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Effect of multiple scattering on experimental Compton profiles: a Monte Carlo calculation

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Abstract

A Monte Carlo technique is used to calculate the total intensity and spectral distribution of multiple scattered photons in a typical γ-ray Compton scattering experiment. The method can be used to correct experimental Compton profiles for the effect of multiple scattering. The procedure is applied to two profiles of water measured on samples of different thicknesses and the resultant corrected profiles are seen to be independent of the original sample thickness; furthermore their agreement with a recent calculation using a near Hartree–Fock wave function is significantly improved.

§ 1. Introduction

In the high-momentum transfer region the spectrum of inelastically scattered X-radiation or γ-radiation—the Compton profile—corresponds directly to the projection of the electron momentum distribution in the scatterer on to the scattering vector, if, and only if, each photon is scattered no more than once. The growth of interest in Compton scattering as a method of studying electron momentum distributions both with X-rays (Cooper 1971) and γ-rays (Eisenberger and Reed 1972) has been accompanied by an increasing awareness of the associated problems of interpretation. However, until recently multiple scattering has been ignored, or at best minimized by the use of thin samples, and any comparison between experiment and theory has rested on the unwarranted assumption that multiple scattering events are negligible.

Experimental work by Phillips and Chin (1973) on beryllium, using MoKα X-rays, has shown that, in typical experimental configurations, multiple scattering is significant ($\sim$ 10–15%) and in general experimentalists now repeat Compton profile measurements on samples of varying thicknesses, and extrapolate the data to zero thickness (e.g. Manninen, Paakkari and Kajantie 1974). This is both time-consuming and inexact, as is discussed later in this paper.

Williams, Pattison and Cooper (1974) have developed earlier work by DuMond (1930) on multiple scattering in the X-ray regime using approximate classical formulae to produce analytic solutions. Such approximations are not valid at higher energies, nor is it practicable to obtain exact analytic solutions at those energies. Therefore a Monte Carlo approach (see e.g. Cashwell and Everett 1959, for a description of the Monte Carlo method) has been adopted with the object of calculating the effect of multiple scattering sufficiently

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accurately for a reliable correction to be made directly to experimental data. Other work on multiple γ-ray scattering (Brockwell 1965) has assumed a classical cross-section and was restricted to the case of stationary electrons.

The method is similar to that of Lichtenberg and Przybylski (1972) who applied the Monte Carlo technique to the problem of multiple scattering in a Compton polarimeter. The Klein–Nishina (1929) cross-section for a stationary free electron is used, and the polarization of each photon is followed for all scattering events. Photoelectric absorption is allowed for, and the Doppler broadening of the scattered radiation, i.e. the Compton line shape, is taken into account by convoluting the energy spectrum of the scattered photon with the experimental Compton profile, as will be described later. The results for up to three photon–electron collisions are described in this paper; the total intensity of all higher-order processes was calculated and found to be negligible for the geometries considered. As a test of the validity and usefulness of the procedure, calculated multiple scattering corrections are subtracted from two sets of data obtained from water samples of different thicknesses and the resulting Compton profiles compared with each other and with a recent near Hartree–Fock (NHF)calculation for water (Tanner and Epstein 1974).

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§ 2. Monte Carlo procedure

In general if a beam of photons is incident upon an assembly of atomic electrons the incoming photons may undergo one of the following interactions: photoelectric absorption, elastic scattering, or Compton scattering. Assuming for the moment linearly-polarized incident radiation interacting with stationary electrons, the differential Compton cross-section is (Klein and Nishina 1929),

$$d\sigma_{\text{Compton}}\,(\omega,\,\Theta)=\tfrac{1}{4}\,r_0{}^2 d\Omega\left(\frac{\omega'}{\omega}\right)^2\left\{\frac{\omega}{\omega'}+\frac{\omega'}{\omega}-2+4\cos^2\Theta\right\}, \qquad (1)$$

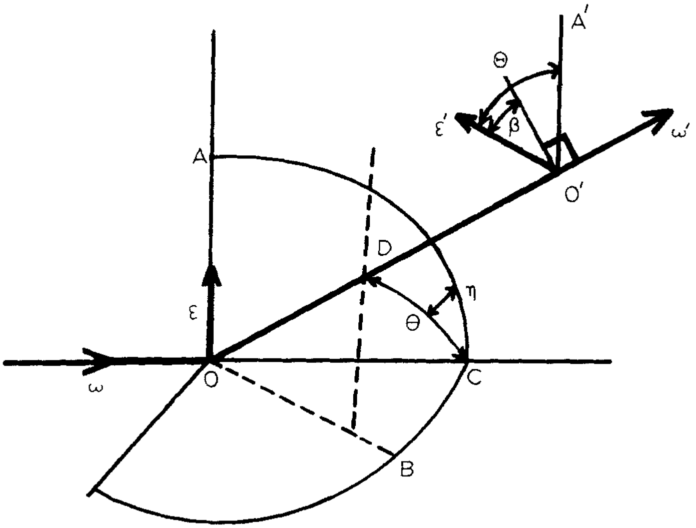
where Θ is the angle between the electric vectors of the incident and scattered photons $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}'$, respectively, r_0 is the classical electron radius, $d\Omega$ is the element of solid angle through which the photon emerges after the collision, and ω, ω' are the energies of the incident and scattered photons, respectively. The relation between ω and ω' is given by the well-known expression for the Compton shift

$$\frac{\omega}{\omega'}=1+\frac{\omega}{m_0c^2}(1-\cos\theta), \qquad (2)$$

where θ is the scattering angle, and m_0c^2 is the electron rest energy. Referring to fig. 1 we denote by η the azimuthal angle between the primary plane of polarization OAC and the scattering plane ODC, and by β the angle between the plane OADB (defined by $\boldsymbol{\epsilon}$ and the direction of scattering) and the plane of polarization after scattering (defined by $\boldsymbol{\epsilon}'$ and the direction of scattering). One can then obtain (see, for example, Evans 1955) the relationship between the various angles

$$\cos^2\Theta=(1-\sin^2\theta\,\cos^2\eta)\,\cos^2\beta \qquad (3)$$

Fig. 1



Scattering event at O. ϵ and ϵ' are the electric vectors of the incident and scattered photons, of energy ω and ω', respectively. The line O'A' is parallel to OA and makes an angle Θ with ϵ'. The angles θ, η and β are defined in the text.

and eqn. (1) becomes:

$$d\sigma_{\mathrm{Compton}}(\omega,\theta,\eta,\beta)=\tfrac{1}{4}r_0^{\,2}\,d\Omega\left(\frac{\omega'}{\omega}\right)^2\left\{\frac{\omega}{\omega'}+\frac{\omega'}{\omega}-2+4(1-\sin^2\theta\cos^2\eta)\cos^2\beta\right\}. \quad (4)$$

It follows that the scattered radiation is partially polarized. In the case of elastic scattering ($\omega'=\omega$), we always have $\beta=0$, i.e. the scattered radiation is completely polarized and the differential cross-section becomes:

$$d\sigma_{\mathrm{el}}(\theta,\eta)=r_0^{\,2}d\Omega\ (1-\sin^2\theta\cos^2\eta). \quad (5)$$

In the following sections the steps in the Monte Carlo calculation needed for simulating the path of one photon are described.

(1) *Point of entrance into the specimen*: The photon is assumed to arrive at right angles to the base of a cylindrical specimen, and the point of entrance is selected at random (i.e. the photon flux is considered uniform).

(2) *Forced first collision*: In order to save computer time, the photon is forced to have a first collision by using the following Monte Carlo relation between the depth of penetration l and the total attenuation coefficient μ (Cashwell and Everett 1959):

$$l=-\frac{1}{\mu}\log_e(1-r[1-\exp(-\mu L)]). \quad (6)$$

L is the thickness of the specimen, and r is a random number in the interval (0, 1). To allow for that part of the flux which would otherwise be transmitted

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through the specimen without collision, the photon is assigned a weight W according to the expression

$$W = 1 - \exp(-\mu L). \tag{7}$$

(3) *The nature of the scattering*: To take account of the possibility that the photon may be photoelectrically absorbed, the weight W is reduced by the ratio, R, of the photoelectric cross-section to the total attenuation coefficient, according to the relationship

$$W' = W(1 - R). \tag{8}$$

The type of scattering process is then determined by dividing the random number interval (0, 1) in proportion to the fractions of elastic and Compton scattering in the scattering attenuation coefficient (the attenuation coefficients were taken from the tables of Hubbell (1969)).

(4) *Geometrical considerations*: The scattering angles θ and η following the collision are selected at random in the intervals $(0, \pi)$ and $(0, 2\pi)$, respectively, and in the case of Compton scattering the polarization angle β is also selected at random in the interval $(0, \pi)$. The weight W of the photon is then reduced according to the differential cross-section for either a Compton collision (eqn. (4)) or an elastic collision (eqn. (5)), normalized with respect to the total cross-section.

(5) *The path after the collision*: The path length l following the collision is then calculated using the formula (Cashwell and Everett 1959):

$$l = -\frac{1}{\mu'} \log_e(r), \tag{9}$$

where μ' is the total attenuation coefficient for the new photon energy and r is a random number in the interval (0, 1). The quantity l, and the angles θ and η, are then used to determine whether the photon escapes before suffering another collision, or if not the position of the next scattering is ascertained.

(6) *The next collision*: If the photon has another collision the procedure described in §§(3), (4) and (5) is repeated. This cycle can be continued until the photon leaves the specimen, or can be stopped after an arbitrary number of collisions. (In the present calculation up to three collisions were considered.) It should be noted that the angles θ, η and β are calculated with respect to the coordinate frame of the photon at each collision. This photon frame is not in general equivalent to the laboratory frame and therefore these angles must be transformed back to the laboratory frame.

(7) *Exit of photon*: If the photon leaves the specimen, the information relating to its energy and to its scattering angle (in the laboratory frame) is stored by adding the final weight W of the photon into an appropriate register. Several registers were available according to the number and nature of the collisions suffered by the photon. Since the initial beam was considered to be linearly polarized, the intensity of the outgoing photons, at a given angle of scattering θ, would depend upon the azimuthal angle η. However, as sources used in current experiments provide unpolarized beams of photons, it is necessary to average over all possible directions of the electric vector of the initial photon.

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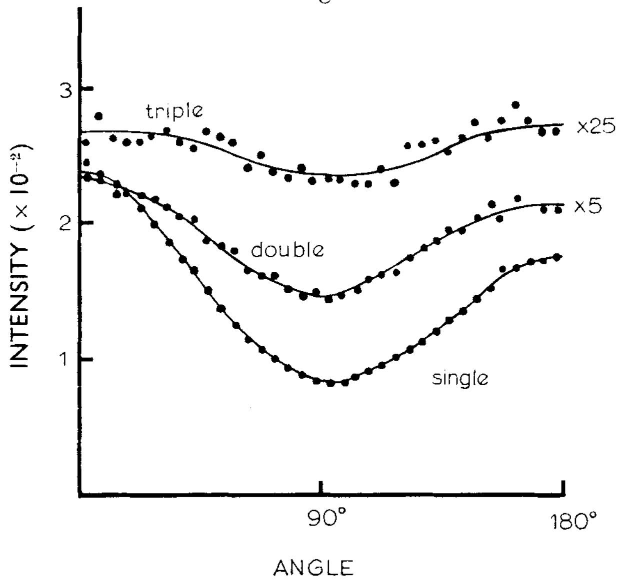
Since the assumed experimental geometry has axial symmetry, this can be achieved in the above calculation by averaging the final intensity (for initially polarized radiation) over all angles η for each angle θ.

§ 3. Results for stationary electrons

The angular and energy distributions of the scattered photons were calculated assuming a monochromatic primary photon beam, having an energy of 59·54 keV (^{241}Am gamma source energy), incident upon a cylinder of radius 2·5 cm and thickness 3·0 cm with the absorption properties of water. The paths of 10^6 photons were followed.

Figure 2 shows the angular distributions of photons scattered once, twice or three times (single elastic events are not shown). The angular distribution

Fig. 2



Calculated angular distributions of photons scattered once, twice or three times in a specimen of thickness 3 cm. The energy of the incident photons is 59·54 keV. The intensity is relative to the incident photon flux.

for single Compton scattering is seen to follow the Klein–Nishina formula for unpolarized incident radiation (see, for example, Evans 1955), and this serves as a check on the Monte Carlo procedure. Since any total scattering angle for multiple events is made up from many combinations of intermediate scattering angles, a general trend away from any angular dependence for higher-order scattering can be expected : this is clearly demonstrated. Furthermore, the angular distribution for double scattering shows qualitative agreement with the distribution predicted analytically by DuMond (1930). (Quantitative agreement would not be expected because DuMond employed a classical cross-section in his calculations.)

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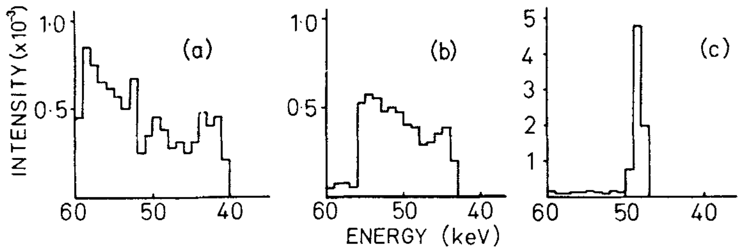
Figure 3 shows the energy distributions of photons scattered twice and leaving the specimen in three different directions, 5°–15°, 85°–95° and 165°–175°. It can be seen that the double-scattering profiles become narrower as the total

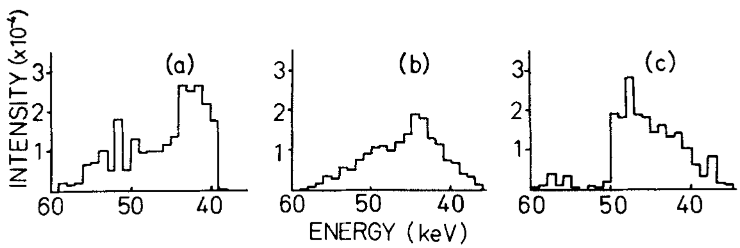
Fig. 3



Calculated energy distributions of photons scattered twice and leaving the specimen in the directions (*a*) 5°–15°, (*b*) 85°–95°, (*c*) 165°–175°. The intensity is relative to the incident photon flux.

scattering angle increases. This is to be expected since, for a total scattering angle θ, the range of angles through which a photon may be deflected extends from θ to $(360°-\theta)$. As the energy loss depends upon the angles of deflection of the photon, this condition will lead to wide profiles at low angles of θ, and to narrow profiles as θ approaches 180°. It can also be seen that a region of

Fig. 4



Calculated energy distributions of photons scattered three times and leaving the specimen in the directions (*a*) 5°–15°, (*b*) 85°–95°, (*c*) 165°–175°. The intensity is relative to the incident photon flux.

low and rather uniform intensity extends from the incident photon energy to the main profile. This is due to photons which suffer one Compton and one elastic collision.

Figure 4 shows the same distributions as fig. 3 for the case of photons scattered three times. Again it can be seen that for higher-order scatterings there is a loss of angular dependence, as well as a reduction in intensity.

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§ 4. Application to experimental Compton profiles

The Monte Carlo technique described above is now used to correct experimental Compton profiles for the effect of multiple scattering. The profiles used were measured in the Technion, Haifa, by one of the authors (J.F.) for two thicknesses of water, as a part of a current international project organized by the International Union of Crystallography. These profiles (for 1 and 3 cm sample thicknesses) are listed in table 1 and also shown in fig. 5, together with a

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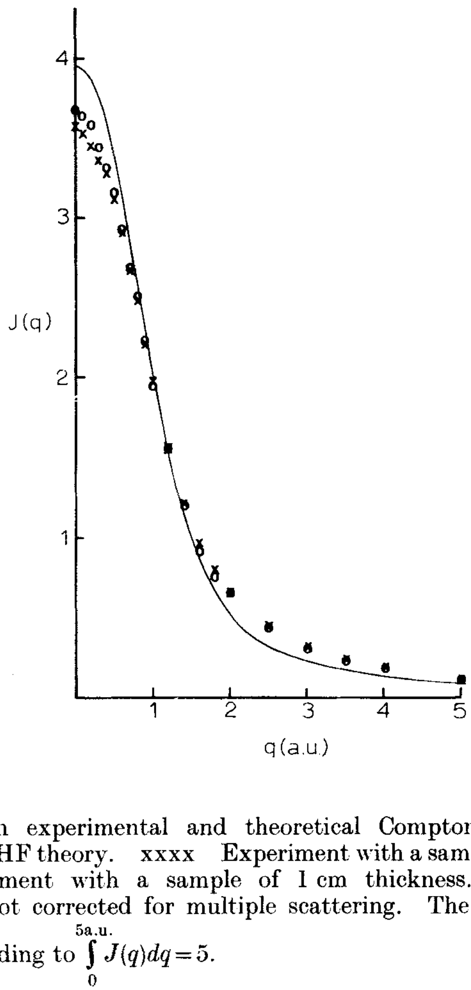
Table 1. Experimental and theoretical Compton profiles of water. The experimental profiles are given for two different sample thicknesses and have not been corrected for multiple scattering. The profiles are all normalized according to $\int_0^{5\text{a.u.}} J(q)dq=5$.

q(a.u.)	Experiment		NHF theory
	1 cm	3 cm	
0·0	3·666 ± 1%	3·584 ± 1%	3·9546
0·1	3·635	3·528	3·9354
0·2	3·574	3·447	3·8749
0·3	3·432	3·363	3·7673
0·4	3·303	3·274	3·6087
0·5	3·147	3·096	3·3997
0·6	2·929	2·892	3·1491
0·7	2·682	2·668	2·8700
0·8	2·502	2·458	2·5779
0·9	2·227	2·196	2·2872
1·0	1·939 ± 2%	1·971 ± 2%	2·0097
1·2	1·551	1·459	1·5223
1·4	1·199	1·210	1·1422
1·6	0·911	0·966	0·8627
1·8	0·752	0·797	0·6636
2·0	0·650 ± 3·5%	0·656 ± 3·5%	0·5240
2·5	0·438	0·452	0·3284
3·0	0·301	0·317	0·2359
3·5	0·234	0·237	0·1901
4·0	0·173	0·185	0·1443
5·0	0·113 ± 7%	0·114 ± 7%	0·0936

recent near Hartree–Fock (NHF) calculation (Tanner and Epstein 1974). The measurements were made using 59·54 keV gamma rays from a 300 mCi ^{241}Am source scattered at an angle of 157° ± 2° and detected with a Ge (Li) counter. The experimental technique has recently been described (Felsteiner, Fox and Kahane 1972 a). The profile of water (1 cm thickness) has also been measured independently by another of the authors (P.P.) for the same international project. That profile is in good agreement with the 1 cm profile shown in table 1.

It is clear that the experimental profiles vary significantly with the sample thickness, and both are in marked disagreement with the NHF theory. Since the measured profiles have already been corrected for sample absorption (and other systematic effects) it is assumed that the dependence upon sample thickness shown above is due to multiple scattering. However, in the procedure described earlier, only stationary electrons were considered. In order to take into

Fig. 5



Comparison between experimental and theoretical Compton profiles of water. ———— NHF theory. xxxx Experiment with a sample of 3 cm thickness. oooo Experiment with a sample of 1 cm thickness. The experimental profiles are not corrected for multiple scattering. The profiles are all normalized according to $\int_0^{5\text{a.u.}} J(q)dq = 5$.

account the momenta of the scattering electrons, the energy distribution of the scattered photons, derived initially from the Klein–Nishina formula, was convoluted for each scattering event with the appropriate Compton profile. Since the Compton profile for single scattering, needed for this convolution, is not known exactly (because of multiple scattering), an iterative procedure was

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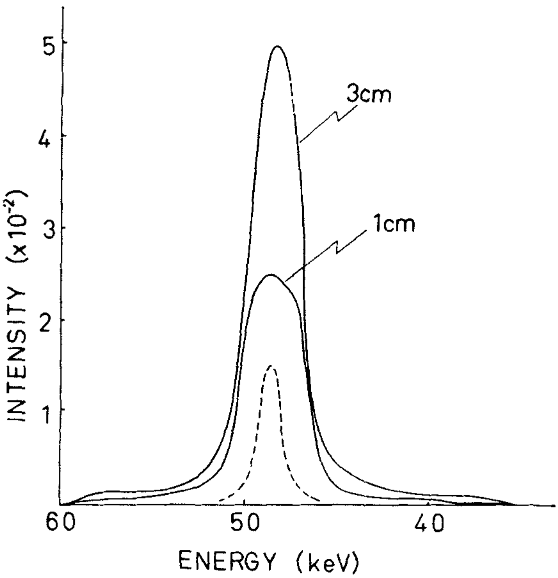
used. The experimental Compton profile was taken as a first approximation to the single-scattering profile and the contribution of multiple scattering obtained in this was was then subtracted from the experimental Compton profile. This corrected profile, renormalized, served as a new approximation for the iterative procedure. Three or four iterations proved sufficient to obtain *self-consistent profiles.*

The final energy distributions of the photons which have undergone two or three collisions and leave the specimen at a total scattering angle of $157° \pm 2°$ are given in fig. 6, for both thicknesses. It was assumed that the effect of the

Fig. 6



Calculated energy distributions of multiple scattered photons which emerge in the angular range $157° \pm 2°$ are shown for two sample thicknesses. The distributions include the broadening effect of the electron momenta. The intensity of each distribution is relative to the number of photons which have a single Compton collision, and leave the sample in the same angular range. An experimental profile (dashed line) which is not to scale, is shown for comparison.

sample holder (brass) was to make the cylindrical walls totally absorbing for 60 keV γ-radiation. Table 2 gives the final Compton profiles corrected for double scattering, and for both double and triple scattering. It is seen that when the effect of both double and triple scattering is taken into account, the corrected profiles for both thicknesses agree well. Thus it seems clear that the discrepancy between the experimental profiles shown in table 1 is due to multiple-scattering effects. Furthermore, it is demonstrated in table 2 that the effect of triple scattering is much more significant in the thicker sample and must be

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included in order to obtain good agreement between the two profiles. It follows that the triple-scattering correction can be neglected only when thin samples are considered. The contribution from scatterings of higher order than three was found to be negligible for both thicknesses considered.

Table 2. Experimental Compton profiles of water for two sample thicknesses after correction for multiple scattering. The profiles are normalized according to $\int_0^{5\text{a.u.}} J(q)dq = 5$.

	Corrected for double scattering		Corrected for double and triple scattering	
(a.u.)	1 cm	3 cm	1 cm	3 cm
·0	3·937	3·883	3·942 ± 1·5%	3·930 ± 1·5%
0·1	3·901	3·820	3·908	3·867
0·2	3·831	3·727	3·837	3·773
0·3	3·670	3·630	3·676	3·674
0·4	3·521	3·529	3·527	3·572
0·5	3·345	3·321	3·350	3·361
0·6	3·096	3·082	3·101	3·117
0·7	2·815	2·818	2·819	2·849
0·8	2·611	2·573	2·615	2·599
0·9	2·298	2·266	2·301	2·286
1·0	1·972	2·004	1·973 ± 3%	2·019 ± 3%
1·2	1·533	1·515	1·534	1·521
1·4	1·140	1·130	1·139	1·129
1·6	0·820	0·861	0·819	0·855
1·8	0·652	0·685	0·651	0·677
2·0	0·551	0·544	0·550 ± 5%	0·534 ± 6%
2·5	0·357	0·369	0·356	0·358
3·0	0·250	0·266	0·248	0·255
3·5	0·208	0·209	0·206	0·198
4·0	0·156	0·168	0·154	0·156
5·0	0·104	0·104	0·103 ± 10%	0·091 ± 12%

Inspection of tables 1 and 2 indicates an increase in the statistical errors after the multiple-scattering correction has been made. A larger number of photons used in the Monte Carlo calculation would have resulted in a smaller increase in these errors but this was not practicable in view of the limited computational facilities available. It can also be seen from these tables that the agreement between the NHF theory and experiment has been considerably improved following the multiple-scattering correction. This is illustrated in fig. 7 where the difference curves between theory and experiment are given.

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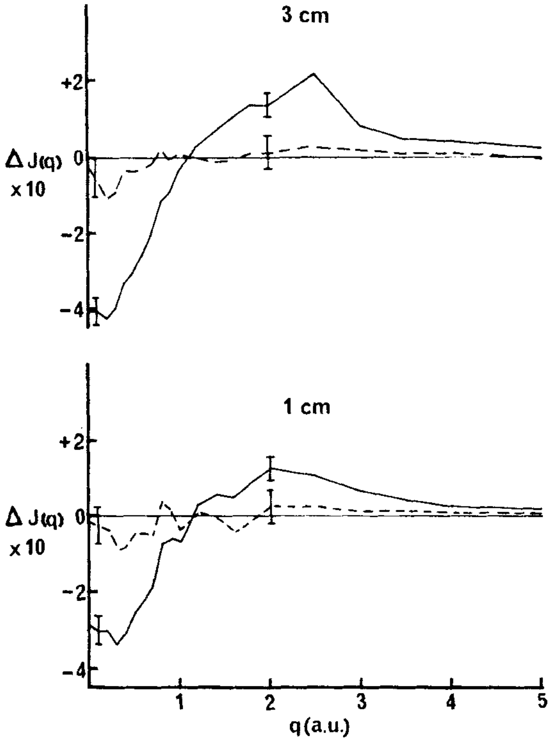
Fig. 7



Difference curves between experimental Compton profiles and the NHF theory. ——— Before correction for multiple scattering. — — — — — After correction for multiple scattering. The range of statistical uncertainty is indicated by the error bars.

§ 5. Discussion

In this paper a Monte Carlo procedure is introduced to correct for the effect of multiple scattering in experimental Compton profiles. Applying this procedure to measured profiles of water, the corrected profiles appear to be independent of sample thickness, within their statistical error. Furthermore, there is now good agreement between the corrected profiles and a NHF theory.

The other methods previously employed to correct for multiple scattering involved the measurement of a number of profiles for different sample thicknesses and the subsequent extrapolation of the data to zero thickness. In these extrapolation methods each point in the Compton profile was assumed to vary either linearly (Felsteiner *et al.* 1972 b, Manninen *et al.* 1974), or with the square root (Tanner and Epstein 1974) of sample thickness. The application of these methods to the experimental profiles given in table 1 leads, for example, to values of $J(0)$ of 3·71 for linear extrapolation and of 3·78 for square root extrapolation. Both of these values are still in poor agreement with the value 3·95, given by the NHF theory in table 1.

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In conclusion it should be stated that it is always wise to minimize multiple scattering by performing measurements on samples as thin as possible. In practice it is necessary to make a compromise between this requirement and the limitations arising from the low intensity inherent in such an experiment. The results reported above indicate that the Monte Carlo technique can be used successfully to correct Compton profile data, measured on a single sample, for the effects of multiple scattering.

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