

Relationship of the relativistic Compton cross section to the electron's velocity distribution

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(Received 6 August 1973)

A relativistic treatment of the Compton cross section for free electrons is given. In addition, conditions are specified when it is correct to within 1% to relate in a simple manner the results of Compton-scattering experiments to a simple Compton profile (velocity distribution of electrons). Many different approaches previously used to achieve this simple relationship have been arbitrary and thus have resulted in the possibility that two investigators with the same experimental data would deduce different Compton profiles. The relationship derived here differs from all the previous ones, and in some cases, would yield a significantly different Compton profile from reported data.

The literature contains the experimental Compton-scattering results of various authors on a variety of materials. These authors, whether they used x rays, 60-keV γ rays, or 160-keV γ rays, have developed their own recipe for the relationship between the Compton-scattering cross section and the momentum distribution (Compton profile). Rather than going into the various incorrect approaches used, we will provide a correct general treatment of the cross section appropriate for all sources. We will then investigate the conditions that must be satisfied in order to relate the cross section to the Compton profile. In general, it is found that for low photon energies the previously derived¹ nonrelativistic calculation is correct to order v/c . For high-energy photons terms of order v/c do appear and must be accounted for. Terms to order v^2/c^2 cannot be included and still preserve a simple interpretation of the scattering results in terms of a Compton profile. Second, it is found that if the experiments are performed with higher-energy photons at a scattering angle (difference between the direction of the input and output photon) differing greatly from 180° then one will deduce erroneous results for the case of an anisotropic velocity distribution. Finally, we conclude that all previous recipes for relating the Compton-scattering experimental results to a Compton profile are formally incorrect and in some cases (higher-atomic-number systems) give rise to significant errors.

In the calculations which follow we assume the validity of the impulse approximation.¹ Specifically, we assume that the ratio of the binding energy of the electron E_B to the recoil energy given the electron in the scattering process E_R is much less than unity. As was previously discussed¹ this approximation is equivalent to assuming that the electron sees the same potential in the initial and final state (i. e., that it is moving in a constant potential and can therefore be regarded as a free electron).

Since $E_B \approx \frac{1}{2} m\bar{v}^2$ for hydrogenic systems, rela-

tivistic effects of the order v^2/c^2 for the ground state vary as E_B/m_0c^2 , where m_0 is the rest mass of the electron. Thus for all photon energies used to date, where $E_B \ll m_0c^2$, the impulse approximation breaks down before v^2/c^2 effects become important. Consequently, in the calculations which follow we eventually remove v^2/c^2 effects keeping in mind that one still may have to consider the validity of the impulse approximation. Final-state relativistic effects depend upon the magnitude of the final velocity of the scattering electron or approximately as E_R/m_0c^2 . That is they depend upon the incident photon energy, ω_1 , since to first order $E_R = 2\omega_1^2/m_0c^2$ for backward scattering. Thus final-state relativistic effects are more important for the higher-energy experiments.

Throughout this relativistic calculation we use the notation, formalism, and results given by Jauch and Rohrlich.² Our contributions are to (i) include a distribution of initial electron velocities in the manner appropriate for scattering from a fixed number of electrons, (ii) calculate the cross section appropriate for the way Compton-scattering experiments are performed and analyzed, and (iii) derive an approximate cross section and specify its range of validity such that to within 1% one can relate the results of the experiments to the Compton profile.

The geometry is shown in Fig. 1 and is the same as in Jauch and Rohrlich.² For $\hbar = 1$, $c = 1$ and with (E, \vec{p}) electron properties and (ω, \vec{k}) photon properties one has from Jauch and Rohrlich² the following relationship (1 are the initial properties and 2 are the final properties):

$$E_1 + \omega_1 = E_2 + \omega_2, \quad (\text{energy-momentum}) \quad (1)$$

$$\vec{k}_1 + \vec{p}_1 = \vec{k}_2 + \vec{p}_2, \quad (\text{conservation}) \quad (2)$$

with other useful quantities defined to be

$$K_1 = E_1\omega_1(1 - p_1 \cos \alpha/E_1), \quad (3)$$

$$K_2 = E_1\omega_1(1 - p_1 \cos \alpha'/E_1), \quad (4)$$

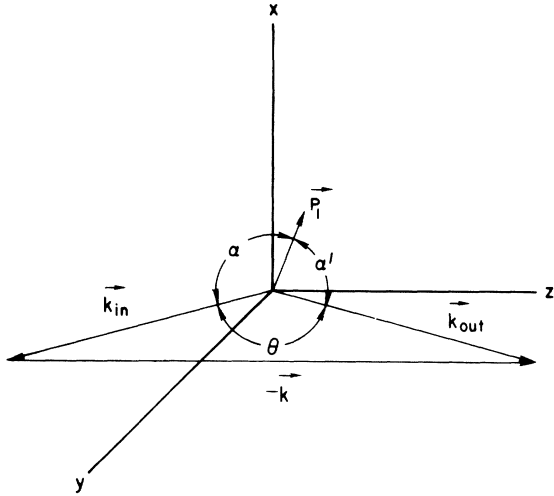


FIG. 1. Geometry of the scattering process.

$$\bar{X} = \frac{K_1}{K_2} + \frac{K_2}{K_1} + 2m^2 \left(\frac{K_2 - K_1}{K_2 K_1} \right) + m^4 \left(\frac{K_2 - K_1}{K_2 K_1} \right)^2 \quad (5)$$

Equation (11-9) in Jauch and Rohrlich² is the total Compton cross section and is the basic starting relationship. It must be modified in two ways to be appropriate for scattering from electrons in solids, atoms, or molecules in which the energy distribution of the scattered radiation is measured. The first and major change is that the flux factor² which is appropriate for scattering from a beam of electrons (K_1) is replaced by ($m\omega_1$), the flux factor appropriate for scattering from a fixed number of electrons with a distribution of velocities. We are evaluating the cross section in a reference frame in which the crystal is at rest and where the recoil of the crystal is ignored. This approach is the standard one in which the matrix element for the interaction as calculated by Jauch and Rohrlich is inserted in the Golden Rule to obtain the cross section. The transition rate is then only dependent upon the rate of photons hitting the electrons which for the case of a stationary crystal is independent of the velocities of the electron. In projecting the bound electrons onto plane wave states, the basis for the Jauch and Rohrlich calculation, errors to order v^2/c^2 may be made and

have been ignored in these calculations. The second change is that the differential cross-section must be calculated since experimentally one measures the energy distribution of the radiation scattered at a fixed angle θ into a solid angle $d\Omega$ within an energy bandwidth $d\omega_2$. These formal modifications are straightforward and yield

$$\frac{d\sigma}{d\omega_2 d\Omega} = \left(\frac{e^2}{4\pi} \right)^2 \int \frac{N(\vec{p}_1)}{2m\omega_1 E_2 \omega_2} \times \int \omega_2^2 \bar{X} \delta^3(\vec{p}_2 + \vec{k}_2 - \vec{p}_1 - \vec{k}_1) \times \delta(E_2 + \omega_2 - E_1 - \omega_1) d^3 p_1 d^3 p_2, \quad (6)$$

where $N(\vec{p}_1)$ is the probability that an electron has momentum \vec{p}_1 . Performing the integral over $d^3 p_2$ with the presence of the δ function yields

$$\frac{d\sigma}{d\omega_2 d\Omega} = \left(\frac{e^2}{4\pi} \right)^2 \int \frac{N(\vec{p}_1) \omega_2 \bar{X} \delta(E_2 + \omega_2 - E_1 - \omega_1) d^3 p_1}{2m\omega_1 E_2} \quad (7)$$

In a standard manner Eq. (7) can be rewritten

$$\frac{d\sigma}{d\omega_2 d\Omega} = \left(\frac{e^2}{4\pi} \right)^2 \times \int \frac{\bar{X} N(\vec{p}_1) \omega_2 \delta(p_x - p_{x0}) dp_x dp_y dp_z}{2m\omega_1 E_2 d(E_2 + \omega_2 - E_1 - \omega_1)/dp_x}, \quad (8)$$

where the z direction is chosen to be antiparallel to the vector $\vec{k} = \vec{k}_1 - \vec{k}_2$. Utilizing the energy-momentum-conservation equations (1) and (2) and the relativistic energy-momentum relationship $E^2 = m^2 + p^2$, one can easily show

$$-\frac{p_{x0}}{E_1} = \frac{(\omega_1 \omega_2 / E_1)(\cos\theta - 1) + \omega_1 - \omega_2}{(\omega_1^2 + \omega_2^2 - 2\omega_1 \omega_2 \cos\theta)^{1/2}} \quad (9)$$

and

$$\frac{d(E_2 + \omega_2 - E_1 - \omega_1)}{dp_x} = \frac{1}{E_2} \left(\frac{p_x}{E_1} (\omega_2 - \omega_1) - (\omega_1^2 + \omega_2^2 - 2\omega_1 \omega_2 \cos\theta)^{1/2} \right) \quad (10)$$

Substituting Eq. (10) into Eq. (8), one finds

$$\frac{d\sigma}{d\Omega d\omega_2} = \left(\frac{e^2}{4\pi} \right)^2 \int \frac{N(p_1) \omega_2 \bar{X} \delta(p_x - p_{x0}) dp_x dp_y dp_z}{2m\omega_1 [(\omega_1^2 + \omega_2^2 - 2\omega_1 \omega_2 \cos\theta)^{1/2} + (p_x/E_1)(\omega_1 - \omega_2)]} \quad (11)$$

The goal of Compton-scattering experiments is to find the Compton profile which is defined by

$$J(p_x) = \int_{p_x = p_{x0}} N(\vec{p}) dp_x dp_y. \quad (12)$$

We would like to be able to rewrite Eq. (11) in the form

$$\frac{d\sigma}{d\omega_2 d\Omega} = C(\omega_2, \omega_1, \theta, p_{x0}) J(p_x), \quad (13)$$

but there are essentially three features of Eq. (11) which prevent us from rewriting it in this form.

The first problem is that E_1 in Eqs. (8) and (11) depends not only on p_x but also on p_x and p_y . Electrons with the same p_x , but different p_x and p_y , will not only scatter over a range of energies given by Eq. (9) but will scatter with a variable probability as given by Eq. (11). The calculation of Eq. (11) under these conditions is almost untractable. An approximate solution to this problem is the replacement of E_1 by m_0c^2 . This replacement is accurate to

$$E_1/m_0c^2 = (1 - v^2/c^2)^{-1/2} \approx 1 + \frac{1}{2}v^2/c^2. \quad (14)$$

Since, in Eq. (9), $p_x \propto E_1(\omega_1 - \omega_2)$, one must restrict v/c to be less 0.14 in order to get the relationship between $\omega_2 - \omega_1$ and p_x correct to 1%.

The second problem is that even more severe restrictions on v/c are needed in Eq. (11). The last two terms in X [Eq. (5)] become for the case of backward scattering ($\theta = 180^\circ$, $p_1 \cos \alpha = p_x$, $p_1 \cos \alpha = -p_x$).

$$\frac{4(1 - v^2/c^2)}{(1 - v_x^2/c^2)} - \frac{4(1 - v^2/c^2)^2}{(1 - v_x^2/c^2)^2} \cong 4v_1^2/c^2, \quad (15)$$

where we still let $E^2 = m^2c^4 + p^2c^2$, v_1 is the perpendicular component of the velocity and we have ignored higher-order terms. To first order then

$$\bar{X} = 2 + 4v_1^2/c^2 = 2(1 + 2v_1^2/c^2), \quad (16)$$

and thus from Eq. (11)

$$\frac{m_0c^2\bar{X}}{E_1} = \frac{2(1 + 2v_1^2/c^2)}{1 + (v^2/2c^2)} = 2 \left(1 + \frac{3}{2} \frac{v_1^2}{c^2} - \frac{p_x^2}{2c^2} \right). \quad (17)$$

The correction terms in Eq. (17) will have the general effect of sharpening the Compton-scattered spectrum for the tightly-bound electrons since at $p_x = 0$, the center of the Compton profile

$$m_0c^2\bar{X}/E_1 \propto 1 + v^2/c^2$$

(\bar{v} is the average velocity), while at large $|p_x|$, where $v_1 \rightarrow 0$,

$$m_0c^2\bar{X}/E_1 \propto 1 - p_x^2/2c^2. \quad (19)$$

Thus to obtain the correct shapes of the Compton profile from the measured spectrum to 1% one requires that \bar{v}/c be less than $\frac{1}{10}$ or $v < 13.7$ a. u. This corresponds to hydrogenic binding energies of about 3000 eV.

The third problem in achieving the relationship given in Eq. (13) is the presence in \bar{X} of K_1 and K_2 which involve the projection of \vec{p}_1 on \vec{k}_{in} and \vec{k}_{out} instead of \vec{k} . This has the consequence that electrons with the same p_x but different p_x and p_y , will contribute differently to the scattered intensity in a manner which not only depends on the

magnitude of p_x and p_y , but also on the direction of \vec{p} . This problem is not severe because in zeroth order \bar{X} is a constant and so small changes in the geometry are not crucial, though for other reasons which we will now discuss backward scattering is obviously preferable.

If $\theta = 180^\circ$, backward scattering, then $p \cos \alpha = -p \cos \alpha' = p_x$ and the angle between \vec{k}_{in} and \vec{k} and \vec{k}_{out} and \vec{k} is 180° and 0° , respectively. In general when $|k_{in}| \neq |k_{out}|$ and $\theta \neq 180^\circ$ then the direction of \vec{k} is not such that it bisects the angle between $-\vec{k}_{in}$ and \vec{k}_{out} (i. e., makes $\frac{1}{2}\pi + \frac{1}{2}\theta$, $\frac{1}{2}\pi - \frac{1}{2}\theta$ angles with \vec{k}_{in} and \vec{k}_{out}). The general expression for the angle that \vec{k} makes with \vec{k}_{in} and \vec{k}_{out} is $(\frac{1}{2}\pi \pm \frac{1}{2}\theta \mp \Delta)$, where Δ is given by

$$\Delta = \frac{[(\omega_1 - \omega_2)/\omega_2] \sin \theta}{1 - \cos \theta + (\omega_1 - \omega_2)/\omega_2}. \quad (20)$$

From Eq. (20) we immediately note that for anisotropy measurements not made near 180° or 0° then the symmetry axis of the crystal which one wants to study should be aligned $(\frac{1}{2}\pi \pm \frac{1}{2}\theta \mp \Delta)$ away from \vec{k}_{in} and \vec{k}_{out} and not $(\frac{1}{2}\pi \pm \frac{1}{2}\theta)$, and second that \vec{k} will vary in direction as well as magnitude as one moves across the Compton spectrum. The magnitude of Δ at the center of the Compton profile can be obtained from Eqs. (9) and (20) is

$$\Delta = \frac{\omega_1/m \sin \theta}{1 + \omega_1/m}, \quad (21)$$

which is obviously greatest at $\theta = 90^\circ$ and increases with increasing ω_1 . For example, with ω_1 equal to 160 keV and $\theta = 90^\circ$ one finds from Eq. (21) that $\Delta \cong 15^\circ$. A variation of 15° in direction of the axis on to which one is projecting the momentum distribution of the electrons is large enough to cause serious problems when making anisotropy measurements.

To achieve a relationship of the form given in Eq. (13) one must in light of the previous discussed features make the following modifications in Eqs. (9) and (11); (i) replace E_1 by m_0c^2 ; (ii) ignore the v^2/c^2 contributions of the last two terms in \bar{X} ; (iii) scatter nearly in the backward direction so that to first order $p \cos \alpha = -p_x = -p \cos \alpha'$. If one does these things one finds

$$-\frac{p_x}{m_0} = \frac{(\omega_1\omega_2/m_0)(\cos \theta - 1) + (\omega_1 - \omega_2)}{(\omega_1 + \omega_2 - 2\omega_1\omega_2 \cos \theta)^{1/2}} \quad (22)$$

and

$$\frac{d\sigma}{d\Omega d\omega_2} = C(\omega_1, \omega_2, \theta, p_x) \int_{p_x^2 \neq p_{x0}} N(\vec{p}_1) dp_x dp_y, \quad (23)$$

where

$$C(\omega_1, \omega_2, \theta, p_{\#}) = \left(\frac{e^2}{4m_0^2 \pi^2 c^2} \right)^2 \left(\frac{\omega_1(1+p_{\#}/m_0c)}{\omega_2(1-p_{\#}/m_0c)} + \frac{\omega_2(1-p_{\#}/m_0c)}{\omega_1(1+p_{\#}/m_0c)} \right) \times \frac{\omega_2 m_0 c}{2\omega_1[(\omega_1^2 + \omega_2^2 - 2\omega_1\omega_2 \cos\theta)^{1/2} + (p_{\#}/m_0c)(\omega_1 - \omega_2)]} \quad (24)$$

This result to order v/c does converge in the limit of low photon energy to the result obtained from a completely nonrelativistic calculation³

$$C(\omega_1, \omega_2, \theta, p_{\#}) = \left(\frac{e^2}{4m_0^2 \pi^2 c^2} \right)^2 \left(\frac{\omega_2}{\omega_1} \right) \times \frac{m_0 c}{(\omega_1^2 + \omega_2^2 - 2\omega_1\omega_2 \cos\theta)^{1/2}} \quad (25)$$

The difference between Eqs. (24) and (25) is of the form $1 + [(\omega_1 - \omega_2)/\omega_1]v/c$ and thus is in some sense the combined effect of the relativistic ground state (v/c) and the relativistic final state $(\omega_1 - \omega_2)/\omega_1$. Although Eqs. (24) and (25) differ considerably at 160 keV in absolute magnitude

(12%), it turns out that their variation across the Compton spectrum is not that much different. Since the Compton profile is obtained from the Compton spectrum after a normalization process which does not depend on the rate of scattering it turns out that using Eq. (25) even at 160 keV will not result in greater than a 2% error in the shape of the Compton profile found from the Compton spectrum. Of course, Eq. (24) is more accurate.

Unfortunately, in working with higher photon energies, Eq. (24) was not used but either Eq. (15) or incorrect forms of Eq. (24) were used.⁴⁻⁸ Some of the forms can result in as much as 10% errors in the shape of the Compton profile for high-atomic-number systems.⁶ We have also

TABLE I. Corrected compton profiles using Eqs. (22)–(24) to process data.

q	Diamond (valence)	Silicon (valence)	Germanium (valence)	Nitrogen	Argon	Krypton
0	1.788	2.658	2.759	5.325	5.118	7.312
0.1	1.781	2.637	2.728	5.282	5.082	7.260
0.2	1.758	2.567	2.640	5.153	4.976	7.109
0.3	1.717	2.437	2.485	4.947	4.806	6.871
0.4	1.661	2.236	2.254	4.676	4.581	6.559
0.5	1.587	1.965	1.954	4.354	4.310	6.191
0.6	1.501	1.640	1.608	4.000	4.007	5.787
0.7	1.399	1.291	1.248	3.630	3.686	5.367
0.8	1.284	0.953	0.911	3.259	3.357	4.950
0.9	1.154	0.659	0.626	2.901	3.034	4.552
1.0	1.008	0.430	0.412	2.568	2.726	4.185
1.1	0.853	0.272	0.277	2.266	2.441	3.859
1.2	0.696	0.176	0.182	1.997	2.184	3.577
1.3	0.549	0.124	0.137	1.762	1.959	3.341
1.4	0.421	0.100	0.116	1.559	1.765	3.146
1.5	0.315	0.088	0.102	1.384	1.602	2.989
1.6	0.233	0.082	0.090	1.234	1.467	2.863
1.7	0.175	0.077	0.086	1.104	1.357	2.761
1.8	0.135	0.074	0.084	0.991	1.266	2.676
1.9	0.109	0.071	0.082	0.892	1.191	2.602
2.0	0.094	0.065	0.081	0.805	1.128	2.535
2.2	0.075	0.055	0.077	0.664	1.023	2.405
2.5	0.055	0.045	0.063	0.521	0.899	2.213
3.0	0.032	0.034	0.049	0.396	0.737	1.886
3.5	0.017	0.026	0.035	0.295	0.626	1.582
4.0	0.014	0.023	0.025	0.234	0.525	1.271
5.0	0.005	0.008	0.007	0.143	0.357	0.916
6.0	0.001	0.005	0.000	0.083	0.252	0.673
7.0	0.000	0.001		0.046	0.174	0.503
8.0		0.000		0.029	0.131	0.382
9.0				0.018	0.099	0.301
10.0				0.008	0.074	0.240
15.0				0.005	0.023	0.091

used an incorrect form in our previous work. One error was our inclusion in Eq. (6) of the wrong flux factor K_1 instead of $m\omega_1$. We have included in Table I our corrected Compton profiles for the high- Z elements. Though the changes are larger than our experimental errors no change in the conclusions reached in the study of those systems is required by the correction.

Since we have now shown that for $v/c > 0.1$, the Compton profile is distorted by more than 1%, the question of data analysis still remains for systems with elements of atomic number greater than 20. If the goal of Compton scattering is to measure accurately the velocity distribution of the outer electrons then the problem is how to subtract the contribution of the tightly bound core electrons. It is usual practice in the analysis of Compton-scattering experiments to integrate the corrected spectrum out to some maximum p_x where only the atomlike core electrons contribute. One then equates the area under that part of the Compton spectrum to the area expected on the basis of atomic calculations. By Eq. (17) one sees that the core 1s electrons will contribute to the scattered intensity proportionally greater than the other electrons because of their large \bar{v} . Thus the change in over-all intensity of the 1s electrons causes not only the wrong shape to be subtracted but also the wrong magnitude. Since a core electron's profile is very flat, this has the effect of giving a long tail to the outer electron's profile and thus reducing the values in the low- p_x region. For example the $J(p_x)$ value for a 1s core

electron in copper is about $\frac{1}{30}$ that of the outer electrons in the small- p_x region. Thus if the normalization integration is restricted to as small a region as possible (i. e., five times the half-width of the profile), then even an overall 6% error in the core will only cause a 1% error in the deduced $J(p_x)$ values for the outer electrons in the small p_x region. The error in the tail of outer electrons profile, will be in most cases within the statistical uncertainty of the experiment. It is exactly the preferred sensitivity of the Compton profile that makes this technique more successful than other techniques in obtaining information about outer electrons.

We have calculated the differential cross section for Compton scattering and stated the conditions and validity of relating this cross section to a Compton profile. The difficulties discussed together with corrections that may be necessitated because of the failure of the impulse approximation may in the future limit the usefulness of Compton profiles to the extent that comparison with very accurate theories is not easily made. However, the measurement of anisotropies in momentum distributions is to first order unaffected by all the difficulties and hence can continue to play a very important role in our investigation of solid state systems.

We would like to point out that the cross section problem was brought to our attention by T. Paakkari. We also gratefully acknowledge the very helpful discussions with P. M. Platzman and P. C. Hohenberg.

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