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Impulse Approximation in Compton Scattering

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IMPULSE APPROXIMATION IN COMPTON SCATTERING

by

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ABSTRACT

The purpose of this paper is to review the current literature on the theory and the use of Compton x-ray scattering and the validity of the impulse approximation in Compton scattering analysis.

Introduction

The development of high-resolution methods [1,2,3] for the measurement of Compton x-ray scattering in solids provides a particularly sensitive tool for investigating the momentum distribution of outer shell atomic electrons. Thus, it offers a very good test of the accuracy of theoretical band calculations, since the Compton profile appears to depend on the details of the valence-electron wave functions. Until today all measurements have been made on light elements, $Z \leq 15$, and their compounds, and all experimental results have been analyzed utilizing a theory which assumes that the electrons which take part in scattering may be treated as free [1]. Eisenberger gives the theoretical justification for this approximation[4]; and comes to the conclusion that impulse approximation, IA, gives very accurate results for weakly bound electrons. And since the light elements have all their electrons (even the core-electrons) weakly bound, the earlier measurements give reliable results.

The impulse approximation is valid if (1) the photon interacts with only a single electron and (2) the binding forces between the ejected electron and the other particles in the system are essentially constant during the time of the collision. If the incoming-photon energy is large compared

with the energies of the system, condition (1) is satisfied. Furthermore, if the final energy of the Compton electron is much greater than its initial energy, the collision time will be much shorter than the time required for any rearrangement of the remaining electrons, and condition (2) will be satisfied. The net effect is that the photon and electron exchange energy and momenta in an essentially constant potential field.

Theory

Consider the incoherent scattering of x-rays from a system containing electrons. Such a scattering process is shown schematically in Fig.1.

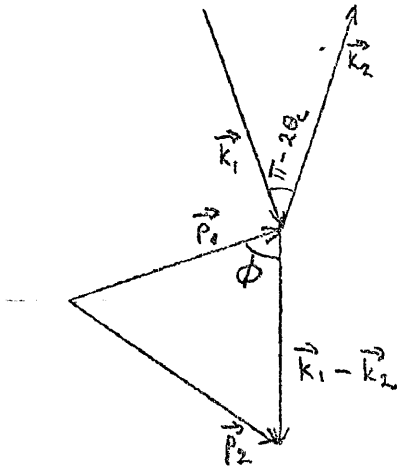

Fig.1. Schematic diagram of Compton scattering

The final and initial photons have been characterized by the wave vectors $\vec{k}_2$ and $\vec{k}_1$, respectively, and before collision the electron momentum is $\vec{p}_1$, being after collision $\vec{p}_2$. Now we can characterize the scattering cross section by the two quantities

$$w = w_1 - w_2 \qquad \vec{k} = \vec{k}_1 - \vec{k}_2 \qquad (1),$$

where w_1 and w_2 are the initial and final frequencies of the photon. Using the energy conservation laws for the free moving electron we get the equations

$$\vec{k} = \vec{p}_2 - \vec{p}_1 \qquad w = \frac{p_2^2 - p_1^2}{2m} = \frac{k^2}{2m} + \frac{\vec{k}\cdot\vec{p}_1}{m} \qquad (2),$$

where $\hbar=1$.

Referring to Fig.1

$$p_2^2 = p_1^2 + |\vec{k}_1 - \vec{k}_2|^2 - 2p_1|\vec{k}_1 - \vec{k}_2|\cos\phi$$

$$\left[(\vec{k}_1 - \vec{k}_2)\cdot\vec{p}_1\right] / |\vec{k}_1 - \vec{k}_2| = p_1\cos\phi = -q \qquad (3),$$

where q is the momentum projection of the initial electron on the scattering vector k. Using Eqs.(2) and (3) we can express q by the frequency of the system

$$q = \frac{mw}{|\vec{k}_1 - \vec{k}_2|} - \frac{|\vec{k}_1 - \vec{k}_2|}{2} \qquad (4).$$

According to definition

$$\frac{\vec{k}_1\cdot\vec{k}_2}{|\vec{k}_1||\vec{k}_2|} = \cos 2\theta_c \qquad (5).$$

Finally we solve from Eqs.(4) and (5) by reinserting $\hbar$ that

$$q = \frac{mc(\lambda_2 - \lambda_1) - 2h\sin^2\theta_c}{\lambda^*} \qquad (6),$$

where λ^* is given by:

$$\lambda^* = (\lambda_1^2 + \lambda_2^2 - 2\lambda_1\lambda_2\cos 2\theta_c)^{1/2}.$$

λ_1 and λ_2 are the wave lengths of the initial and final photons, respectively. Equation (6) clearly shows that the momentum projection of the electron depends linearly on the wave length of the scattered photon. For the change of the wave length of scattering photon, if it ejects the electron that is originally at rest we get the formula

$$\lambda_2 - \lambda_1 = \frac{2h}{mc}\sin^2\theta_c \qquad (7)$$

that is a familiar formula from elementary physics courses.

Thus, if k_2 and k_1 are fixed experimentally, $p_1\cos\phi$ is uniquely determined, and we can relate the distribution of wave lengths, scattered from the sample in a fixed angle , to the distribution of q's of the electronic system.

For the x-rays and scattering angles used in current experiments the recoil energies of electrons are typically of the order of 1 keV and one is concerned with values of $\omega_1 \cong 20$ keV and $k_1 = \frac{2\pi}{\lambda_1} \sim 10^{-1}$ Å^{-1} in the x-ray region so that a non-relativistic description of the cross section is adequate. For the weak scattering, we can calculate the cross section

by using lowest order Born approximation, BA, when the Hamiltonian contains the external field in the first order. We can write for the electronic system the Hamiltonian in a form

$$H = \frac{p_1^2}{2m} + V(r) = H_0 + V(r) \qquad (8),$$

where the quantity V(r) is the external potential. The coupling to the electromagnetic field can be obtained by replacing $\vec{p}_1$ by $\vec{p}_1 - e/c\cdot\vec{A}$, where $\vec{A}$ is the vector potential of the field.

$$H_c = \frac{e^2A^2}{2mc^2} - e\frac{\vec{p}_1\cdot\vec{A}}{mc} \qquad (9).$$

Appendix 1 gives a more detailed discussion the Hamiltonian for charges in a radiation field.

Of the $\vec{p}_1\cdot\vec{A}$ and A^2 terms in the interaction of the electrons with the electromagnetic field, the former makes a contribution to the Compton scattering which is estimated to be quite small in the x-ray region, $w_1 \approx 20$ keV [4], so we can consider the contributions to the Compton cross section from the A^2 term in lowest order pertubation theory. Now, using the description of individual electromagnetic processes in terms of Feynman diagrams [see e.g. 7,8] we can write the differential cross section for Compton scattering from a one electron atom [4,5]

$$\frac{d^2\sigma}{d\Omega\, dw} = \frac{w_2}{w_1} r_0^2 (\vec{e}_1\cdot\vec{e}_2)^2 I(w) \qquad (10),$$

$$I(w) = \sum_i \delta(E_f - E_i - w)\,|\langle f|e^{i\vec{k}\cdot\vec{r}}|i\rangle|^2$$

where $r_0 = \frac{e^2}{mc^2}$ is the classical electron radius, $\vec{e}_1$ and $\vec{e}_2$ are the polarization vectors of the incoming and outgoing photon beams, respectively, and $|i\rangle$ is the initial state wave function and the sum over f runs over final states of the recoiling electron.

Equation (10) is the exact formula for the cross section of one electron atom. Using the proper wave functions for the one electron states the cross section can be found from that equation by fixing the magnitude of p_2 from the energy-conservation δ-function

$$p_2^2/2m = -|E_B| + w \qquad (11),$$

where $|E_B|$ describes the binding energy of the electron. Now, we can derive the formula for Compton cross section in IA and after that make some comparisons between it and the exact formula, Eq.(10).

Impulse Approximation

Suppose we consider the incoherent scattering of x-rays from the electronic system. If the frequency of the incoming x-ray beam is much higher than the binding energy of the electron we can write Eq.(10) in a form [6]

$$\left[\frac{d^2\sigma}{dw\,d\Omega}\right]_{IA} = \frac{w_2}{w_1} r_0^2 (\vec{e}_1 \cdot \vec{e}_2)^2 \int_{-\infty}^{\infty} \langle a_{p_1}^{+}(t) a_{p_1} \rangle e^{i(w - E_3)t}\, dt \qquad (12),$$

where a_{p_1} is the annihilation operator for an electron in a state of momentum p_1 and $\langle\ \rangle$ represents the ground-state expectation value, or

expectation value, and

$$a_{p_1}(t) = e^{iHt} a_{p_1} e^{-iHt} \tag{13}$$

which is the creation operator for an electron into momemtum p_2. The ground-state of the electronic system is competely specified by the momemtum distribution

$$n_{p_1} = \langle a_{p_1}^{+} a_{p_1} \rangle \tag{14}$$

In Eq.(2) we present the energy of the electron after collision

$$E_f = \frac{(\vec{p}_1 + \vec{k})^2}{2m} \tag{15}$$

Our approximations rest so far on the following arguments. The wave length of the photon is so small (large k) that it interacts with an individual electron and ejects it from the atom instantaneously, and furthermore we assume that the ejected electron behaves like a free particle. Thus we can say that for short times, the potential the electron is moving in may be thought of as a constant. That is the essence of the IA.

Neglecting the time dependence of $\langle a_{p_1}^{+}(H) a_{p_1} \rangle$ introduces an error of the order $p_1^2/2m$ relative to $k^2/2m$. To be consistent then we write

$$E_f = \frac{k^2}{2m} + \frac{\vec{p}_1 \cdot \vec{k}}{m} \tag{16}$$

and obtain

$$\left[\frac{d^2\sigma}{d\omega\, d\Omega}\right]_{IA} = \frac{w_2}{w_1} r_0^2 (\vec{e}_1 \cdot \vec{e}_2)^2 \frac{1}{(2\pi)^3} \int n_{p_1} d^3p_1\, \delta\left(\omega - \frac{k^2}{2m} - \frac{\vec{k}\cdot\vec{p}_1}{m}\right) \quad (17),$$

where we have used Eq.(14), too. n_{p_1} is the probability of an electron having momemtum p_1 and the δ-function ensures that at each w_2 only those electrons with the right momemtum projection to satisfy Eq.(4) will contribute to the integral. It is obvious that in the IA equation (17), the binding energy does not appear.

One can rewrite Eq.(17)

$$\left[\frac{d^2\sigma}{d\omega\, d\Omega}\right]_{IA} = \frac{w_2}{w_1} r_0^2 (\vec{e}_1 \cdot \vec{e}_2)^2 J(q) \quad (18),$$

where

$$J(q) = \frac{1}{(2\pi)^3} \int_q^\infty |f(p_1)|^2 d^3p_1 \quad (19),$$

and

$$q = \vec{k} \cdot \vec{p}_1 \quad (20).$$

The quantity $f(p_1)$ is the Fourier transform of the ground-state wave function $\psi(r)$, i.e.,

$$f(p_1) = \int e^{-i\vec{p}_1\cdot\vec{r}} \psi(r)\, d^3r \quad (21),$$

and $J(q)$ is the Compton intensity we use when we compare theoretical and experimental results in Eq.(17). The energy δ-function in Eq.(17) tells us that the scattered photon is shifted in frequency both by the momemtum transfer term $k^2/2m$ and the Doppler shift component $(\vec{k}\cdot\vec{p}_1)/m$. Thus in the IA, the essential nature of the Compton scattering process is

revealed to be a Doppler broading of the scattered photon energy.

Validity of Impulse Approximation

In deriving the impulse approximation, Eisenberger and Platzman [4] showed that to accuracy $2m|E_B|^2/k^2$, we can replace Eq.(10) by Eq.(17). For light elements $2m|E_B|^2/k^2$ is of the order 10^{-3}. Thus, the IA can be used for analyzing experimental results in that case.

Eisenberger [4] has compared the exact Compton spectrum and the IA Compton spectrum with different Z's (Fig.2). The dotted curves are the exact results. The solid curves are

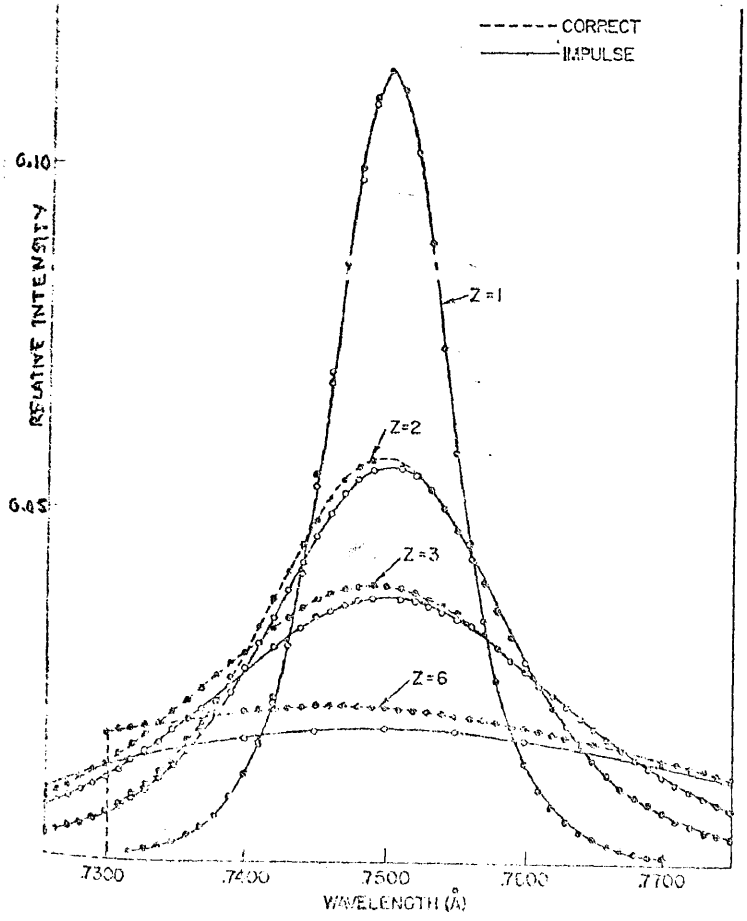

FIG. 2 Compton spectrum for hydrogenic systems with different Z's. A comparison between the results of the exact calculation [Eq. (11)] and the IA [Eqs. (15) and (20)] for Mo K_{α_1} radiation ($\omega_i \cong 17.4$ keV and $E_R \sim 940$ eV).

obtained by using the IA results. It is seen that the long wave length large recoil portion of the spectrum is given very accurately by the IA. When we approach threshold , the deviations become larger. For $\omega > k^2/2m$, the IA holds uniformly to something of order $(E_B/E_R)^2$, where $E_R = k^2/2m$.

Eisenberger [4] has also shown (Fig.3) that if we increase the energy of incident x-rays the IA gives more accurate results for the Compton cross section.

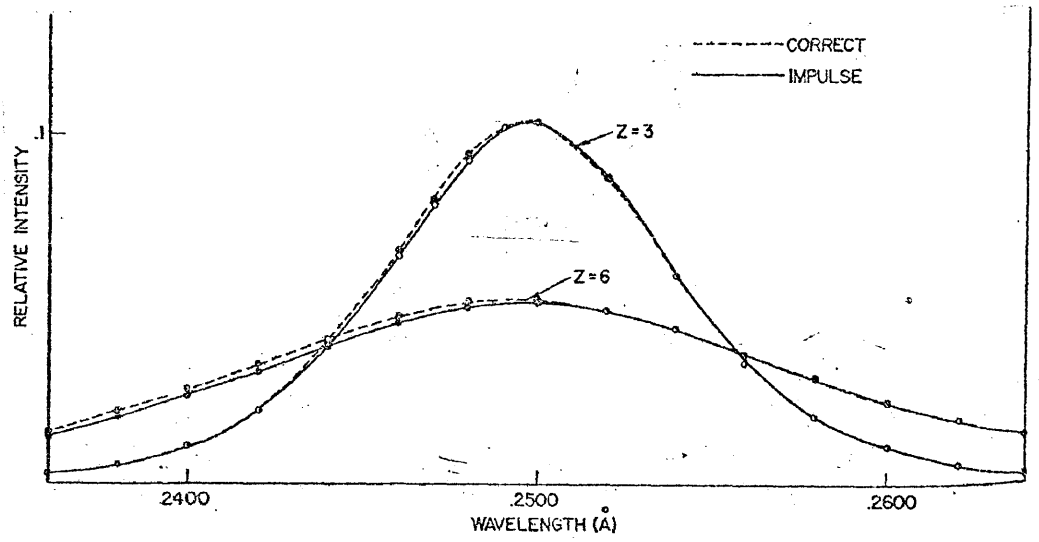

FIG. 3. Compton spectrum for hydrogen systems with different Z's, for tungsten K_{α_1} radiation ($\omega_1 \cong 59.3$ keV and $E_R \sim 9.7$ keV).

As mentioned before, until recently all measurements have been made in the x-ray region using x-rays from a molybdenum spectrometer tube, powered by a very stable constant potential generator. In that case we came to a

conclusion that impulse approximation holds for light elements, $Z \leq 15$. Thus in the case we want to study elements or their compounds beyond this limit we have to use harder radiation for irradiating sample. Nowadays some experimentalists[9] have measured the Compton spectrum using 59.54 keV γ-rays. In this case we can believe that our approximation, the photon interacts with only a single electron, have more evidence because the probability that the photon finds an electron increases if the wave length of the photon becomes smaller. It seems to me that in the future Compton experimentalists will more and more change their x-ray spectrometers into the γ-ray ones.

Appendix 1

Classical Hamiltonian For Charges In A Radiation Field

An external field in electromagnetic theory can be described by means of a scalar potential ϕ and a vector potential $\vec{A}$, according to equations

$$\vec{E} = -\overrightarrow{grad}\,\phi - \frac{\partial \vec{A}}{\partial t} \quad , \quad \vec{B} = curl\ \vec{A} \qquad (A1),$$

where $\vec{E}$ is the electric field and $\vec{B}$ is the magnetic induction. Then we can show that the Hamiltonian of a system of charges, such as electrons and nuclei, in this external field, and acting on each other by Coulomb forces, is

$$H = \sum_j \left\{ \frac{\left[\vec{P}_j - e_j \vec{A}(r_j)\right]^2}{2m_j} + e_j \phi(r_j) \right\} + V(x_1 \ldots z_N) \qquad (A2),$$

where m_j is the mass of the j:th particle, e_j its charge, p_j its momemtum, r_j its vector position, $A(r_j)$ and $\phi(r_j)$ are the vector and scalar potentials at its position, and $V(x_1 \ldots z_N)$ is the potential energy of the Coulomb interactions between the pairs of particles.

It is easy to show that using Hamilton's equations for the Hamiltonian (A2) we have the equations of motions for the charged particles, with an additional force

$$\vec{F}_i = e_i \left\{ \vec{E}(r_i) + \left[\vec{V}_i \times \vec{B}(r_i) \right] \right\} \qquad (A3),$$

where $E(r_i)$ is the external electric field at the position r_i of the i:th particle, and $B(r_i)$ is the external magnetic field at the same position.

Because we can see the Hamiltonian of Eq.(A2) leads to the correct equation of motion for the particle moving in an external field, we are justified in adopting it for our treatment of an atom in an external field. If we wish to denote the unperturbed Hamiltonian of the atom in the absence of the field as H_0, where we have

$$H_0 = \sum_j p_j^2/2m_j + V(x_1, \ldots z_N) \qquad (A4)$$

we can then write the whole Hamiltonian as $H_0 + H_c$, where H_c is the pertubative Hamiltonian arising from the field. We then have

$$H_c = \sum_j \left[-\frac{e_j}{m_j} \vec{p}_j \cdot \vec{A}(r_j) + \frac{e_j^2}{2m_j} A^2(r_j) + e_j \phi(r_j) \right] \qquad (A5),$$

where we have three types of terms arising from the external field: the term linear in $\vec{A}$, that quadratic in $\vec{A}$, and that in ϕ. Now we do not need the term in ϕ, because the radiation field can be described in terms of a vector potential only. We have also to remember that the Hamiltonian (A2) is not entirely complete for an atomic system, it does not take account of magnetic interactions between the particles of the atomic system, but it is adequate for the problem of this paper.

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