CHAPTER 1

RECENT DEVELOPMENTS IN THE THEORIES OF PHOTON SCATTERING.

1.1. INTRODUCTION.

The scattering of photons in matter is divided into two classes:

i) The scattering of photons by atomic electrons.

ii) The scattering of photons by nuclei or fields.

At lower photon energies, the contribution of the scattering by nuclei or fields is very small compared to that by the atomic scattering, which can again be divided into two categories: Incoherent(inelastic) scattering and coherent(elastic) scattering, known as atomic Rayleigh scattering.

1.1.2. Incoherent(inelastic) scattering.

In this scattering reaction, the incident photon undergoes a change in both momentum and energy and the state of the scattering atom after the scattering is excited or ionized. The processs is incoherent, because the wavelengths of scattered radiation from different electrons are different resulting in no difinite phase relation between the scattered radiation from different electrons. The incoherent scattering cross section is the probability of occurrence of such an intraction with an electron. If a_i is the amplitude for incoherent scattering by the i th atomic electron, then the probability of incoherent scattering by the atom of atomic number Z is $\sum_{i}^{Z} |a_i|^2$. This means that the scattering cross section for the entire atom is not Z times the scattering cross section per electron, because a_i's are different due to differing binding of electrons in the atom. For sufficiently high photon energies, when the binding energy of atomic electrons can be neglected, each scattering electron can be considered as free, all amplitudes of scattering ~~am~~ by the free electrons are

the same 'a' and the probability is $Z|a|^2$. The value of the incident photon energy above which each atomic electron can be considered as free depends on the angle of scattering and Z. Incoherent scattering of photons by free electrons is known as Compton scattering. The assumption of free electron is valid when for scattering at an angle θ of photon with energy $E = h\nu$ the momentum transfer to the electron $q = 2E/c \sin \theta/2$ (for $\nu - \nu' \simeq 0$) is very large compared to the initial momentum of the electron in the atom. Taking the approximate value $Z \propto mc$ for the momentum of a k-electron, this condition can be written as $q = 2k \sin \theta/2 \gg Z\alpha = Z/137$. Here, q is expressed in units of mc, k is, photon energy in unit of mc^2, the electron's rest energy, $\alpha = e^2/\hbar c = 1/137$, and $h\nu'$ is the energy of the scattered photon.

The theory of Compton scattering was formulated by Klein and Nishina (K 29) using Dirac's relativistic theory of the electron. Interaction between a photon and a free electron, in the quantum electrodynamics, involves an initial state, an intermediate state and a final state. Momentum and energy are conserved between the initial and final state but in the intermediate state, in requirement to the theory, only momentum should be conserved. During the intermediate state an electron at rest can emit a virtual photon, violating the ordinary energy conservation law, and then can absorb an incident photon. Consequently the photon scattering process by a free electron at rest is the sum of two processes (i) the incident photon $h\nu$ is absorbed by the electron. In the intermediate state, the electron momentum is $h\nu/c$ and no photon is present. The electron emits the photon $h\nu'$ in the transition to the final state, (ii) The electron emits the photon $h\nu'$. In the intermediate state, the electron momentum is $-h\nu'/c$ and two photons $h\nu'$ and $h\nu$ are present. The electron absorbs $h\nu$ in transition to the final state. This representation of the scattering mechanism was used to obtain the well-known Klein-Nishina differential cross section per electron for unpolarized

incident photon beam.

$$\sigma_{K\text{-}N}(\theta) = \frac{r_0^2}{2} \frac{1 + \cos^2\theta}{[1 + k(1-\cos\theta)]^2} \left\{ 1 + \frac{k^2(1-\cos\theta)^2}{(1+\cos^2\theta)[1 + k(1-\cos\theta)]} \right\} \qquad (1.1)$$

Here $\sigma_{K\text{-}N}(\theta) = \frac{d\sigma}{d\Omega}$ in cm^2/electron stradian of solid angle is the cross section for scattering of photons in $d\Omega$ at an angle θ. $r_0 = e^2/mc^2/cm^2 = 2.82 \times 10^{-13}$ cm is the classical radius of electron. For small incident photon energies and scattering angles, the formula can be written approximately as

$$\sigma_{K\text{-}N}(\theta) = \frac{r_0^2}{2} \frac{1 + \cos^2\theta}{1 + 2k(1+\cos\theta)} \qquad (1.2)$$

As $k \to 0$

$$\sigma_{K\text{-}N}(\theta) \longrightarrow \frac{r_0^2}{2}(1 + \cos^2\theta) = \sigma_T(\theta) \qquad (1.3)$$

where $\sigma_T(\theta)$ is the differential cross section for Thomson scattering. The total cross section for Compton scattering by an electron

$$\sigma_{TOT} = \int \sigma_{K\text{-}N}(\theta)\, d\Omega = 2\pi \int_0^{\pi} \sigma_{K\text{-}N}(\theta) \sin\theta\, d\theta \qquad (1.4)$$

values of $\sigma_{K\text{-}N}(\theta)$ and σ_{TOT} were computed and tabulated by Nelms (N 53) and Evans (58, 68). The cross section for an atom is Z times the cross section for a single electron.

When the binding energy of the scattering atomic electrons cannot be neglected, an exact calculation of incoherent scattering cross section proved very difficult so far. In all approximate theory, the differential cross section per atom is formulated as

$$\sigma_{\text{INCOH.}}(\theta) = \sigma_{K\text{-}N}(\theta) \cdot Z \cdot S(\underline{q}, Z) \qquad (1.5)$$

where the function $S(\underline{q}, Z)$ [to be written hereafter simply S] is called incoherent scattering function. It represents the probability that the atom be raised to an excited or ionised state as a result of one of atomic electrons receiving a momentum q.

If the electron receiving the momentum q does not make a transition, then the atom as a whole absorbs the momentum, and because of relatively large atomic mass, the momentum absorbtion q means negligible energy absorption.

For high energy photon interacting with the loosely bound electrons in low Z atoms, each atomic electron acts as a free and stationary electron and the incoherent scattering function S approaches its maximum value 1.

Evaluations of S is based on the expression

$$S(\underline{q},Z) = \frac{1}{Z}\sum_{\epsilon>0} |F_\epsilon(\underline{q},Z)|^2 \qquad (1.6)$$

where F_ϵ is the generalised form factor to include excited states and defined as

$$F_\epsilon(\underline{q},Z) = \langle\epsilon| \sum_j^Z e^{i\,\underline{q}\cdot\underline{r}_j/\hbar} |0\rangle \qquad (1.7)$$

Here $|0\rangle$ represents the ground state of the atom, $\langle\epsilon|$, an excited state and r_j represents position of the j the electron relative to the nucleus of the atom. The sum of (1.6) is taken, excluding the ground state $\epsilon = 0$, to mean a sum over the excited states and an integral over the continuum states. The expression for S $(\underline{q},Z)$ can be written as

$$\begin{aligned} S(\underline{q},Z) &= \frac{1}{Z}\left\{\sum_{\epsilon=0}\langle 0|\sum_j e^{-i\,\underline{q}\cdot\underline{r}_j/\hbar}|\epsilon\rangle\langle\epsilon|\sum_j e^{i\,\underline{q}\cdot\underline{r}_j/\hbar}|0\rangle \right. \\ &\quad \left. - \left|\langle 0|\sum_j e^{i\,\underline{q}\cdot\underline{r}_j/\hbar}|0\rangle\right|^2\right\} \\ &= \frac{1}{Z}\left\{\langle 0|\left|\sum_j e^{i\,\underline{q}\cdot\underline{r}_j/\hbar}\right|^2|0\rangle - |F(\underline{q},Z)|^2\right\} \end{aligned} \qquad (1.8)$$

where $F(\underline{q},Z)$ is the common coherent scattering form factor $\langle 0|\sum_j^Z e^{i\,\underline{q}\cdot\underline{r}_j/\hbar}|0\rangle$ of the atom. S can be evaluated exactly only for hydrogen atom where ground state wave function $\langle 0|$ is known exactly.

$$\begin{aligned} S &= 1 - |F(q, Z=1)|^2 \\ F(q, Z=1) &= \left\{1 + \frac{aq}{2}\right\}^{-2} \end{aligned} \qquad (1.9)$$

where a = $\hbar^2/mc^2 = 5.29 \times 10^{-9}$, Bohr radius. For all other atoms approximate atomic models have been used to calculate the ground state wave function.

Thomas-Fermi(TF) Model.

This statistical model,valid for high Z atoms, is based on treating the atomic electrons as a Fermi gas at zero temperature confined to a region by spherically symmetric atomic potential $V(r)$. If $V(r)$ does not change significantly over a distance of the order of deBroglie wavelength of electrons, then the maximum kinetic energy at any distance r from the nucleus is $-V(r)$ and hence the density of Fermi gas is expressed interms of potential. The potential is evaluated using Poisson's law. This procedure leads to an equation for potential

$$x^{1/2} \frac{d^2\chi(x)}{dx^2} = \chi^{3/2}(x) \qquad (1.10)$$

where the quantities x and χ are given by

$$V(r) = \frac{Ze^2}{r}\chi \quad , \quad r = bx \quad , \quad b = 0.885\, a/Z^{1/3} = 0.47/Z^{1/3}\,(\text{Å})$$

with the boundry conditions: $\chi(x) = 1$ at $x = 0$, and $\chi = 0$ at $x = \infty$. Heisenberg (H 31) derived the following expression for S interms of χ and the universal variable v

$$S(v) = 1 - \int_0^{x_0} \left\{\left(\frac{\chi}{x}\right)^{1/2} - v\right\}^2 \left\{\left(\frac{\chi}{x}\right)^{1/2} + \frac{v}{2}\right\} x^2\, dx \qquad (1.11)$$

$$v = \frac{a}{3Z^{2/3}} q = \frac{a}{3Z^{2/3}} \cdot 4\pi \frac{\hbar}{mc} \frac{\sin\theta/2}{\lambda} = \frac{a}{3Z^{2/3}} 4\pi \frac{\hbar}{mc} \chi$$

with $\chi = \frac{\sin\theta/2}{\lambda}$, where λ is the wavelength of incident photon. Bewilogua (B 31), Wheeler and Lamb (W 39) computed numerically S values, as a function of v. These values agree fairly with those calculated from the analytical expression for S obtained by Tietz (T 59) by integrating equation (1.11).

Hartree(H) and Hartree-Fock(HF) self consistent field (SCF) models.

The nonrelativistic H-model is based on the assumption that each electron moves in a central field due to all other electrons and the nucleus. Shröedinger equation is solved for each electron in its own field and the resulting wavefunctions made consistent with the potentials from which they are calculated. The final single-particle wave functions determined are taken to give the wave function for the ground state of the atom through the antisymmetrized product

$$|0\rangle = \prod_{n=1}^{Z} |n\rangle \tag{1.12}$$

where $|n\rangle$ denotes the nth electron state in the ground state of the atom. Substituting (1.12) in (1.8)

$$\begin{aligned} S(\underline{q},Z) &= \frac{1}{Z}\left\{ \prod_{n=1}^{Z}\langle n| \left| \sum_j e^{i\underline{q}\cdot\underline{r}_j/\hbar}\right|^2 \prod_{n'=1}^{Z}|n'\rangle \right. \\ &\quad \left. - \left| \prod_{n=1}^{Z}\langle n| \sum_j e^{i\underline{q}\cdot\underline{r}_j/\hbar} \prod_{n'=1}^{Z}|n'\rangle \right|^2 \right\} \\ &= \frac{1}{Z}\left\{ Z - \sum_{i=1}^{Z} \left| \langle i| e^{i\underline{q}\cdot\underline{r}_i/\hbar}|i\rangle \right|^2 \right\} \end{aligned} \tag{1.13}$$

Evaluated in the position representation, $S(\underline{q},Z)$ becomes,

$$S(\underline{q},Z) = \frac{1}{Z}\left\{ Z - \sum_{i=1}^{Z} |f_i(\underline{q})|^2 \right\} \tag{1.14}$$

where $f_i(\underline{q}) = \int u_i^*(\underline{r})\, e^{i\underline{q}\cdot\underline{r}/\hbar}\, u_i(\underline{r})\, d^3r$

$u_i(\underline{r})$ is the wave function of the ith electron in the ground state of the atom.

The HF model takes for the ground state wave function of the atom, a symmetrized product of single electron wave function u_i expressed in Slater determinant.

$$\psi_o = \frac{1}{\sqrt{Z!}} \begin{vmatrix} u_1(1) & \cdots & \cdots & \cdots & u_Z(1) \\ \vdots & & & & \vdots \\ u_1(Z) & \cdots & \cdots & \cdots & u_Z(Z) \end{vmatrix} \qquad (1.15)$$

with $u_i(j) = u_i(\bar{r}_j)\,\chi_i(\sigma_j)$

where $\chi_i(\sigma_j)$ is the spin function for a single electron. Substituting this in equation(1.8)

$$S(\underline{q}, Z) = \frac{1}{Z}\left\{ Z - \sum_{i=1}^{Z} |f_i(\underline{q})|^2 - \sum_{i \neq j} \delta(m_{si}, m_{sj}) |f_{ij}(\underline{q})|^2 \right\} \qquad (1.16)$$

where $f_{ij}(\underline{q}) = \int u_i^*(\underline{r})\, e^{i\,\underline{q}\cdot\underline{r}/\hbar}\, u_j(\underline{r})\, d^3r$

Basic calculations for evaluation of S on nonrelativistic HF model have been done by Freeman (F 59) and Freeman and Watson (F 59). Some other HF model calculations by Milberg and Brailsford (M 58) for a few low Z atoms are also available. Zerby et al (Z 66) calculated S values for some 27 elements using the basic calculations on H-model for S by James and Brindley (J 31). TF model has been used by Veigele (V 65) to calculate S for a few elements.

Recently Cromer and Mann (C 67) used relativistic SCF HF wave functions for computation of S for all atoms upto Z = 94. These wave functions in numerical form were calculated by Mann (M 67). Cromer's S values form a most comprehensive set so far available.

Incoherent scattering factors from different calculations.

Calculations of incoherent scattering factors S using TF model have some limitations. There are (i) The effects of atomic shells are smoothed out (ii) Near the nucleus, the model predicts high density of electrons, resulting in an underestimate of incoherent scattering at large momentum transfer. (iii) The electron density near the periphery of the atom does not decrease rapidly enough resulting in inaccuracy in S.

These limitations have been removed in the H-model. One of the drawback

of this nonrelativistic model is that the exchange effect is not considered for a system of Fermi particles. However, the theory has been modified in the HF model to take into account exchange effect by using a symmetrized product of single electron wave functions, although the electron motion is not considered relativistically. This drawback has been eliminated in the calculations of S by Cromer and Mann who used numerical non-relativistic wave functions derived on the HF model. So these incoherent scattering factors of Cromer and Mann appear to be the best because of inclusion in the HF model complete exchange effect ~~relativity effect which is particularly important for high Z atoms and large momentum transfers.~~

The total cross section for incoherent scattering is evaluated by integrating equation (1.5) over the full solid angle. This is

$$\sigma_{\text{INCOH.}} = 2\pi \int_0^{\pi} \sigma_{K\text{-}N}(\theta)\, Z\, S(q,Z) \sin\theta\, d\theta \qquad (1.17)$$

Bewilogua (B 31), Wheeler and Lamb (W 39) numerically computed S values using Heisenberg's TF model derivation of S (q,Z). For Z = 100 maximum value of S tabulated corresponds to X = 10 Å^{-1}. H model computations of S after James and Brindley have been given by Compton and Allison (Co 35) for X upto about 1.1 Å^{-1} for a number of elements. The S results on HF model over the range $0.1 \leq X \leq 1.1$ for some elements have been given by Curien. A comparison is given in table 1.1 and graph (fig.1.1) over the X range of earlier calculations. SCF HF model calculations for S have been given by Cromer and Man (C 67, 69) over the range $0 \leq X \leq 61$ Å^{-1} $(0 \leq q \leq 3.89\, mc)$

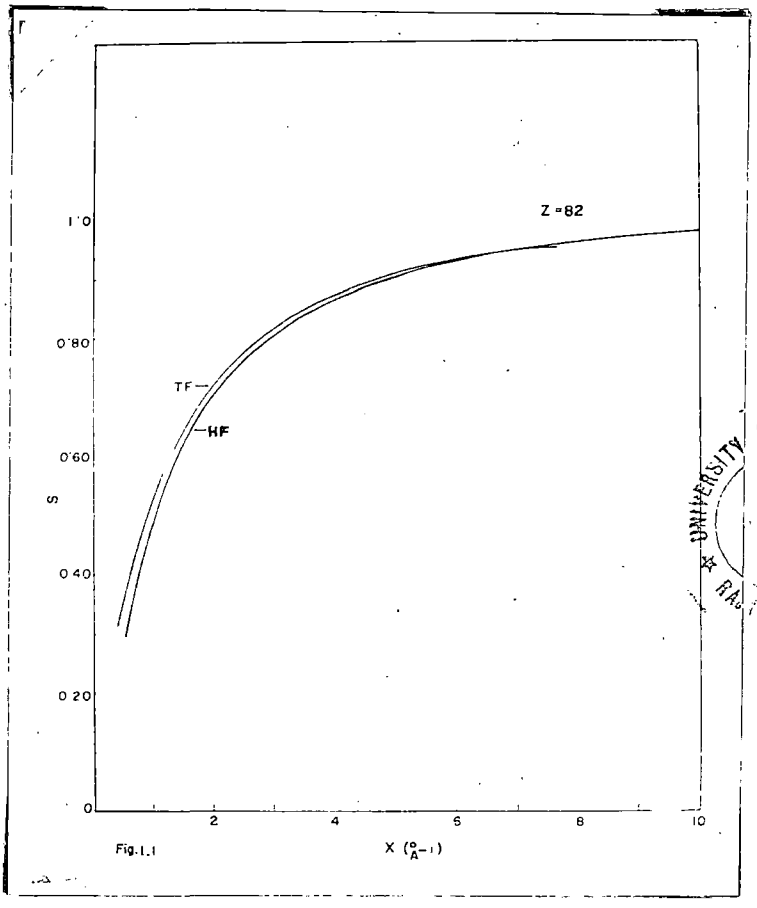

Fig. I.1

TABLE 1.1

Comparison of incoherent scattering factor S (q, Z) from TF, H, HF and Cromer models for some selected elements over a range of momentum transfer q corresponding to $0.1 \leq x \leq 1.1$ (H and HF values are not available for $X > 1.1$)

$$q = 4\pi \cdot \frac{\hbar}{mc} (\text{Å}) \times \frac{\sin\theta/2}{\lambda} (\text{Å}^{-1}) = 4.8 \times 10^{-2} (\text{Å}) \cdot X (\text{Å}^{-1})$$

Z	Method	X (Å^{-1})					
		0.1	0.2	0.3	0.4	0.5	0.6
6	TF	0.38	0.57	0.674	0.74	0.80	0.839
	H	0.33	0.55	0.70	0.75	0.78	0.83
	HF	0.17	0.42	0.59	0.67	0.74	0.78
	Cromer	0.17	0.43	0.64	0.71	0.75	0.78
13	TF	0.28	0.43	0.53	0.62	0.67	0.72
	H	0.22	0.40	0.54	0.65	0.74	0.80
	HF	0.18	0.31	0.40	0.49	0.58	0.65
	Cromer	0.17	0.31	0.40	0.50	0.58	0.65
29	TF		0.30			0.52	
	H	0.17	0.38	0.52	0.59	0.66	0.69
	HF	0.07	0.18	0.28	0.37	0.44	0.51
	Cromer	0.08	0.19	0.29	0.37	0.45	0.51

TABLE 1.1 (Contd.)

Z	Method	X ($\AA^{-1}$)					
		0.7	0.8	0.9	1.0	1.1	1.2
6	TF	0.88		0.909			0.929
	H	0.87		0.90		0.93	
	HF	0.81		0.87		0.91	
	Cromer	0.81		0.87	0.89		
13	TF	0.76		0.82	0.84		
	H	0.83		0.87		0.89	
	HF	0.71		0.79		0.84	
	Cromer	0.71		0.79	0.82		
29	TF				0.72		
	H	0.76		0.79		0.86	
	HF	0.57		0.66		0.72	
	Cromer	0.57		0.66	0.69		

The values of the differential and the total cross sections have been computed by Brown (B 66) using TF model calculations of S (H 31, B 31, W 39). Recently Veigele et al (V 71) have computed values of total scattering cross section using S values of Cromer and Mann over a wide range of momentum transfer corresponding to the X values $0 \leq X \leq 81\ \AA^{-1}$.

1.1.3. Atomic Rayleigh Scattering.

This scattering is elastic, because the state of the atom before scattering is identical to its state after scattering. The scattering electron does not make a transition and so the atom as a whole absorbs the recoil momentum. As the mass of the atom is much larger than the electron mass, this recoil momentum absorption means negligible amount of energy absorption from the incident photon. Consequently, the scattered photon has an energy almost the same as the incident photon.

Under the conditions of elastic scattering the wavelength of the radiation scattered by each electron of the atom is same and a definite phase relation between the scattered radiations from different electrons exists. This means a constructive interference between these coherent radiations. The probability of this coherent scattering by the atom is $\left|\sum_{i=1}^{Z} a_i\right|^2$ where a_i is the amplitude of coherent scattering by the ith electron in the atom. Rayleigh scattering is important when the scattering electrons can be taken to be bound in the atom. For K-shell electrons of an atom with atomic number Z coherent scattering is important if the momentum transfer $q = 2k\sin\theta/2 \ll Z\alpha$. This means, the Rayleigh scattering is significant at low energy of incident photon or at small scattering angle.

Theoretically Rayleigh scattering has been treated by two methods.

a) Exact calculation of scattering amplitudes in the second order perturbation theory.

In an exact calculation, there are difficulties in using bound state wave functions in the initial, intermediate and final states and other considerations that are involved in the exact description of the scattering process. So far, only a few accurate calculations (B 54, B 55, B 57) by this method have been published.

b) Calculation of scattering cross section under the form factor approximation employed by Franz (F 35) and Bethe (Be 52).

Under the approximations that the binding on the electrons in the intermediate state is negligible and $q \ll mc$ for photons of nonrelativistic energy, the differential cross section for the coherent Rayleigh scattering of photons by an atom is written as

$$\sigma_{coH}(\theta) = \left[\tfrac{1}{2} r_0^2 (1+\cos^2\theta)\right] |F(q,Z)|^2 \qquad (1.18)$$

The first factor is the differential cross section for Thomson scattering of the incident radiation by a free point charge. The second factor gives the probability that Z electrons of the atom absorb the recoil momentum q without absorbing any energy from the photon. F (q,Z), the form factor, is defined as $\langle o| \sum_{i=1}^{Z} e^{iq\cdot r_i/\hbar} |o\rangle$ in the notation already explained in the section 1.1.2. For spherically symmetric atoms, the expression for form factor is

$$F(q,Z) = 4\pi \int \rho(r) \frac{\sin qr/\hbar}{(qr)/\hbar} r^2 dr \qquad (1.19)$$

where $\rho(r)$ is the density of electrons at r . The effect of charge distribution in the atom on the elastic scattering by a point charge is expressed through the form factor-part of the cross section formula.

The form factor F (q,Z) has been calculated using TF, H and HFS models. The HF model has been modified by including Slater's approximate exchange potential and the model is known as HFS model.

In the TF model the charge density is given by

$$\rho = \frac{Z}{4\pi b^3} \left[\chi(x)/x\right]^{3/2} \qquad (1.20)$$

in the notation already explained in the section 1.1.2. Using a new variable u given by

$$u = bq/\hbar = b(4\pi/\lambda)\sin\theta/2$$

the form factor F, equation (1.19), becomes

$$F = \frac{Z}{u} \int_0^{\infty} \frac{\chi^{3/2}(x)}{x^{1/2}} \sin(ux)\, dx \qquad (1.21)$$

Franz(F 35, 36) has made an analysis of the above scattering function and obtained under nonrelativistic approximation $q \ll mc$ the following result (M 50) for the Rayleigh differential cross section per atom for angles greater tha a characteristic angle θ_c

$$a\sigma_R(\theta) = \frac{8.73 \times 10^{-33}}{\sin^3 \theta/2} \left(\frac{Z}{k}\right)^3 \frac{1}{2} \left(1 + \cos^2\theta\right) cm^2/Sr \qquad (1.22)$$

with $\theta_c = 2 \sin^{-1}\left[0.026\, Z^{1/3}/k\right]$

For angles $\theta < \theta_c$ Debye's (D 30) calculations show that the scattering cross section is propertional to Z^2 and independent of energy.

The H model calculations of $F(q, Z)$ in the range $0 \leq q \leq 0.5$ mc were carried out by Nelms and Oppenheim (N 55) using electron charge distribution computed from the SCF Hartree wave functions.

Herman and Skillman (H 63) calculated wave functions for all elements upto Z = 103 using the SCF Hartree-Fock-Slater (HFS) method, in which Slater-approximation (S51) is made to eliminate the difficult calculation of exchange potentials. The HF model formfa factors for X from 0 to 1.9 $\mathring{A}^{-1}$ for some elements have been tabulated by Ibers (I 62).

All these models are nonrelativistic. Liberman et al (L 65) have made a relativistic Dirac-Slater (DS) calculation, for all elements using Slater's method. Cromer and Waber (C 64, C65, C68) have computed DS form factors for all elements for a ~~larger~~ range of momentum transfers, corresponding to the value of the variable X in the range $0 \leq X \leq 2\ \mathring{A}^{-1}$ $(0 \leq q \leq 0.096 mc)$. Viegele et al (V 71) have obtained the average coherent Rayleigh scattering cross section using the Cromer's non-relativistic F values by numerically over the range of $\sin\theta/2/\lambda$ $0 \leq X \leq 81\ \mathring{A}^{-1}$ by numerically evaluating the integral

$$\sigma_{COH-R} = \frac{r_0^2}{2} \int_0^{\pi} \left(1 + \cos^2\theta\right) \left|F(q, Z)\right|^2 2\pi \sin\theta\, d\theta \qquad (1.23)$$

The form factors based on nonrelativistic HFS model have been evaluated by Hanson et al (Ha 64). Storm and Israel (St 67) have used these HFS form factors to evaluate the integral for σ_{COH-R} for all elements. Evaluations of σ_{COH-R} based on TF model have been given by White-Grodstein (W 57) and Davisson (D 65). Form factors have also been predicted in taking into account the exchange effect in the TF model. This is Thomas-Fermi-Dirac model (TFD) and it overestimates the form factor for small q when compared with H, HFS and DS form factor. The differences between the H, HFS and DS form factors (and hence the differential cross sections) increase with increase in Z. For low Z ($Z \leq 40$) the difference between HFS and DS form factors is negligible. A comparison is made in table 1.2 among various form factors for some selected elements.

TABLE 1.2

Comparison of form factors $F(q, Z)$ from TF, TFD, HF and DS models for some selected elements over a range of momentum transfer q corresponding to $0.1 \leq X \leq 1.5$ (TF, TFD and HF form factors are not available for $X > 1.5$ $\mathring{A}^{-1}$).

Z	Method	X ($\mathring{A}^{-1}$)							
		0.1	0.2	0.4	0.6	0.8	1.0	1.2	1.5
29	TFD	26.54	22.21	15.98	12.07	9.49	7.70	6.40	5.02
	HF	27.19	23.63	16.48	11.44	8.61	7.13	6.25	5.25
	DS	27.08	23.54	16.48	11.46	8.61	7.12		5.26
47	TFD	43.63	37.57	28.16	21.85	17.52	14.42	12.12	9.64
	HF	43.88	37.68	27.17	21.37	17.96	15.16	12.62	
	DS	43.93	38.14	27.57	21.44	17.93	15.16		9.48
80	TF	75	66	50	41	33	28		
	TFD	75.31	66.66	52.06	41.59	34.06	28.50		
	HF	75.48	67.14	52.65	42.31	34.64	28.59		
	DS	75.80	67.90	52.89	42.37	34.77	28.61		

Bethe (B 52) calculated K-shell form factor F_k using Dirac K-shell wave function. Levinger (L 52) obtained relativistic corrections to F_k in the near relativistic change of momentum region ($q \leq mc$). The calculation for L-shell for $q > mc$ made by Brown and Woodward (B 52) and by Rohrlich and Rosenzweig (R 52) gave a L-shell contribution about one eighth of K-shell contribution. The correct amplitude of Rayleigh scattering is complex. The imaginary of absorptive part was found by Greifinger et al (G 52) to be about three-fifth as large as the real or dispersive part, if electron binding in the intermediate state is neglected. The imaginary part has been neglected in the form factor calculation.

As already mentioned, Brown et al (B 52-57) have developed an exact method of calculating Rayleigh scattering amplitudes taking electron binding in the intermediate state and making no nonrelativistic approximation. They have calculated by this method only the K-shell amplitudes for mercury at photon energies 0.32, 0.64, 1.26 and 2.56 mc^2. These calculations using circular polarization states gave two K-shell amplitudes a_R^{nsf} and a_R^{sf}. The amplitudes a_R^{nsf} called non-spin-flip amplitude, represents the scattering when the outgoing photon has the same polarization as the incoming photon. When the polarizations are different, the amplitude is called spin-flip amplitude a_R^{sf} . It has been shown that real part of the K-shell amplitude $a_{R,K}^{sf}$ can be very well approximated by

$$r a_{R,K} = r_0 F_K (1-\cos\theta)/2 \qquad (1.24)$$

when F_k is K-shell form factor calculated by Bethe. For $a_{R,K}^{nsf}$ however a modified form factor F'_k is used for calculation using the form

$$r a_{R,K} = r_0 F_K' (1+\cos\theta)/2 \qquad (1.25)$$

F'_k may be calculated from the modified form factor expression

$$F'(\underline{q}, z) = \int \rho(r)\, e^{i \underline{q}\cdot\underline{r}/\hbar \frac{mc^2}{E+V(r)}}\, d^3r \qquad (1.26)$$

where E is the total energy of the scattering electron and $V = Ze^2/r$.

The relations (1.24) and (1.25) form the basis for calculation of K-shell amplitudes for other elements at slightly different energies using the calculated amplitudes for mercury at the specified energies. The L-shell amplitudes are estimated using the calculated K-shell and L-shell form factors and assuming that

$$\frac{{}_{r}a^{nsf}_{R,L}}{{}_{r}a^{nsf}_{R,K}} = \frac{F_L'}{F_K'} \qquad (1.27)$$

and

$$\frac{{}_{r}a^{sf}_{R,L}}{{}_{r}a^{sf}_{R,K}} = \frac{F_L}{F_K} \qquad (1.28)$$

The contribution to the cross section from the imaginary amplitudes becomes important above 2 MeV. These, related to an absorptive process (photoelectric effect) in the K-shell, have been obtained naturally from calculations at 1.31 MeV and can be extrapoled to other elements and energies.

1.1.4. Delbrück scattering and nuclear elastic scattering.

Interaction of photons with the atomic nucleus results in a few more elastic scattering processes. These are the nuclear Thomson scattering, Delbrück scattering and Nuclear resonance scattering. Above about 1 MeV, nuclear Thomson scattering and Delbrück scattering can be important at scattering angles where atomic Rayleigh scattering is considerably reduced.

Delbrück scattering:- The scattering of photons by the strong electric static field such as the coulomb field of atomic nuclei is known as Delbrück (D 33) scattering. The scattering is elastic if the incident photon energy is very small compared with the rest energy of the nucleus so that the nuclear recoil is negligible. The scattering is described as occuring through the production of an electron-positron pair in the static electric field and subsequent annihilation emitting a photon of the same energy as the incident photon. The scattering amplitude is complex consisting of the

real or dispersive part ${}_r a_D$ and the imaginary or the absorptive part ${}_i a_D$. The theoretical calculations of forward Delbrück scattering carried out by Rohrlich and Gluckstern (R 52) lead to the following expressions for ${}_i a_D$ and ${}_r a_D$ in the limit of low and high photon energy

$$ {}_r a_D(E) = \frac{73}{72} \cdot \frac{1}{32} (\alpha Z)^2 r_0 \left(\frac{E}{mc^2}\right)^2 \quad \text{for} \quad E \ll mc^2 \tag{1.29} $$

$$ {}_r a_D(E) = \frac{7}{8} (\alpha Z)^2 r_0 \left(\frac{E}{mc^2}\right) \quad \text{for} \quad E \gg mc^2 \tag{1.30} $$

The expression (1.29) is a good approximation for energy close to $2\,mc^2$.

The imaginary part ${}_i a_D$ which has the same threshold ($2\,mc^2$) as the pair production is

$$ {}_i a_D = \frac{1}{24} (\alpha Z)^2 r_0 \left(\frac{E}{m} - Z\right)^3 \quad \text{for} \quad E - 2mc^2 \ll mc^2 \tag{1.31} $$

The high energy limit of ${}_i a_D$ is

$$ {}_i a_D = \frac{7}{9\pi} (\alpha Z)^2 r_0 \frac{E}{mc^2} \left(\ln \frac{2mc^2}{m} - \frac{109}{42} \right) \quad \text{for} \quad E \gg 2mc^2 \tag{1.32} $$

For small angles, other calculations include those by Toll (T 52) and the approximate results only for high energies given by Bethe and Rohrlich (Be 52). The imaginary part of the amplitude has been calculated by Kessler (K 58) and these results have been used by Zernik (Z 60) to obtain the numerical values of ${}_i a_D$ at 2.62 and 6.14 MeV at various scattering angles. Ehlotzky and Sheppey (E 64) have given numerical calculations in the energy range 1 MeV to 20 MeV for angles 0° - 120° for the real and imaginary parts of Delbrück amplitude using Kessler's calculation and a simple fixed angle dispersion relation. Sannikov (Sa 63) has given an approximate calculation for high energies and large scattering angles. In the common range of energy, Sannikov's results are in serious disagreement with those of Ehlotzky and Sheppey. Eftimiu and Verjoih (Ef 60) have given an expression for the differential cross section for energy near 1 MeV. Several features

of Delbrück scattering as revealed from the calculations done so far are as follows:(i). In the forward scattering, the real part of the amplitude is dominant compared to the imaginary part not only below threshold ($2\,mc^2$) where $i a_D$ vanishes also above threshold upto about 10 MeV. Above 10 MeV, $i a_D$ is dominant at all angles.(*ii*). The dispersive part of the cross-section falls off with θ much faster than the absorptive part when $E \gg mc^2$ and $\theta \leq \frac{mc^2}{E}$. At lower energies, the variation of the dispersive part with θ is less rapid.(*iii*) The real part of the Delbrück amplitude at zero angle has been shown to be out of phase with the real Rayleigh amplitude. Since the amplitudes a^{sf} vanish at zero angles, this phase relation is applicable to amplitudes a^{nsf} only.For scattering at other angles, the phase relation between the Rayleigh and Delbrück amplitudes are not fixed exactly in the calculations so far reported.

Nuclear Thomson scattering:- Atomic Rayleigh and Delbrück scattering occur coherently with nuclear Thomson scattering. The differential cross section for nuclear Thomson scattering is obtained when $r_0 \left(= \frac{e^2}{mc^2}\right)$ in equation (1.3) is replaced by the classical nuclear radius $R = Z^2 (m/M) r_0$.

$$\sigma_{N\text{-}T}(\theta) = \frac{1}{2} R_0^2 (1+\cos^2\theta) = 2{\cdot}39 \times 10^{-32} \cdot \frac{Z^4}{A^2} \frac{1}{2} (1+\cos^2\theta)\ cm^2/sr$$

The cross-section is independent of energy and the scattering shows up at large angles for energies at which Rayleigh scattering amplitude is small.

Nuclear Resonance scattering:- In the KeV energy range, when the photon energy corresponds to one of the nuclear resonance levels, the nuclear level is excited and subsequently deexcited reemitting the whole photon energy. Since the condition for resonance excitation is difficult to obtain, this resonant scattering is negligible under the common scattering experiments.

The nuclear resonance scattering in the case when the incident photon energy is far from resonance has been investigated by Levinger (L 51). It has been shown that the corresponding nuclear resonance amplitude is small, at least upto 2.80 MeV compared to that for nuclear Thomson scattering.

Three nonresonant elastic scattering processes which take place coherently give rise either to constructive or destructive interference depending on the relative phases among their amplitudes. For each of these processes we have two amplitudes a^{nsf} and a^{sf}. So, the total differential cross section separates out into two parts, corresponding to non-spin-flip and spin-flip amplitude.

Since Rayleigh and Delbrück amplitudes are complex, so there are four amplitudes for each of these two scattering processes. This means that there are several possibilities involving relative phases and magnitudes of the various amplitudes. The magnitudes of these amplitudes and the relative phases among them must be known for calculation of the total differential coherent scattering cross section

$$a\sigma_{coH}(\theta) = \frac{1}{2}\left\{|A^{nsf}|^2 + |A^{sf}|^2\right\}$$

where, for all the three processes taken together

$$A^{nsf} = r_o\left(a_T^{nsf} + a_R^{nsf} + a_D^{nsf}\right)$$

$$A^{sf} = r_o\left(a_T^{sf} + a_R^{sf} + a_D^{sf}\right)$$

The labels T, R and D refer to nuclear, Thomson, Rayleigh and Delbrück scattering.

It seems that at an energy and scattering angle where all the three amplitudes a_T, a_R and a_D are of comparable magnitudes, an exact knowledge of the relative phases associated with all the amplitudes and of the magnitudes of Rayleigh and Thomson scattering amplitudes is necessary to interpret the experimental coherent scattering data.

1.1.5. Conclusion.

In the summary given above, we have not given the detailed descriptions of different calculations on scattering of photons. We have attempted only to indicate (i) that the theoretical calculation of Cromer for the whole atom incoherent scattering function seems to be adequate until additional shell-wise calculations of incoherent scattering function are available.

(ii) The relativistic calculation of atomic form factor has been improved using the DS atom model. These form factors now provide the most comprehensive set so far available for calculation of cross sections in the photon energy range where effects of other coherent processes are negligible. An exact shellwise calculation of Rayleigh scattering amplitude has been available only for K-shell of mercury at a few specified photon energies. In absence of an accurate knowledge of K-shell and higher shell amplitudes for lower and higher Z atoms at various arbitrary photon energies the theoretical shape of angular distribution is not predicted exactly. (iii) The calculation on Delbrück scattering process appears to be inadequate so far as the exact angular distribution of dispersive Delbrück scattering at lower photon energies are concerned. Some uncertainty exists in fixing the relative phases among the amplitudes of Rayleigh and Thomson scattering on the one hand and the Delbrück scattering on the other which together determine the final shape of the angular distribution of coherent scattering.