, the form factors $F(x, Z)$ with the assumption that the atom is spherically symmetric is

$$F(x, Z) = 4\pi \int_{0}^{x} \rho(r) \frac{\sin(4\pi xr)}{4\pi xr} r^2 dr$$

(2.31)
The form factor so defined may be understood either to describe coherent scattering from all the bound electrons, as characterized by a charge distribution $\rho(r)$, or the contribution to scattering due to a given sub-shell characterized by its charge distribution.

In the form factor approximation, the Rayleigh scattering amplitudes in the circular polarization description are given by

$$A_R^{NSF} = -\frac{r_e}{2} (1 + \cos \theta) F(q, Z) \quad (2.32)$$

and

$$A_R^{SF} = \frac{r_e}{2} (1 - \cos \theta) F(q, Z) \quad (2.33)$$

Where $r_e = e^2 / mc^2$ is the classical electron-radius. Hence, the differential cross section for the Rayleigh scattering of unpolarized photons through an angle $\theta$ and averaged over final polarizations may be written as,

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

$$= \frac{d\sigma_T}{d\Omega} |F(q, Z)|^2 \quad (2.34)$$

Thus, the differential Rayleigh scattering cross section in the form factor approximation can be expressed as the product of two factors. The first factor is the expression for the Thomson scattering cross section $\frac{d\sigma_T}{d\Omega}$) which concerns the probability that the photon is deflected by a certain angle and transfer to the electron a corresponding amount of momentum as though the electron were free. The second factor is the square of the atomic form factor, which takes into account the electron-charge distribution and expresses the probability that the $Z$ electrons of an atom take up a recoil momentum without absorbing any energy.

### 2.3.2a Calculation of form factor

To calculate the form factor, the ground state wave function $\psi_0(r_1 ... r_2)$ for the atom must be known. hydrogen is the only atom for which it is known exactly. If the coulomb wave function describing the ground state of hydrogen is inserted into equation (2.29), the integration can be performed analytically, resulting in (Pirenne 1946),

$$F(q, Z = 1) = [1 + \left(\frac{a_0 q}{\lambda}\right)^2]^2 \quad (2.35)$$

in which $a_0 = \hbar^2 / me^2 = 0.529177$ Å is the first Bohr radius,
or, from equation (2.31), we get

$$F(x, l) = [1 + 4\pi^2 a_0^2 x^2]^{-2}$$  \hspace{1cm} (2.36)

For all other atoms, we have to take recourse to different approximate models of charge distribution within the atom, such as Thomas-Fermi, Hartree-Fock, and others to determine the atomic form factor (Thomas 1927; Fermi 1928; Hartree 1928; Fock 1930, 1934; Slater 1951). White Grodstein (1957) has discussed several of these approximate models in detail of these various models, only the Thomas-Fermi and Hartree-Fock-Slater models are important from the standpoint of applicability and accuracy.

### 2.3.2b Thomas-Fermi statistical model

The distribution proposed by Thomas (1927) and Fermi (1928) considers the electrons as a gas surrounding the nucleus, with a charge density which is a function only of the distance from the nucleus. The average charge density \(\rho(r)\) is a radial function of the potential \(V(r)\) given by

$$\rho(r) = \frac{8\pi e}{3h^3} [2meV(r)]^{\frac{1}{2}}$$  \hspace{1cm} (2.37)

which in turn can be substituted in the Poisson's equation

$$\nabla^2 V(r) = 4\pi \rho(r)$$

to get,

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dV(r)}{dr} \right) = \frac{32\pi^2 e}{3h^3} [2meV(r)]^{\frac{3}{2}}$$  \hspace{1cm} (2.38)

The above equation is to be solved for \(V(r)\) under the condition that \(\lim_{r \to \infty} V(r) = 0\) and that \(\lim_{r \to 0} V(r) = Ze\). Thomas (1927) solved this equation numerically for the case of Cesium (\(Z=55\)) and obtained \(V(r)\). The average charge density \(\rho(r)\) is in turn obtained by using equation (2.37) and thence \(F(x, Z)\) by using equation (2.31), again with assumed spherical symmetry. The Thomas-Fermi charge distributions for different atoms are related to each other such that once \(F(x', Z_0)\) has been calculated for a “standard” atom \(Z_0\) (e.g. Cs, \(Z_0 = 55\)), \(F(x, Z)\) for any other atom \(Z\) is given by

$$F(x, Z) = \frac{Z}{Z_0} F(x', Z_0)$$  \hspace{1cm} (2.39)

Where \(x\) is the desired argument and if \(x\) is the tabulated argument for \(Z_0\) then

$$x' = x \left( \frac{Z}{Z_0} \right)^{\frac{1}{3}}$$  \hspace{1cm} (2.40)
Also, exchange effects have been incorporated into the Thomas-Fermi model by Dirac(1930), taking into account the fact that electrons are identical particles which must be described by a totally anti symmetric wave function.

2.3.2c Hartree-Fock model

The most accurate computations of wave functions of many-electron atoms are based on the self consistent field (SCF) method of Hartree (1928). This is an independent particle model in which each electron is assumed to be in the field of the nucleus and in an average field due to the other electrons. Thus, the charge distribution $\rho(r)$ can be written

$$\rho(r) = \sum_{j=1}^{Z} \rho_j(r) = \sum_{j=1}^{Z} \psi_j^*(r)\psi_j(r)$$  \hspace{1cm} (2.41)

Where $\rho_j(r)$ is the charge density distribution of the $j$th electron and $\psi_j(r)$ is its wave function. The Hartree scheme has been generalized by Fock (1930, 1934) to include the effects of exchange, and Slater (1951) has shown that the Hartree and Hartree-Fock wave functions arise out of variational treatments in which the wave functions of the many electron atom is assumed to be a product of individual electron wave functions. Recently, Hubbell et al (1975) and Hubbell and Overbo (1979) have published respectively the tables of non-relativistic and relativistic atomic form factors for all elements $Z=1$ to 100 over wide range of momentum transfer values ($x = 0.01-10^9\text{Å}^{-1}$).

2.3.3a Qualitative features predicted by form factor approximation

Although form factor predictions are often wrong in quantitative detail, their qualitative features give considerable insight into the behavior of the Rayleigh amplitudes (Kissel et al 1980). The behavior of the total atom Form-factor $F(q) = \sum F_i(q)$ can be better understood by considering the behavior of its components $F_i(q)$ contributed by each particular electron, sub-shell or shell, as a function of momentum transfer. For zero momentum transfer, the integral for a sub-shell form factor reduces to an integral over the corresponding sub-shell charge density and is equal to the number of electrons in that sub-shell. As the momentum transfer increases, the value of $F_i(q)$ remains approximately constant until the typical momentum $q_{typ}$ of electrons in that sub-shell is reached. This $q_{typ}$, for inner shells such as K-shell, is inversely proportional to the radius of that shell. Beyond this, $q_{typ}$, the magnitude of the form factor becomes small. For nodeless sub-shell (such as the K-shell), the value of the form factor for $q > q_{typ}$ decreases monotonically. For sub-shells with nodes (such as the L_1 sub-shell), there is a region of more rapid variation or oscillation for $q > q_{typ}$ before reaching the asymptotic region, where $F_i(q)$ decreases monotonically. For large $q$, $F_i(q)$ decreases rapidly with $q$ (but most slowly for $l = 0$) and is larger for heavy atoms. Thus, for small momentum transfers, each sub-shell
contributes to the total-atom form factor proportional to the number of electrons in that sub-shell. As the momentum transfer increases, the contributions to the total atom form factor of more and more of the outer electrons become small. This process continues until the K-shell's typical momentum ($Z\alpha$) is exceeded. Beyond this point contributions to the total atom form factor due to all sub-shells are monotonically decreasing. In this asymptotic region the S states ($l=0$) dominate, with the shells yielding the largest contribution. Therefore, for a heavy element such as lead, the form factor approximation predicts that the K-shell dominates at large momentum transfer, with the next largest contribution coming from the L₁ sub-shell and so on.

The differential Rayleigh scattering cross sections are obtained from the atomic form factors using equation (2.34). The range of momentum transfers possible for a fixed photon energy $\omega$ are $0 \leq q \leq 2 \omega$. Thus, for low photon energies, the form factor predicts little variation in the differential scattering cross sections. For high photon energies, the form factor is equal to the number of electrons in the forward direction but becomes very small at the backward angles, giving a highly forward peaked angular distribution. For small $q$, the cross section varies as $Z^2$, while for large $q$ it will vary as $Z^8$.

The form factor approximation also predicts the importance of screening of the nuclear charge by the atomic electrons. For small $q$, the form factor reduces to the number of electrons, which is independent of the potential used and suggests that screening effects are small. For large $q$, small radial distances are most important. For small radial distances, screening corrections to the Coulomb wave functions appear only in their normalization (Pratt and Tseng 1972). Thus, the form factor approximation predicts that, for large $q$, screening effects in the matrix elements can be expressed as the squared ratio of screened to unscreened bound state wave function normalizations.

**2.3.3b Limitations of form factor approximation.**

The range of validity of the form factor approximation for the description of the elastic photon scattering by bound electrons is limited (Kissel et al 1980). The effects of binding, although crucial in the low energy scattering of photons, are neglected by the form factor approximation. At high energies one might expect that binding effects would become less important and that scattering would approach that for free electrons. In fact, corrections of the order of $(Z\alpha)^2$ remain at all energies and angles, because of the use of zero-order Born approximation for intermediate states. For a given atomic electrons, the form factor approximation is not valid for larger angles (high momentum transfers) or lower energies (compared with electron binding energy). With decreasing energy, the approximation first fails for inner electrons (or larger binding energies) which, however, give a dominant contribution at large momentum transfers (larger angles at higher energies). In addition,
corrections due to relativity have been neglected, again implying deviations of the form factor for the inner shells of heavy atoms or for high photon energies.

2.3.3.3 Dispersions corrections to the form factor

All deviations of the form factor approximations have assumed that the photon energy \( \omega \) is much greater than the electron binding energy \( \varepsilon \) (\( \omega >> \varepsilon \)). But in many cases of interest the photon energy is comparable to the binding energy of the electron, especially for medium- and high-\( Z \) atoms where K-shell binding is tens of keV. In such cases, the form factor \( F(q) \) may be replaced by a structure factor \( F^D \) given by,

\[
F_D = F(q) + (\Delta F') + i(\Delta F'')
\] (2.42)

The corrections \( \Delta F' \) and \( \Delta F'' \) have been referred to as the dispersion corrections to the form factor, anomalous scattering factor or anomalous dispersion corrections. The word "anomalous" refers to the observed rapid variations of the photon energy around \( \omega = \varepsilon \). Cromer and Liberman (1970) performed numerical calculations of the anomalous scattering factors using Dirac-Hartree-Fock-Slater (DHFS) wave functions. However, these anomalous scattering factors have been derived for the case of forward scattering only (i.e. \( \theta = 0 \)). It has been the practice to transform these zero angle corrections to non-zero value of \( \theta \) by multiplying the zero angle value of \( \Delta F' \) and \( \Delta F'' \) for each electron by its corresponding form factor, which is unity at \( \theta = q = 0 \). These forward angle dispersion corrections are usually applied (James 1965) at other angles through the use of the following expression,

\[
F_D = F_0 + \sum_i \Delta F'_i \frac{F_0'(q)}{F'(0)} + \sum_i \Delta F''_i \frac{F_0''(q)}{F''(0)}
\] (2.43)

Where \( F_0'(q) \) is the form factor per electron for the \( i \)th sub-shell. However, this procedure of transforming the zero angle corrections to other angles has not been justified.

2.3.4 Modified Form Factor

Within the relativistic framework, an electron binding correction to the form factor approximation was originally suggested by Franz (1935, 1936) and the resulting approximation later developed is known as the modified form factor (MFF) approximation. Brown and Mayers (1957) compared this modified form factor due to Franz with their numerical scattering amplitudes and found that it gave improved results. The modified form factor is defined by

\[
g(q, Z) = \sum_{j=1}^{Z} g_j(q, Z)
\]
Where \( \varepsilon_j \) is the binding energy of the \( j \)th electron and \( V(r_j) \) is the electrostatic potential at \( r_j \), both in units of \( mc^2 \). For the spherically symmetric charge distribution, \( g(q, Z) \) is,

\[
g(q, Z) = \sum_{j=1}^{Z} 4\pi \rho(r) \frac{\sin qr}{qr} \frac{1}{1 - \varepsilon_j - V(r)} r^2 dr
\]  

(2.45)

The additional denominator factor has its origin in the Green's function propagator of the intermediate states and represents a binding corrections. In the modified form factor approximation, the differential cross section for the Rayleigh scattering of unpolarised photons is obtained by replacing \( F(q, Z) \) by \( g(q, Z) \) in equation (2.34).

A general investigation of the validity of the modified form factor has been carried out by Kissel et al (1978, 1980, 1983) and has resulted in the conclusion that the modified form factor is superior to the form factor in a wide range of momentum transfers. For the K-shell of light atoms, the modified form factor continues to provide good predictions for momentum transfers up to 0.5 \( mc \) (10 \( \text{Å}^{-1} \)). Errors in the K-shell amplitudes of light Z atoms predicted by the modified form factor are at the 10% level by about 5\( \varepsilon_K \), the 5% level by about 10\( \varepsilon_K \), and 1% level by about 25\( \varepsilon_K \). For the K-shell of medium and heavy atoms, the predictions of the modified form factor at finite energies is a major improvement over the ordinary form factor, and this improved agreement also extends to the higher momentum transfer of 0.5 \( mc \). Errors in the K-shell amplitudes of heavy Z elements predicted by the modified form factor are at the 10% level by about 3\( \varepsilon_K \), the 5% level by about 5\( \varepsilon_K \) and the 1% level by about 10\( \varepsilon_K \). Improved agreement over the form factor is also found in the predictions of the modified form factor for higher shells for \( \omega \geq \varepsilon_K \). Thus, accurate total-atom differential scattering amplitudes may be calculated using the modified form factor approximation for all shells of all atoms for forward angles and photon energies greater than K-shell binding.

Non-relativistic Hartree-Fock wave functions of Hubbell et al (1975) reported the coherent and incoherent scattering cross section of elements. Also, using relativistic Hartree-Fock wave functions of Hubbell and Overbo (1979) have tabulated coherent as well as incoherent scattering cross section of elements from \( Z = 1 \) to 100. These values have been used in the present study for the purpose of comparison.

**2.3.5 S-matrix calculation**

The scattering matrix (commonly called the S-matrix) is an operator which connects the final state of a time dependent system with that of the initial state. Therefore, for Rayleigh
scattering, the matrix element \( S_{fi} = \langle f | S | i \rangle \) represents the amplitude of a specific stationary state \( |f\rangle \) that evolved through scattering from the initial state \( |i\rangle \). Such scattering calculations usually start with atomic potential obtained in the independent particle approximation, which assumes that the independent electrons interact electrostatically with a central potential resulting from the charge distribution of the nucleus and electrons. In independent particle approximation, the amplitude for scattering \( (S_{fi}) \) of each atomic electron should be calculated separately. Numerical methods for the calculation of the Rayleigh scattering amplitudes in this way were first developed by Brown and his group. The calculation starts with the Feynman-Dyson representation of scattering in second order, as shown in Fig.2.2. The effect of binding in the intermediate state (times between \( t_1 \) and \( t_2 \) in Fig 2.2) is important (it has been neglected in form factor approximation) and was

Fig. 2.2. Feynman diagram for lowest order contributions to the Rayleigh scattering amplitude: (a) the "Absorption first" (b) the "Emission first" contribution.

explored analytically in the relativistic theory of Brown and Woodword (1952). This calculation was done in Born approximation. The realization that higher order Born correction terms are important in calculating the Rayleigh scattering amplitude led to the development of numerical partial wave methods (Brown et al., 1955). Brown and coworkers (Brenner et al., 1955; Brown and Mayers; 1956, 1957) applied this numerical method to the elastic scattering of 0.32, 0.64, 1.28, 2.56 \( mc^2 \) (\( mc^2 \sim 511 \) keV) from the K-shell electrons of mercury (\( Z = 80 \)). The atomic potential assumed in these calculations was a point Coulomb potential. Later Cornille and Chapdelaine (1959) extended Brown's calculation for 2.62 MeV scattering from the K-shell electrons of mercury. These calculations were very lengthy in terms of the computers available at that time and the calculations were limited to only the K-shell of only one atom and for five photon energies.
Later work has suggested that for high energies and back angles, not enough partial waves and multipoles were included.

S-matrix calculation needs increasing number of multipoles to converge for a given sub-shell of electrons as the photon energy increases. This can be related to the binding energy of the electron sub-shell. The number of photon multipoles to be included increases as the ratio of incident photon energy to the binding energy of the sub-shell electron increases. Therefore, it is often found to be impractical to calculate Rayleigh scattering amplitudes for all electrons using S-matrix calculation for an extensive set of cases, particularly for high Z elements and for high photon energies. The usual procedure in such cases is to calculate using numerical partial waves for the contributions for which the scattering is significant (inner electrons) and then to calculate the contributions from outer electrons by some approximate method. The original and most common procedure is to use the amplitude predicted by modified form factor. It makes modified form factor as an useful tool to calculate outer shell contributions at the level of 1% since in most cases incident photon energy is very high compared to the binding energy of the outer shell. For photon energies below the K-edge, either all the outer electrons are to be included using S-matrix calculations or modified form factor predictions may be used with anomalous correction including (Zhou et al., 1990).

This method of calculating Rayleigh amplitudes using partial wave methods is often referred to as "exact" calculation, which may require some explanation. As understood from figure 2.2, calculation of Rayleigh scattering amplitudes must include binding effects in the initial, final and intermediate states. The numerical partial wave calculations included the binding effects in these states exactly to all orders in the independent particle approximation potential and hence are referred to as "exact" calculation. However, one may realize that as the calculation was done in the lowest non-vanishing order in the S-matrix expansion, electron correlation (important for very low energy photons) was neglected, making the calculation far from exact. It will be seen in the next section that correlation effects are not very important in the region of photon energies of this article. Nonetheless, such predicted independent particle approximation scattering amplitudes and cross sections are so far the most accurate. The calculated scattering amplitudes are accurate within an order of 1%.