CHAPTER - 4

THEORETICAL CALCULATIONS OF COHERENT DIFFERENTIAL SCATTERING CROSS SECTION.

The present set of experimental data of differential cross sections listed in tables 10-13 expressed in units of Thomson cross section $d\sigma(\theta)_T = \frac{r_0^2}{2}(1+\cos^2\theta)$, where r_0 is the classical electron radius and θ is the angle of scattering are compared with theoretical values of cross sections also expressed in units of Thomson cross section as a function of momentum transfer q in mc unit. The momentum transfer covered in these comparisons lies between 0.01 mc and 10.0 mc.

4.1 Theoretical calculation of differential coherent scattering cross sections.

For the interpretation of the experimental data and examining their status in terms of the theories, theoretical differential coherent scattering cross sections are computed from the following calculations(mentioned in Chapter 2.)

i) Non-relativistic Hartree-Fock (NRHF) calculations of the atomic factor by Cromer and Mann[89] compiled by Hubbell[9].

ii) Relativistic Hartree-Fock (RHF) calculations of the atomic form factor (f) by Doyle and Turner[30], Cromer and Waber[31] and Øverbø[32] obtained from the compilation of Hubbell and Øverbø[10].

iii) Atomic shellwise calculations of the Rayleigh scattering amplitudes by Johnson and Cheng[5] (JC), Kissel and Pratt[6,7,8] (KP).

iv) Atomic K-shell Rayleigh amplitudes by Florescu and Gavrila[11] (FG).

v) Atomic coherent scattering factors corrected for forward angle dispersion terms by Cromer and Liberman[81] (CL).

vi) Delbruck scattering amplitudes by Papatzacos and Mork[12,82] (PM)

Theoretically the differential coherent scattering cross section are calculated by the following relation

$$\frac{d\sigma}{d\Omega}_{Theo.} = \frac{r_0^2}{2}\left(a_{\parallel} + a_{\perp}\right)^2 cm^2 sr^{-1} \qquad \ldots (4.1.1)$$

where r_0 is the classical electron radius and a_{11} and $a_{\perp}$ are the scattering amplitudes parallel and perpendicular to the plane of scattering respectively. For circularly polarized photons

$$\frac{d\sigma}{d\Omega} = r_0^2 \left(a_{N.S.F.} + a_{S.F.} \right)^2 \, cm^2 sr^{-1}$$

... (4.1.2)

where the spin flip $a_{S.F}$ and no-spin-flip amplitudes are related to a_{11} and $a_{\perp}$ by

$$a_{S.F} = \frac{a_{11} - a_{\perp}}{2} \quad \text{and} \quad a_{NSF} = \frac{a_{11} + a_{\perp}}{2}$$

... (4.1.3)

The amplitudes a's are complex for Rayleigh (R), nuclear resonance (NR) and Delbruck (D) scattering, containing both real and imaginary parts while the nuclear Thomson (NT) scattering amplitudes are real.

4.2 Nuclear Thomson amplitudes (NT).

The nuclear Thomson (NT) scattering amplitudes are found from

$$a_{\perp}^{(NT)} = -\frac{Z^2 m}{M} \quad \text{and} \quad a_{\parallel}^{(NT)} = -\frac{Z^2 m}{M} \cos\theta$$

... (4.2.1)

where m and M are the electron and nuclear masses respectively and $\frac{m}{M}$ is approximately equal to $\frac{1}{1823A}$ where A is the atomic weight. The nuclear Thomson scattering amplitudes are independent of photon energy but dependent on atomic number of target atoms. For example nuclear Thomson amplitudes for Lead and Uranium could be written as

$$a_{\perp}^{(NT)}(Pb) = -0.0178 \, , \quad a_{\parallel}^{(NT)}(Pb) = -0.0178 \cos\theta$$

$$a_{\perp}^{(NT)}(U) = -0.0195 \, , \quad a_{\parallel}^{(NT)}(U) = -0.0195 \cos\theta$$

... (4.2.2)

4.3 Rayleigh amplitudes

Rayleigh amplitudes using form factors are given by

$$a_{\perp}^{(R)}(FF) = -f(q,Z)$$

$$a_{\parallel}^{(R)}(FF) = -f(q,Z)\cos\theta$$

... (4.3.1)

These atomic form factors are corrected by forward angle dispersion terms $\Delta f'$ and $\Delta f''$ in the case of photon energies comparable to electron binding energy. These forward angle dispersion corrections are usually applied at other angles through the use of the following expression

$$\frac{\frac{d\sigma}{d\Omega_{coh}}}{\frac{d\sigma}{d\Omega_{T}}} = \left| f_0 + \sum \Delta f' \frac{f_0'(q)}{f'(0)} \right|^2 + \left| \sum \Delta f'' \frac{f_0'(q)}{f'(0)} \right|^2$$

... (4.3.2)

where $f_0^i(q)$ is the form factor per electron for the ith subshell.

The Rayleigh scattering amplitudes for a given subshell electron calculated from S-matrix formalism depend on incident photon energy, atomic number of the target atoms and scattering angles. The exact inner shell amplitudes calculated by Johnson and Cheng and Kissel and Pratt are used. These shell wise amplitudes are added before they are coherently summed up with other elastic scattering amplitudes and squared to get the theoretical value of the differential cross section. In most cases Kissel and Pratt Rayleigh amplitudes are used because they are available for a wide number of target atoms, wide range of photon energy and scattering angles. In the present work experimental and theoretical results are compared for a wide range of photon energy (from 28 KeV to 2.754MeV) and scattering angles from 1^{o} to 150^{o} for various target atoms.

Exact Rayleigh scattering amplitudes for such photon energies which are not available are found out by Lagrange's numerical method of interpolation (Ref. 6 Kissel, Thesis page 94). For example the K-shell Rayleigh amplitudes for photon energies of 1.70 MeV and 2.09 MeV are found by such interpolation from exact calculations of K-shell amplitudes for photon energies of 0.889, 1.1205, 1.1732, 1.3325 and 2.754 MeV. To check the reliability of this method a trial interpolation of K-shell amplitudes are made for photon energy of 1.1732 for Lead, assuming it to be unknown, from the amplitudes for 0.889, 1.1205, 1.3325 and 2.754 MeV photon energies at different scattering angles. These interpolated amplitudes are found to agree excellently with the exact calculation available. The best agreement is obtained if logarithm values of the amplitudes are used in interpolation. The differential cross section using 1.1732 MeV interpolated amplitudes are found to be within 1.5% error at all scattering angles when compared to the cross section obtained with exact Rayleigh amplitudes at this energy. A difficulty arises when the sign of the amplitudes changes with energy of the photon at a particular angle of scattering. This is overcome by interpolating real spin flip amplitudes (eqn. 4.1.3) which are all positive in sign and by interpolating real $a_1^{(R)}$ amplitudes which are all negative in sign. The $a_{11}^{(R)}$ amplitudes are then found from the relation given in eqn. 4.1.3. In the case of imaginary parts of the amplitudes the signs are reversed.

Another problem arises due to non availability of exact L, M, N shell Rayleigh amplitudes for photon energies greater than 889 KeV. For photon energies above 1 MeV the contribution of Rayleigh scattering is due to K-shell electrons mostly. But contribution of both real and imaginary parts of L, M, N shell amplitudes are significant relative to Delbruck scattering amplitudes. To have a meaningful estimate of those inner shell amplitudes consistent with the exact calculation, those amplitudes are to be found out based on exact calculation of K-shell amplitudes. In their paper Kissel, Pratt and Roy[8] have suggested the use of modified form factors for estimating these amplitudes based on their exact K-shell amplitudes. We have made a comparative study with the help of table 14 to estimate the real part of these amplitudes based on the exact K-shell amplitudes by using ordinary form factors (FF) and modified form factors (MF) and their ratios etc. The highest photon energy for which exact calculation of L-shell amplitudes are available due to Kissel and Pratt is 889 KeV. We can easily estimate the L-shell amplitudes at this energy via, form factors, modified form factors, their ratios etc and compare these estimate with the exact calculation of L-shell amplitudes at the energy. It has been found that ordinary form factors give higher while modified form factors give lower estimations of L-shell amplitudes when compared to exact L-shell amplitudes at 889 KeV. Consequently, use of ratios of ordinary form factors f(q) and modified form factors g(q) to scale the exact K-shell amplitudes to obtain L, M, N etc shell amplitudes and the method of obtaining spin flip amplitude $a^{(R)}_{S.F}$ using ratio of modified form factors g(q) and no-spin-flip amplitudes $a^{(R)}_{N.S.F}$ using ratios of ordinary form factors f(q) are discussed.

In column one of the table 14, the cross sections are obtained with exact values of K and L shell amplitudes of Kissel and Pratt for Z = 82 for photon energy of 889 KeV. In the second column the L-shell amplitudes are found by

$$a^{(R)}_{L\text{-}SHELL} = \frac{LFF}{KFF} \times a^{(R)}_{K\text{-}SHELL\,exact} \qquad \ldots (4.3.3)$$

In the third column the L-shell amplitudes are expressed by

$$a^{(R)}_{L\text{-}SHELL} = \frac{LMF}{KMF} \times a^{(R)}_{K\text{-}SHELL\ exact} \qquad \ldots (4.3.4)$$

And in the fourth column the L-shell amplitudes are obtained from the following relations.

$$a^{(R)}_{S.F.\ L\text{-}SHELL} = \frac{LFF}{KFF} \times a^{(R)}_{S.F.\ K\text{-}SHELL}$$

$$a^{(R)}_{N.S.F.\ L\text{-}SHELL} = \frac{LMF}{KMF} \times a^{(R)}_{N.S.F.\ K\text{-}SHELL}$$

and where $a^{(R)}_{S.F} = \frac{a^{(R)}_{\parallel} - a^{(R)}_{\perp}}{2}$

And $a^{(R)}_{NSF} = \frac{a^{(R)}_{\parallel} + a^{(R)}_{\perp}}{2}$ ... (4.3.5)

In all these expressions LFF, KFF are the ordinary L and K shell form factors and LMF and KMF are the corresponding modified form factors.

Table 14 Theoretical Cross Sections of 899 KeV photons in $10^{-26}cm^2/sr$, Z = 82 (including Rayleigh and nuclear Thomson amplitudes)

W	θ	1	2	3	4	A $\frac{1-2}{1}$ x 100	B $\frac{1-3}{1}$ x 100	C $\frac{1-4}{1}$ x100
899 KeV	1°	609.83	587.021	696.7784	696.78	-14.3%	1.08%	1.08%
	10°	103.07	95.945	103.2460	103.2424	- 6.9%	0.17%	.16%
	30°	3.5852	4.0738	3.6841	3.6878	4.66%	2.70%	2.86%
	60°	2.2420-01	2.3466 -01	2.2979 -01	2.3129 -01	4.6%	2.49%	3.16%
	90°	5.9219-02	6.1624 -02	6.16614-02	6.1625 -02	4.06%	4.12%	4.05%
	120°	4.3336-02	4.5206 -02	4.5956 -02	4.5205 -02	4.3%	5.76%	4.31%
	150°	3.9274-02	4.0888 -02	4.12596-02	4.0883 -02	4.1%	6.58%	4.10%

1. L-Shell Exact
2. L-Shell using ratios of ordinary form factors
3. L-Shell using ratios of modified form factors
4. L-Shell using ratios of both ordinary and modified form factors ratios.

It appears from the comparison in the table 14 that the ratios of ordinary form factors give higher estimates of L-shell amplitudes at angles starting from 1° to 60° while ratios of modified form factors give higher estimates at angles greater than 60°. L-shell amplitudes obtained in the fourth column seems to provide consistent estimate at all scattering angles.

The estimate of the imaginary parts of these inner shell amplitudes, which have either been neglected or not mentioned how they have been obtained by almost all experimental researchers is obtained following a method suggested by Kissel[55]. The imaginary parts of the forward angle Rayleigh scattering amplitudes are related to the total absorption cross sections by optical theorem based on the unitarity of the S-matrix by

$$
\begin{aligned}
I_m a_{\parallel}^{(R)}(\theta=0) &= I_m a_{\perp}^{(R)}(\theta=0) \\
&= \frac{\alpha\omega}{4\pi\, 0.0794}\left(\sigma_{P.E.} - \sigma_{P.C.}\right)
\end{aligned}
$$

... (4.3.6)

where

α = fine structure constant.

$\sigma_{P.E}$ = photo effect cross section in barns

$\sigma_{P.C.}$ = bound electron pair creation cross section in barns.

ω = photon energy in mc^2

For photon energies less than required for bound electron pair creation the ratio of $I_m a_{\parallel}^{(R)}$ or $I_m a_{\perp}^{(R)}$ are equal to the ratio of photo-effect cross sections. The ratio

$$R = \frac{I_m a_{\parallel}^{(R)}(SS)}{I_m a_{\parallel}^{(R)}(ms)} \qquad \ldots (4.3.7)$$

is used to scale the inner shell imaginary amplitudes where $I_m a_{\parallel}^{(R)}(SS)$ is the S-matrix prediction for sum of shells at $\theta = 0$ and $I_m a_{\parallel}^{(R)}(ms)$ is the S-matrix prediction for model shell at $\theta = 0$.

The agreement between pure S-matrix predictions and the photo-effect cross section ratio scaled inner shell predictions are excellent in case of photon energy at 889 KeV. Another method of scaling also suggested by Kissel[54] is done by using ratio of bound S state normalizations for large momentum transfer. We find good agreement of imaginary amplitudes estimated by both methods suggested above for photon energy of 2.754 MeV. It is found that inclusion of imaginary parts of Rayleigh amplitudes changes differential cross sections by 0.116 to 5% at various scattering angles at different photon energies around and above 1 MeV. We have taken photo-effect cross sections from the work of Scoffield[55] to calculate the imaginary parts of Rayleigh amplitudes. The values of Rayleigh amplitudes from S-matrix formalism for photon energies of 0.0843, 1.70 and 2.09 MeV which are not available in literature are given in tables 15-18. All other Rayleigh amplitudes relevant to our present set of measurements and experimental data from other workers used for comparison are available in literature.

4.4 Nuclear resonance (NR) amplitudes.

The nuclear resonance scattering amplitudes (NR) are calculated using Lorentz parameters from Veyssiere et al[53,54]. The nuclear resonance amplitudes perpendicular and parallel to the plane of scattering are given by

$$a_{\perp}^{(NR)} = (\alpha_1 + \alpha_2) + i(\beta_1 + \beta_2)$$

$$a_{\parallel}^{(NR)} = (\alpha_1 + \alpha_2)\cos\theta + i(\beta_1 + \beta_2)\cos\theta$$

... (4.4.1)

where α_i's and β_i's are related to the complex scattering amplitudes by

$$\alpha_i + i\beta_i = \frac{E^2\sigma_i\Gamma_i}{2r_0 c\hbar} \; \frac{(E_i^2 - E^2) + i\Gamma_i E}{(E_i^2 - E^2)^2 + (\Gamma_i E)^2}$$

... (4.4.2)

where E_1, Γ_1, σ_1 are the peak energy, the width at half maximum and peak cross section of low energy resonance while E_2, Γ_2, σ_2 are the corresponding quantities at high energy resoname of the giant dipole resonance. In the case of Lead (Z = 82) the Lorentz curve is single peaked while in the case of Uranium (Z = 92) the nucleus is deformed and there are two Lorentzian peaks. In calculating the nuclear resonance amplitudes the following parameters were used from the work of Veyssiere et al[56,57]. In the case of Lead, $\sigma_1 = 640$ mb, $E = 13.42$ MeV, $\Gamma = 4.05$ MeV; and in the case of Uranium $\sigma_1 = 301 \pm 6$ mb, $\sigma_2 = 369 \pm 6$ mb, $E_1 = 10.96 \pm 0.09$ MeV, $E_2 = 14.04 \pm 0.13$ MeV, $\Gamma_1 = 2.90 \pm 0.14$ MeV and $\Gamma_2 = 4.35 \pm 0.13$ MeV were used.

The values of nuclear resonance scattering amplitudes perpendicular to the plane of scattering $a_{\perp}^{(NR)}$ for 1.70 MeV and 2.09 MeV are found to be for Lead as .0006025 + i.0000234 and .000917 + i.000044 and for Uranium as .00066 + i.0000269 and .00101 + i.000051. Nuclear resonance scattering amplitudes are not added in the calculation of cross sections for Lead for photon energies below 2 MeV.

4.5 Delbruck amplitudes (D)

The Delbruck amplitudes calculated by Papatzacos and Mork for photon energies of 1.115, 1.1205, 1.1732, 1.3325, 1.70, 2.09 and 2.754 MeV are used in calculating the coherent differential scattering cross sections. Delbruck amplitudes at 1.3325 and 2.754 are available in the literature[12,14,15]. Dolbruck amplitudes at photon energies at 1.115, 1.70 and 2.09 MeV have been calculated by Papatzacos and Mork and communicated[52] for the present work. The values of those Dolbruck amplitudes are given in table 15-19.

Table 15

Z = 79

E = 84.20

Rayleigh Scattering Amplitudes (K+L+M Shells)

	R	I	R	I
0	-24.7661	0.5892	-24.7619	0.5892
5	-24.2501	0.5716	-24.5609	0.5749
10	-22.7129	0.5605	-23.1391	0.5732
15	-20.4450	0.5422	-21.2919	0.5704
20	-17.8443	0.5177	-19.1338	0.5664

Table 15

Z = 82
E = 1.70 MeV.

RAYLEIGH AMPLITUDES

Θ (°)	R_{11}	Im_{11}	R_{1}	Im_{1}	
30.00	-0.1571478	0.0050167	-0.209118	0.018078	
45.00	-0.0158996	0.0048837	-0.0573314	0.015563	×
60.00	0.0138852	0.0052736	-0.0202869	0.013749	
75.00	0.0130153	0.0039254	-0.0141717	0.011573	
90.00	0.012098	0.0015479	-0.0075804	0.009358	
120.00	0.0088879	-0.0031914	-0.0065665	0.006204	
135.00	0.007216	-0.0045235	-0.0062352	0.006491	≠ ·005491
150.00	0.007014	-0.0072234	-0.0066024	0.002938	

Z = 82
E = 1.70 MeV.

DELBRUCK AMPLITUDES.

Θ (°)	D_{11}	Im_{11}	D_{1}	Im_{1}
30.00	0.04908	0.009171	0.03528	0.006771
45.00	0.03045	0.006269	0.01615	0.002934
60.00	0.02095	0.004478	0.006735	0.0006699
75.00	0.01518	0.003454	0.001565	-0.0005875
90.00	0.01171	0.002869	-0.001436	-0.001275
120.00	0.007938	0.002335	-0.004406	-0.001873
135.00	0.007021	0.002217	-0.005123	-0.001992
150.00	0.006376	0.002149	-0.005587	-0.002059

Table 16

Z = 82 RAYLEIGH AMPLITUDES.

E = 2.09 MeV.

Q (°)	R_{11}	Im_{11}	R_1	Im_1
30.00	−0.06396	0.003583	−0.1023	0.01389
45.00	−0.001302	0.002996	−0.02112	0.01036
60.00	0.009215	0.002912	−0.007475	0.008763
75.00	0.003112	0.002219	−0.004835	0.006921
90.00	0.006468	0.001235	−0.004117	0.005411
120.00	0.003647	−0.000161	−0.004042	0.003401
135.00	0.003451	−0.001255	−0.003578	0.002816
150.00	0.003197	−0.001837	−0.003312	0.002451

Z = 82 DELBRUCK AMPLITUDES.
E = 2.09

Q (°)	D_{11}	Im_{11}	D_1	Im_1
50.00	0.05839	0.01991	0.03708	.01204
45.00	0.03475	0.01239	0.01497	.003905
60.00	0.02325	0.008454	0.008553	.0002329
75.00	0.01675	0.006140	0.00072	− .001464
90.00	0.01275	0.004979	−0.002031	− .002267
120.00	0.009347	0.003726	−0.004621	− .002880
135.00	0.007236	0.003403	−0.005302	− .002984
150.00	0.006520	0.003203	−0.005692	− .003034

Table 17

Z = 92 RAYLEIGH AMPLITUDES ~~SHELLS K L M~~

E = 1.70 MeV

θ (°)	R_{11}	Im_{11}	R_1	Im_1
30.00	-0.205754	0.007997	-0.27813	0.031020
45.00	-0.022473	0.0036649	-0.093994	0.0233799
60.00	0.0180758	0.0034915	-0.0458049	0.019969
75.00	0.0185538	0.0024924	-0.025616	0.0152768
90.00	0.0101128	0.0140874	-0.0194411	0.0121025
105.00	0.016734	0.0008943	-0.0162223	0.00940772
120.00	0.0150937	-0.00064527	-0.0148527	0.00754335
135.00	0.0136770	-0.0019893	-0.0134193	0.0059472
150.00	0.0128404	-0.00316936	-0.0127542	0.00476643

Z = 92 DELBRUCK AMPLITUDES.

E = 1.70 MeV

θ (°)	D_{11}	Im_{11}	D_1	Im_1	
30.00	0.06173	0.011544	0.044419	0.003523	
45.00	0.03833	0.0070917	0.020339	0.005693	
60.00	0.020245	0.0056369	0.0084779	0.0008452	
75.00	0.0190754	0.0045607	0.00197067	-0.0007395	
90.00	0.014746	0.003612	-0.0018033	-0.0016054	
105.00	0.011905	0.0031927	-0.0040586	-0.0020079	
120.00	0.010056	0.002940	-0.0064367	-0.0025073	62 3 5 8
135.00	0.008838	0.0027914	-0.0064367	-0.0025073	
150.00	0.008027	0.0027037	-0.0070349	-0.0025929	

Contd...

Table 18

Z = 92 RAYLEIGH AMPLITUDES.

E = 2.09 MeV.

Θ (°)	R_{11}	Im_{11}	R_1	Im_1
30.00	-0.1084	0.006064	-0.1555	0.02422
45.00	-0.006037	0.003582	-0.04282	0.01650
60.00	0.01001	0.003360	-0.01942	0.01473
75.00	0.01069	0.002563	-0.01275	0.01162
90.00	0.009671	0.0008212	-0.01019	0.009112
120.00	0.007309	-0.0007392	-0.007909	0.005691
135.00	0.006705	-0.00192	-0.007036	0.004770

Z = 92 DELBRÜCK AMPLITUDES.

E = 2.09 MeV

Θ (°)	D_{11}	Im_{11}	D_1	Im_1
30.00	0.07359	0.02494	0.04667	0.01515
45.00	0.04574	0.01560	0.01885	0.004015
60.00	0.02926	0.01064	0.006989	0.0002931
75.00	0.02106	0.007729	0.0003064	-0.001330
90.00	0.01605	0.006269	-0.002556	-0.002354
120.00	0.01051	0.004689	-0.005817	-0.003625
135.00	0.009109	0.004241	-0.006674	-0.003756