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THE UTILITY OF COMPTON SCATTERING IN DETERMINATION OF ELECTRON MOMENTUM DENSITY

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We present new insights regarding the validity of the impulse approximation (IA) in determining electron momentum density (EMD) from Compton scattering. These insights are obtained utilizing the code we have recently developed for the full calculation of the triple differential cross-section (TDCS) for Compton scattering. We find that, due to the averaging, at lower energies IA is more accurate for the double differential cross-section (DDCS) than for TDCS. We conclude that at such energies an EMD determination from the DDCS is more accurate than its direct determination through the measurement of the TDCS at the same energy. We also discuss the validity of IA for calculations of other less averaged Compton observables.

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1. Introduction

We offer some new insights concerning the utility of the impulse approximation (IA) in electron momentum density determination, obtained as we developed a code for calculating the triple differential cross-section (TDCS) for Compton scattering [1]. This work is based on our previous code [2, 3] for the calculation of the double differential cross-section (DDCS), in which the ejected electron is not detected. TDCS corresponds to a scattering situation in which both outgoing particles (photon and electron) are detected in coincidence. Our TDCS and DDCS results are based on the full relativistic second-order S-matrix (SM) theory for Compton scattering within the independent particle approximation (IPA).

We have examined the expected validity of IA by comparing its predictions with our S–matrix (SM) calculations. We confirm that, contrary to one's hope, the requirement for the validity of IA in TDCS is about an order of magnitude stronger than in the case of DDCS, which means that much higher photon energies are required. While for DDCS it is sufficient to require that photon momentum transfer $\boldsymbol{K}$ is similar to or greater than the average momentum p_{av} of the bound electron which is ionized, for TDCS it is required that $|\boldsymbol{K}| \gg p_{av}$. We will discuss the consequences of these findings for the utilization of IA for Compton scattering in atomic, molecular and condensed matter physics.

2. *Theoretical considerations*

Here we will consider only the peak region of the Compton spectrum, for which it is found that IA is generally applicable for DDCS calculations [3–6], and we will examine the corresponding situation for the TDCS. The peak of the DDCS Compton spectrum appears in the vicinity of the energy corresponding to the scattering by a free electron at rest, which is specified by the Compton frequency $\omega_C = \omega_1/[1 + (\omega_1/m)(1 - \cos\theta)]$ for scattering of the photon at an angle θ. For higher incident-photon energies, this kinematical region becomes accessible. The Compton scattering mechanism which also describes scattering by free electrons (in the nonrelativistic region arising from the so–called "$\boldsymbol{A}^2$" term of the interaction Hamiltonian) becomes important when the incident photon momentum $|\boldsymbol{k}_1|$ is similar to or greater than the average momentum p_{av} of the bound electron which is ionized, $|\boldsymbol{k}_1| \gtrsim p_{av}$. For such energies of incident photons, the total cross-section for Compton scattering [7] is comparable to or dominates that of photoeffect as a mechanism of ionization of a given sub-shell.

The usual picture of IA is that the bound electron is treated as a momentum distribution of free electrons, and outgoing electrons are considered as free. A relativistic expression for IA has been given by Eisenberger and Reed [8] and by Ribberfors [9], who used a relativistic expression for Compton scattering from a free electron distribution $\rho(\boldsymbol{p})$[10]. With this approach, based on the usual picture of IA, one can obtain an expression for TDCS in IA, by not performing the integration over the outgoing electron angles, in the form

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\omega_2 \mathrm{d}\Omega_2 \mathrm{d}\Omega_f} = \frac{m^2 r_0^2}{2} \frac{\omega_2}{\omega_1} \frac{p}{E_f} X(K_1, K_2) \rho(\boldsymbol{p}), \tag{1}$$

where

$$K_1 = E\omega_1 - \boldsymbol{p}\cdot\boldsymbol{k}_1,\ K_2 = E\omega_2 - \boldsymbol{p}\cdot\boldsymbol{k}_2, \tag{2a}$$

$$\boldsymbol{p} = \boldsymbol{p}_f + \boldsymbol{k}_2 - \boldsymbol{k}_1,\ E = (p^2 + m^2)^{\frac{1}{2}},\ E_f = (p_f^2 + m^2)^{\frac{1}{2}}, \tag{2b}$$

$$X(K_1, K_2) = \frac{K_i}{K_f} + \frac{K_2}{K_1} + 2m^2\left(\frac{1}{K_1} - \frac{1}{K_2}\right) + m^4\left(\frac{1}{K_1} - \frac{1}{K_2}\right)^2. \tag{2c}$$

In Eqs. (1) and (2), $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ represent the momenta of incoming and outgoing photons, respectively, ω_1 and ω_2 denote the energies of incoming and outgoing photon, respectively, m is the electron rest mass, r_0 is the electron classical radius, and $\boldsymbol{p}_f$ is the momentum of outgoing electron. The electron distribution $\rho(\boldsymbol{p})$ is given by the Fourier transform of the wave function of the bound electron, *i.e.*, $\rho(\boldsymbol{p}) = |\Psi(\boldsymbol{p})|^2$.

In fact Eisenberger and Platzman [11] have shown that the non-relativistic IA results for DDCS can be derived, using the "$\boldsymbol{A}^2$" approximation for the interaction of radiation with matter, without treating the initial and final states as free. The interaction of an electron with the external field (atomic potential) in the initial state and the same interaction in the final state approximately cancel out, when DDCS is considered at high photon energies, in such a way as to reproduce the usual result for IA obtained assuming free electrons. The essential point in obtaining this result is the use of the completeness relation for electron states [12] when integrating over outgoing-electron angles. This extended validity of IA is not obtained for TDCS [13] for double and single differential cross-sections when outgoing electron is observed (averaging over photon observables does not improve the validity of IA [14]), or for other Compton observables which can be considered less averaged, as has been discussed previously [1] in the example of the IA treatment of the total cross-section for double ionization Compton scattering from helium (even though averaged over both outgoing electrons and over the outgoing photon).

The possible validity of IA is restricted to the region of the Compton peak (quasi–free kinematics). The generally accepted criteria for the validity of IA in that region is that the photon momentum transfer $|\boldsymbol{K}|$ must be much larger than the average momentum p_{av} of the bound electron which is ionized [15–17]

$$\frac{p_{av}}{|\boldsymbol{K}|} \ll 1. \tag{3}$$

However, IA has been used in the Compton peak region for the DDCS even when $|\boldsymbol{K}| \approx p_{av}$, and it has been found to be fairly accurate even in such circumstances [18,19]. The explanation for this extended validity of IA in DDCS lies in the fact that the electron does not have to be treated as free, in initial or final state, when considering the DDCS, in order to obtain the usual impulse approximation DDCS. In the case of DDCS, we may use the criterion

$$\frac{p_{av}}{|\boldsymbol{K}|} \lesssim 1\,, \tag{4}$$

if the peak region is discussed. However, we have confirmed [1] that in the case of TDCS, Eq. (4) is not a good criterion for the validity of IA, but rather the generally accepted criterion Eq. (3) must be used.

We illustrate this in Fig. 1. Recently, an absolute measurement of DDCS on K-shell electrons of copper [19] was performed for several scattering angles using 59.32 keV photons. The authors find very good agreement between IA calculations and experimental results measured in the region where, in agreement with the criterion of Eq. (4), $p_{av}/|\boldsymbol{K}| \approx 0.7$. Here we examine this case, calculating both DDCS and TDCS using IA and also our SM code. This is an example of the situation in which there is a good agreement among experiment, IA predictions and SM calculations for DDCS in the region where $p_{av}/|\boldsymbol{K}| \approx 1$, as we illustrate in Fig. 1a for the photon scattering angle $\theta = 140°$. In contrast, we find that IA is poor in treating TDCS in comparison with SM calculations, as shown in Fig. 1b, for the same photon scattering angle and two choices of the electron scattering angle within the scattering plane, defined by momenta of the incoming and outgoing photon. For a free electron at rest and for a given photon scattering angle θ, the outgoing electron momentum is fixed (by energy and momentum conservation) and it is equal to photon momentum transfer. For the photon scattering angle $\theta = 140°$ this

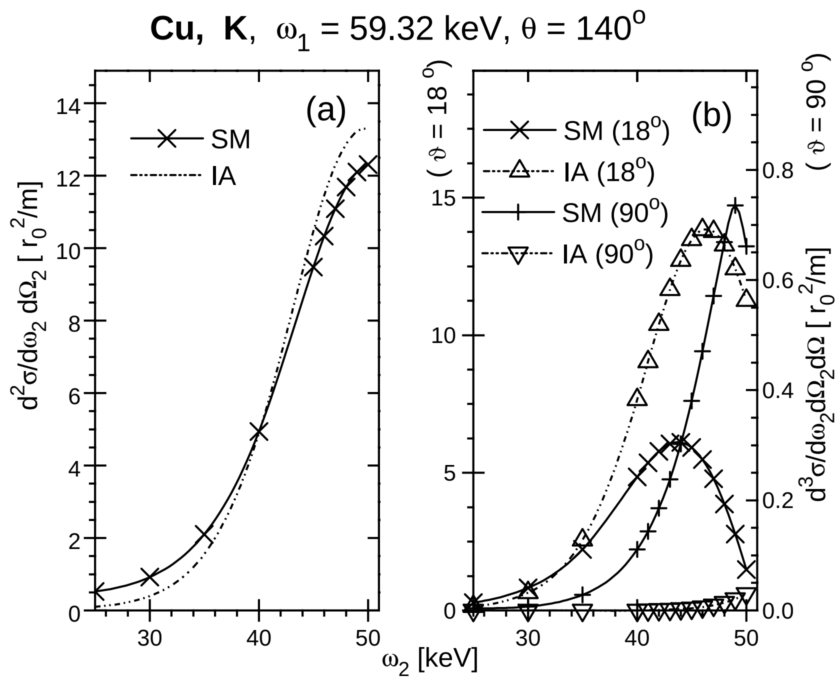

Fig. 1. Scattering of 59.32 keV *photons from a* K*–shell electron of* Cu *into* 140°*, taken from [1]. The cross-sections are obtained using S-matrix IPA calculations and IA. (a) Double differential cross-section, (b) triple differential cross-section for two choices of outgoing-electron angles within the scattering plane,* $\vartheta = 18°$ *(scale shown on the left side of the right panel) and* $\vartheta = 90°$ *(scale shown on the right side of the same panel).*

corresponds to the outgoing electron angle $\vartheta = 18°$, measured from the incident photon direction, and lying in the scattering plane. For such a choice of outgoing-electron angle (which we call free kinematics), in the case of Compton scattering from bound electrons, where all outgoing electron angles are kinematically allowed, the IA is expected to work well. However, as illustrated in Fig. 1b, IA overestimates the TDCS by about a factor of two (for $p_{av}/|\boldsymbol{K}| \approx 1$). In general, we find that for angles close to those corresponding to free kinematics, the IA overestimates TDCS in the peak region. For angles differing much from free kinematics, IA underestimates TDCS. We also illustrate this in Fig. 1b, showing the TDCS for the electron angle $\vartheta = 90^\circ$ with the electron momentum in the scattering plane. By integrating the IA TDCS over outgoing-electron angles, these deviations average, resulting in a quite accurate IA description of DDCS. In contrast to this relatively low-energy situation, our investigation [1] indicates that we can use IA for TDCS near the peak region, with an error of less than about 5%, if the ratio $p_{av}/|\boldsymbol{k}|$ is less than about 0.1.

Now we discuss the consequences of these findings for situations in which IA is used in determining Compton scattering cross-sections.

(1) The IA provides an interpretation of the measured differential cross-section in terms of the momentum density of bound electrons. Due to this fact, Compton scattering has become an important tool in investigating electron momentum density (EMD) in atomic, molecular and condensed matter systems [15]. In most of these experiments, DDCS are measured and interpreted in terms of the so-called Compton profile [15], which is a two dimensional integral over EMD. Complete information about EMD can be obtained by employing reconstruction techniques [20] to a large number of measured Compton profiles. An alternative approach has sometimes been utilized [21] in which the scattered photon and the ejected electron are detected simultaneously. Then in IA there is no integration over EMD and therefore no need for a reconstruction. In such TDCS measurements, information about the three-dimensional EMD can be obtained directly, *e. g.* using Eq. (1) with unpolarized photons. In both types of experiments (*i.e.* in measurements of DDCS or TDCS), the validity of the IA is essential for the simple interpretation of the experimental cross-sections in terms of EMD. Hence, we conclude that at lower energies the EMD from the DDCS is more accurate than its direct determination through the measurement of the TDCS at the same energy. However, in the TDCS experiments known to us [21] which were performed for the purpose of obtaining information about EMD of valence and weakly bound electrons, high photon energies were employed (much higher than one would need for IA to be valid for Compton profile measurements). This was partly motivated by the fact that electrons produced in Compton scattering have mostly small energies. These electrons exhibit multiple scattering in relatively thick targets, which introduces error in determining outgoing electron angles in the Compton process. The problem is reduced at higher photon energies yielding higher energy electrons and less multiple scattering. Our study [1] confirms that for these relatively high photon energies one has achieved validity of IA for TDCS.

Another technique for direct determination of the EMD of bound electrons, electron momentum spectroscopy, is based on (e,2e) collisions near the Bethe ridge. There the direct connection of measured cross-sections with EMD is obtained within IA in the kinematical region where criterion Eq. (3) is satisfied ($|\boldsymbol{K}|$ being momentum transfered from the initial electron) [22], just as in TDCS Compton scattering as discussed here. In measuring EMD of valence electrons by (e,2e) collisions, this means employing electrons of about 1 keV kinetic energy, or higher [22].

(2) IA has also been employed for the calculation of cross-sections for double ionization in Compton scattering [23], a subject of considerable recent experimental and theoretical investigation [24], particularly for the case of the ratio of double to single ionization total cross-sections in helium. There, as in the case of TDCS for single ionization, it had been hoped that a similar region of validity would apply as in DDCS. But, again, the comparison of IA calculations with experiments [25,26] and other calculations [27] indicates that larger energies are required for the IA treatment to be accurate, much larger (approximately an order of magnitude) than one would expect from the single ionization DDCS case. In the derivation of IA for double ionization, explicit use of the plane-wave approximation for the fast outgoing electrons is made, as in the TDCS derivation, and unlike in DDCS. Viewing the double ionization Compton total cross-section as a more differential observable than DDCS for single ionization, as is also TDCS, leads [1] to the expectation that IA for the total cross-section for double ionization in Compton scattering from helium is adequate above about 50 keV.

(3) Recently the utilization of the double-ionization Compton profile (as distinguished from the ordinary Compton profile), also based on IA, in double ionization Compton scattering has been suggested for studying the correlation effects in helium [28]. This means measuring the double differential cross-section (with respect to outgoing-photon energy and angle) for double ionization in Compton scattering, as in the coincidence of scattered photons with double ionized atoms. The arguments [1] used above for estimating the accuracy of IA for the total cross-section for double ionization Compton scattering lead to the conclusion that the double ionization Compton profile interpretation of the cross-section can be valid, for most angles, for photon energies above about 50 keV, the energies which are available with today's synchrotrons.

(4) Compton scattering is one of the primary processes responsible for attenuation of radiation in matter. In modeling electron–photon transport through matter (important in technological and biomedical fields), for energies for which the Compton process is significant, one needs an approach which is both fast and reliable. Some of the more sophisticated transport codes [29] treat Compton scattering using IA. Since we have found that IA is inadequate in predicting the angular and energy distribution (TDCS) of Compton electrons unless $|\boldsymbol{K}| \gg p_{av}$ for a particular shell, caution is needed when there is a significant contribution from several inner shells for which the criterion is not satisfied.

3. Conclusion

We have found that the criteria given by Eq. (4) giving an extended validity for impulse approximation (IA) in DDCS can not be used for less averaged Compton observables. Instead, the criteria Eq. (3) must be used when free electron states are required in the derivation, as in the case of TDCS or the double ionization total cross-section. We have illustrated our findings, using an example for which the validity of IA for DDCS has been demonstrated both experimentally and within our S-matrix calculation, but for which IA gives incorrect predictions for TDCS in comparison with our SM results. Since within IA one may interpret both the measured double differential cross-section (DDCS) (integrated over electron momenta) and the TDCS in terms of the momentum distribution of bound electrons, we have concluded that at lower energies electron momentum density determination from the DDCS is more accurate than its direct determination through the measurement of the TDCS at the same energy.

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PRIMJENLJIVOST COMPTONOVOG RASPRŠENJA ZA ODREĐIVANJE IMPULSNE RASPODJELE ELEKTRONA

Predstavljamo nove poglede o valjanosti impulsne aproksimacije (IA) za određivanje impulsne raspodjele elektrona (EMD) Comptonovim raspršenjem. Ti se pogledi osnivaju na primjeni nedavno razvijenog programa za računanje trostrukog diferencijalnog udarnog presjeka (TDCS) za Comptonovo raspršenje. Nalazimo da zbog računanja prosjeka, IA je na niskim energijama točnija za dvostruke diferencijalne presjeke (DDCS) nego za TDCS. Zaključujemo kako je na tim energijama određivanje EMD na osnovi DDCS točnije nego mjerenjem TDCS na istoj energiji. Raspravljamo također valjanost IA za određivanje drugih Comptonovih manje usrednjenih veličina.