Triply differential cross section for Compton scattering

Z. Kaliman
Pedagogical Faculty, University of Rijeka, 51000 Rijeka, Croatia

T. Surić and K. Pisk
R. Bošković Institute, P.O. Box 1016, 10000 Zagreb, Croatia

R. H. Pratt
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
(Received 7 November 1997)

The triply differential cross section for Compton scattering from atomic electrons is obtained numerically in a full relativistic second-order S-matrix calculation based on the independent particle approximation. We compare our results with the results of more approximate approaches. Special attention is paid to the validity of the impulse approximation (IA), which has often been used for calculating the doubly differential cross section even when the photon momentum transfer $\mathbf{K}$ is similar to the average momentum p_{av} of the bound electron, which is ionized (and IA is found to be fairly accurate even in such circumstances). We here show that, on the contrary, IA calculations of the (less averaged) triply differential cross section are quite inaccurate for $|\mathbf{K}| \sim p_{\mathrm{av}}$, even near the peak in the triply differential cross section (where the free kinematics for scattering from an initial free electron at rest are satisfied and where IA should work the best). We conclude that electron momentum distribution determination through the Compton profile, using the doubly differential cross section, is more accurate at lower energies than direct determination through the measurement of the triply differential cross section at the same energy. In addition, viewing the total cross section for double ionization in Compton scattering as another observable less averaged than the doubly differential cross section in single ionization, we estimate that IA predictions of the total cross section for double ionization in Compton scattering from Helium are adequate above about 50 keV. [S1050-2947(98)07604-5]

PACS number(s): 32.80.Cy

I. INTRODUCTION

We study the triply differential cross section (TDCS) for Compton scattering from atomic electrons using full relativistic second-order S-matrix (SM) numerical calculations within the independent particle approximation (IPA). Our study corresponds to the situation in which polarized or unpolarized incident photons are scattered off an electron in a specified subshell of an unpolarized atom. In our work we have summed over outgoing photon polarizations and outgoing electron spin directions.

The underlying formalism and numerical code are extensions of previous work [1–8] on Compton scattering. Our approach in this paper is based on the framework of Ref. [5], where the doubly differential cross section (DDCS) is calculated, developing a suitable code, within second-order QED S-matrix theory, for Compton scattering from bound electrons within IPA. We here reformulate the theory and extend the code to the case of the observation of the complete kinematics for Compton scattering from bound electrons, i.e., for the calculation of TDCS.

In beginning a more systematic study of TDCS for various photon energies, atomic states and atomic systems, we limit our discussion here mostly to the region of incident photon energy in which the total cross section for Compton scattering [9] is comparable to or dominates that for the photoeffect as a mechanism of ionization of a given subshell. For incident photon momentum $\mathbf{k}_1$ and average bound electron momentum p_{av} this region is roughly determined by $|\mathbf{k}_1| \gtrsim p_{\mathrm{av}}$. Our discussion of TDCS, within this region, focuses mainly on the kinematical region (choice of outgoing photon energy and angles and electron angles) close to that of free particle kinematics for an initial electron at rest. In this kinematical region the momentum transfer to the nucleus is small and the Compton scattering spectrum (by Compton spectrum we generally mean TDCS or DDCS as a function of scattered photon energy for fixed angles) features a peak. We call this the Compton peak region. (This should be distinguished from the resonant Compton peak, which is governed by a different Compton scattering mechanism and is positioned in a different kinematical region.) The position of the Compton peak in TDCS can approximately be determined by considering Compton scattering from a free electron at rest. There, for a given photon scattering angle, the outgoing electron angle is fixed by energy and momentum conservation. For such a choice of outgoing electron angle, in the case of Compton scattering from bound electrons where all outgoing electron angles are kinematically allowed, we use the term ''free kinematics.''

In discussing the Compton peak region we pay particular attention to the validity of the impulse approximation (IA) approach in treating TDCS for Compton scattering. IA has been widely used in discussing DDCS in Compton scattering [10]. The generally accepted criteria for the validity of IA for Compton scattering is that the photon momentum transfer $\mathbf{K}$ must be much larger than the average momentum p_{av} of the bound electron, which is ionized, $|\mathbf{K}| \gg p_{\mathrm{av}}$. However, IA has also been used for the DDCS even when $|\mathbf{K}| \sim p_{\mathrm{av}}$, and it

has been found to be fairly accurate even in such circumstances. We here show that, to the contrary, IA calculations of the (less averaged) TDCS are quite inaccurate for $|\mathbf{K}| \sim p_{\mathrm{av}}$, even near the peak in the TDCS (where the impulse approximation should work the best) [11]. However, we also confirm that, by increasing the incident photon energy (corresponding to momenta $|\mathbf{k}_1| \gg p_{\mathrm{av}}$) and allowing larger momentum transfers, the impulse approximation results, in the region where $|\mathbf{K}| \gg p_{\mathrm{av}}$, approach ours for TDCS [12].

In addition to the Compton peak region, we also discuss to some extent the other two regions of the Compton spectrum, the infrared divergent and the resonant regions, dominated by mechanisms that require relatively large momentum transfers to the nucleus (and cannot occur for free electrons).

We compare our results with experiments. Recently, coincidence measurements of the scattered photon and ejected electron in Compton scattering have been reported [13,14]. In these experiments the photon momentum transfers are much larger than the average momentum of bound electrons involved in scattering (binding effects are not very important). We demonstrate that, for these photon momentum transfers, the IA approach for TDCS is quite accurate. We are aware of only one other reported measurement of the ejected electron in coincidence with the scattered photon, in a situation where binding effects are very important [15], which was performed 30 years ago. We discuss this case too. However, large error bars prevent meaningful comparison of our calculations with the reported results. It is reasonable to expect that today's experimental techniques should allow more precise measurements and we hope that our work will stimulate new measurements of Compton scattering TDCS in the region where electron binding effects are important.

In recent years IA has also been employed for calculating cross sections for double ionization in Compton scattering [16]. Viewing the double ionization Compton scattering total cross section as another Compton observable which is also less averaged than the DDCS in single ionization, we clarify the adequacy of its IA description.

In the next section we describe some features of the Compton spectrum needed for our subsequent discussion and then discuss utilization of IA in Compton scattering and criteria for its validity. In Sec. III we present our formalism for the full SM approach and describe the tests of the code that is based on the formalism. In Sec. IV we compare the computational results from the code with the results of more approximate approaches and with existing experimental data. We discuss the validity of the more approximate approaches, paying particular attention to the IA approach in treating TDCS.

II. IMPULSE APPROXIMATION FOR COMPTON SCATTERING

Generally we may distinguish three regions of the Compton spectrum [5], which correspond to different mechanisms for Compton scattering by a bound electron. These are (1) the infrared divergent region, (2) the resonant region, and (3) the Compton peak region. A full second order S-matrix IPA approach, unlike more approximate approaches, is applicable in all three regions of the spectrum. Most simpler approaches are based on the nonrelativistic photon-electron interaction Hamiltonian, which, in Coulomb gauge, contains two terms: a ''$\mathbf{p}\cdot\mathbf{A}$'' term and an ''$\mathbf{A}^2$'' term. The ''$\mathbf{p}\cdot\mathbf{A}$'' approximation (only the ''$\mathbf{p}\cdot\mathbf{A}$'' interaction term is taken) has been employed in treating Compton spectra in the $|\mathbf{k}_1| \ll p_{\mathrm{av}}$ region [17–19], where the contribution of the ''$\mathbf{A}^2$'' term is negligible. It has also been used in treating the infrared divergent part of the spectrum for higher incident photon momenta, where an approach through the low-energy theorem (LET) is also available [5,20].

For higher incident photon energies ($|\mathbf{k}_1| \sim p_{\mathrm{av}}$) the kinematical region corresponding to the kinematics for photon scattering from a free electron at rest becomes accessible and the ''$\mathbf{A}^2$'' interaction becomes important, giving a Compton scattering mechanism that is also applicable for free electrons [21]. This mechanism becomes significant when $|\mathbf{k}_1| \sim p_{\mathrm{av}}$, and it dominates the region of the spectrum in the vicinity of the energy corresponding to scattering from 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 through angle θ. In the region near ω_C the DDCS Compton spectrum exhibits a peak, which is sometimes described [22–26] within the so-called ''$\mathbf{A}^2$'' approximation (only the ''$\mathbf{A}^2$'' interaction term is taken), often in order to test the more approximate IA approach. We will primarily consider this dominant kinematical region in our discussion of TDCS.

The most widely used approximation for the Compton DDCS has been the impulse approximation (IA). IA is relatively simple to use (it utilizes the atomic potential only through the momentum distribution in the initial electron state) and it is quite accurate (at the level of DDCS) in the incident photon energy region where Compton scattering is comparable to or dominates the photoeffect as a photoionization mechanism. Its validity is not restricted to the nonrelativistic region (unlike the ''$\mathbf{A}^2$'' approximation) and its accuracy increases with increasing photon energy.

The usual picture of IA is that the bound electron is treated as a momentum distribution of free electrons and outgoing electrons are viewed as free. In fact Eisenberger and Platzman [27] have shown that the nonrelativistic IA results for DDCS can be derived, using the ''$\mathbf{A}^2$'' 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 allow the usual interpretation of IA in terms of free electrons. This extended validity of IA does not apply for TDCS. A relativistic expression for IA has been given by Eisenberger and Reed [28] and by Ribberfors [29] using a relativistic expression for Compton scattering from a free-electron distribution $\rho(\mathbf{p})$ [30]. With this approach, based on the usual picture of IA, one can obtain an expression for TDCS in IA, not performing the integration over the outgoing electron angles [31].

Utilizing IA to describe the scattering process, Compton scattering experiments have long been used to provide information on the electron momentum density (EMD) of (mostly) valence electrons [10,32]. In these experiments the DDCS are measured and interpreted in terms of the so-called Compton profile [10], which is a two-dimensional integral over EMD. Complete information about EMD can be ob-

tained by employing reconstruction techniques [33] to a large number of measured Compton profiles. An alternative approach has been utilized [13,14] 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 triply differential cross section (TDCS) measurement information about the three-dimensional EMD is obtained directly. It should be noted that 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.

IA for DDCS is restricted to the region of the Compton peak (quasifree kinematics). The generally accepted criteria for the validity of IA in that region is that the photon momentum transfer **K** must be much larger than the average momentum p_{av} of the bound electron which is ionized [10,26,34],

$$\frac{p_{\mathrm{av}}}{|\mathbf{K}|} \ll 1. \tag{1}$$

However, IA has been used in the Compton peak region for the DDCS even when $|\mathbf{K}| \sim p_{\mathrm{av}}$, and it has been found to be fairly accurate even in such circumstances [35,36]. Hence, in the case of DDCS, we may use the criterion

$$\frac{p_{\mathrm{av}}}{|\mathbf{K}|} \lesssim 1, \tag{2}$$

if the peak region is discussed. Here we will reconsider the validity of criteria Eq. (1) and Eq. (2) for IA when discussing the peak region of Compton spectra. We will show that in the case of TDCS Eq. (2) is not a good criterion for the validity of IA, but rather the generally accepted criterion Eq. (1) must be used.

III. FORMALISM AND NUMERICAL APPROACH FOR SM CALCULATION

The formalism and code for performing calculations of the triply differential cross section for Compton scattering from bound atomic electrons are an extension of previous work [4–8] on DDCS, based on the second-order S-matrix element in QED in Furry's picture. The method is relativistic and it includes the external relativistic atomic field, within the IPA, in all orders. In the IPA all electrons see a common self-consistent central potential and electron-electron correlation effects are neglected.

Our approach allows for calculation of scattering from electrons of any subshell in an atom, described within the IPA, over the whole spectrum of scattered photon energies. Thus far we have concentrated on the cases in which the incident photons are linearly polarized, or unpolarized, the bound electrons are unoriented and no polarization of the scattered photons or spin state of the outgoing electron is detected. This corresponds to the situations that have been investigated experimentally. From an experimental point of view, our present calculation corresponds to a scattering situation in which both outgoing particles, i.e., the scattered photon and the ejected electron, are detected in coincidence, as shown in Fig. 1. The sum of outgoing photon and electron

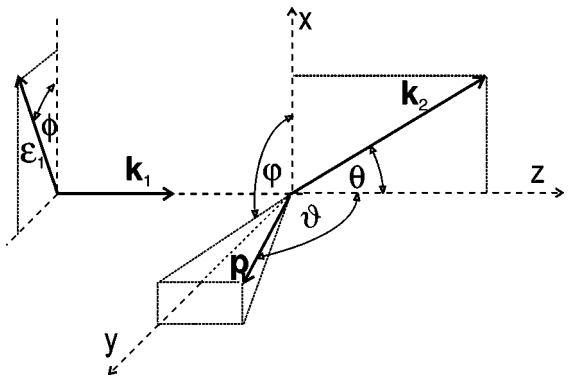

FIG. 1. Scattering geometry used here. The scattering plane is defined by the incoming and scattered photon directions. θ is the photon scattering angle and ϕ is the angle between the vector of incoming photon linear polarization and the scattering plane. The angles ϑ and φ are outgoing electron angles.

energies identifies the subshell from which the scattering occurred.

The Compton matrix element may be written as

$$M = M_a + M_e\,. \tag{3}$$

Following [5], the absorption-first M_a and emission-first M_e amplitudes are expressed (in units $\hbar = c = 1$) as

$$M_{a,e} = 4\pi\alpha i \int d^3y\, \overline{\psi_2}(\mathbf{y})\, \boldsymbol{\gamma}\cdot\mathbf{A}_{2,1}(\mathbf{y}) F(\mathbf{y}, \eta_{a,e}), \tag{4}$$

where $\mathbf{A}_1$ and $\mathbf{A}_2$ represent incoming and scattered photon states, $\eta_a = E_1 + \omega_1$ for M_a and $\eta_e = E_1 - \omega_2$ for M_e, ω_1 is incident and ω_2 is scattered photon energy, and E_1 is energy of the bound electron. In Eq. (4) the spinor function F is defined as

$$F(\mathbf{y}, \eta_{a,e}) = -\int d^3x S^{\mathrm{ext}}(\mathbf{y}, \mathbf{x}, \eta_{a,e})\, \boldsymbol{\gamma}\cdot\mathbf{A}_{1,2}(\mathbf{x})\, \psi_1(\mathbf{x}). \tag{5}$$

F satisfies the inhomogeneous Dirac equation in the external (atomic) potential V for propagator energy η:

$$[\boldsymbol{\gamma}\cdot\mathbf{p} + m + \gamma^0 V(|\mathbf{y}|) - \gamma^0 \eta] F(\mathbf{y}, \eta) = \boldsymbol{\gamma}\cdot\mathbf{A}(\mathbf{y})\, \psi_1(\mathbf{y}). \tag{6}$$

In these expressions the indices 1 and 2 refer to variables associated respectively with the incident and with the scattered photon, and similarly with the initial bound and final continuum electron. The electron wave functions ψ_1, ψ_2 are solutions of the Dirac equation in the potential V, and S^{ext} is the electron propagator in the same field.

In our calculations we use a realistic spherically symmetric atomic potential generated by the nucleus and atomic electrons, namely, the self-consistent screened Dirac-Fock-Slater atomic potential, with a Latter tail. For this purpose, the code of Lieberman, Cromer, and Waber [37] is employed. However, when comparing with calculations employing a hydrogenic atomic model, the Coulombic potential is used. For test purposes, when comparing with analytic expressions in Born approximation, the potential V has been set to zero in portions of the calculation.

After decomposition of the electron wave functions into partial waves, and multipole expansion of the photon field, as

in [5], we factorize the amplitudes M_a and M_e into angular parts and radial integrals. The radial integrals, which contain the whole dynamics of the Compton process, are the same as given by Eqs. (A16) of [5]. In our calculations they are calculated using the previous code, and their numerical accuracy is on the same level as was estimated in [5].

From these factorized amplitudes an expression for TDCS can be obtained in closed form [38] through the algebra of 3-j, 6-j and 9-j coefficients, for example, when the intrinsic states (polarizations and spins) of all particles are summed and averaged. Using such a form we could generate a code for TDCS. However, in general, a large number of angular momenta are required. To achieve adequate convergence it is preferable if numerical computation starts from the factorized matrix element Eq. (4), rather than the cross section. The cross section for scattering polarized and unpolarized incident photons from unoriented bound electrons is then obtained by numerical squaring of the matrix element, with numerical summation and average of the resulting cross sections over the spin polarizations of final and initial states. A similar numerical approach was used in [39] for calculating triply differential electron bremsstrahlung cross sections. For special cases, when only a small number of partial waves and multipoles is required for results to converge, we have performed the calculations both ways, and in matching results we have tested the kinematical structure of the code.

We have further tested the code in a variety of ways: (1) As an additional test of the kinematical structure of the TDCS code we performed comparisons with the Born approximation for scattering from K-shell electrons, which is given analytically [40]. By Born approximation we mean that we set the potential V to zero in the code when solving both the inhomogeneous Dirac equation and the homogeneous Dirac equation for the outgoing electron, keeping V only in calculating the initial bound state. Our numerical results have been compared with the analytical expressions. In the range $Z=1\rightarrow 92$, and for the energy range from 2.5 to 279 keV, we always found agreement within 0.1% between the numerical results from the code and the analytical expression. (2) By numerically integrating the TDCS over outgoing electron angles the DDCS is obtained. In this way we tested the TDCS code against the results of the DDCS code. In the entire range of Z and energy, agreement was always on the level of the errors of the numerical integration. (3) We also tested the code in cases where simpler approximations are expected to be accurate. In the regime where incident photon momentum is much smaller than p_{av} (but the photon has enough energy to eject the electron from the shell) we tested our code by comparing its results with the results of the nonrelativistic ''$\mathbf{p}\cdot\mathbf{A}$'' dipole approximation [17–19]. In the high but nonrelativistic energy regime, and for low Z, we tested our code against the ''$\mathbf{A}^2$'' approximation [22,26]. The results of these tests show excellent agreement between the code results for the TDCS and the results of these more approximate approaches in the region where these approximations are expected to be highly accurate. This is in agreement with the results of the similar tests performed in [4,5] for DDCS. (4) In another test, for high incident photon energies with low outgoing photon energies (this is a region where the dipole ''$\mathbf{p}\cdot\mathbf{A}$'' approximation should not be accurate, because retardation and relativistic effects are important) we obtain, as shown subsequently, good agreement between code results for TDCS and low-energy theorem (LET) predictions.

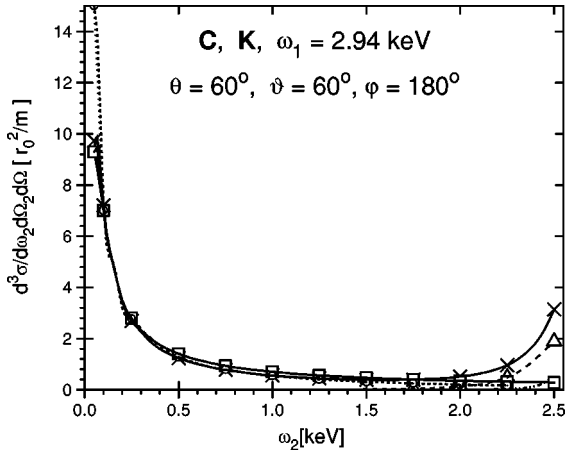

FIG. 2. Triply differential cross section for the scattering of 2.94 keV photons from a K-shell electron of carbon into 60° for electron angles $\vartheta=60°$ and $\varphi=180°$. The cross sections are obtained from nonrelativistic ''$\mathbf{A}^2$'' approximation (triangles), present S-matrix IPA calculations ($\times$), the impulse approximation (dashed-dotted line), results obtained from photoeffect cross sections using the low-energy theorem (squares), and the results of the nonrelativistic ''$\mathbf{p}\cdot\mathbf{A}$'' calculations (circles).

IV. RESULTS AND DISCUSSION

In [5] a wide and systematic investigation of the Compton scattering DDCS was presented, and the results of the relativistic S-matrix IPA calculation were compared with the results from more approximate methods. Here, we extend the discussion to the TDCS. We have examined the region of incident photon energies between tens of eV for H and 662 keV for Au, studying more systematically the case of scattering from a K-shell electron. We have also examined examples of scattering from higher shells of medium- and high-Z elements in order to study resonant and peak regions. We present illustrative results obtained with our code together with the corresponding results of the various simpler methods widely used in Compton calculations, in Figs. 2–4,

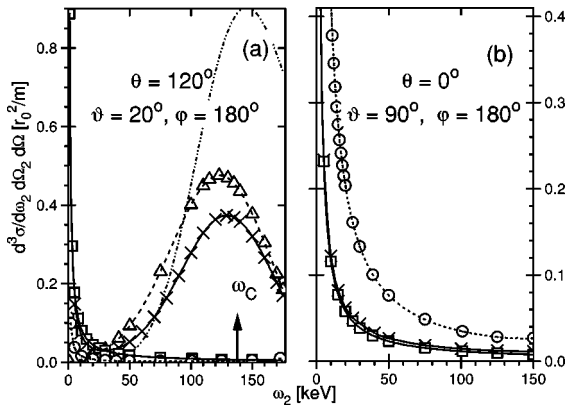

FIG. 3. Same as Fig. 2 except for scattering of 279.11-keV photons from a K-shell electron of lead into (a) 120° for $\vartheta=20°$ and $\varphi=180°$, (b) 0° for $\vartheta=90°$ and $\varphi=180°$.

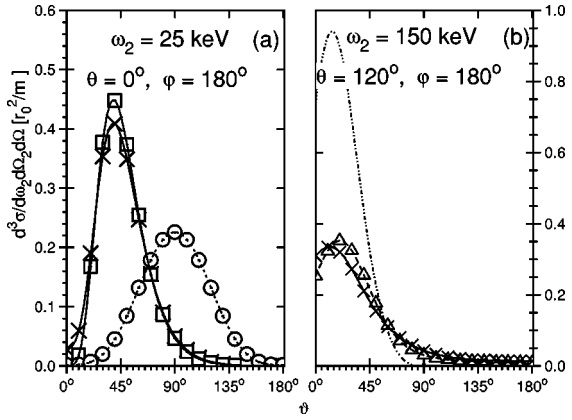

FIG. 4. Triply differential cross sections for the scattering of 279.11-keV photons from a K-shell electron of lead as a function of the outgoing electron angle (ϑ). Energies (ω_2), angles (θ) of the scattered photon, and angles φ of the outgoing electron are indicated in the panels.

showing representative cases of K-shell Compton TDCS of low-, intermediate-, and high-Z elements for $|\mathbf{k}_1| \ll p_{\rm av}$ ($Z=6$) and for $|\mathbf{k}_1| \sim p_{\rm av}$ ($Z=29,82$) We also discuss the existing experimental data, in comparison with our calculations (Figs. 5–7) and we make some suggestions for new experiments in Compton scattering.

For the TDCS we can expect additional differences between the SM results and more approximate approaches, in comparison to the situation in DDCS. We pay particular attention to these circumstances. We find that (1) in the Compton peak region for TDCS and for $p_{\rm av}/|\mathbf{K}| \lesssim 1$ the IA approach in treating TDCS is incorrect unless $p_{\rm av}/|\mathbf{K}| \ll 1$, unlike for DDCS cases where IA is good even for $p_{\rm av}/|\mathbf{K}| \sim 1$. We do find that in the region $|\mathbf{k}_1| \gtrsim p_{\rm av}$, the ''$\mathbf{A}^2$'' approximation (unlike IA) generally reproduces TDCS reasonably well in comparison with our SM results, as in the DDCS case. (2) For large Z and relatively large incident photon energies the dipole ''$\mathbf{p}\cdot\mathbf{A}$'' dipole approximation is much less accurate in describing both the infrared divergent and resonant regions of the TDCS than for DDCS, due to the importance of retardation. (The LET approach gives an adequate description of the infrared divergent region for all Z and all incident photon energies.) (3) In addition, we discuss the consequences of the failure of the IA approach in the $|\mathbf{K}| \sim p_{\rm av}$ region of the TDCS for the treatment of double ionization in Compton scattering at low incident photon energies.

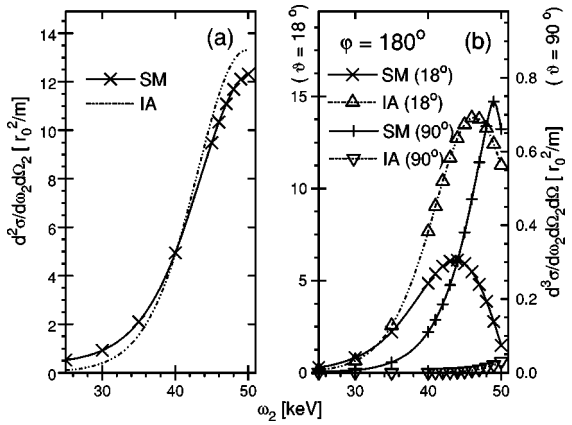

FIG. 5. Scattering of 59.32-keV photons from a K-shell electron of Cu into 140°. The cross sections are obtained using S-matrix IPA calculations and IA. (a) Doubly differential cross section, (b) triply differential cross section for two choices of outgoing electron angles $\vartheta=18°$ and $\vartheta=90°$ with the same $\varphi=180°$.

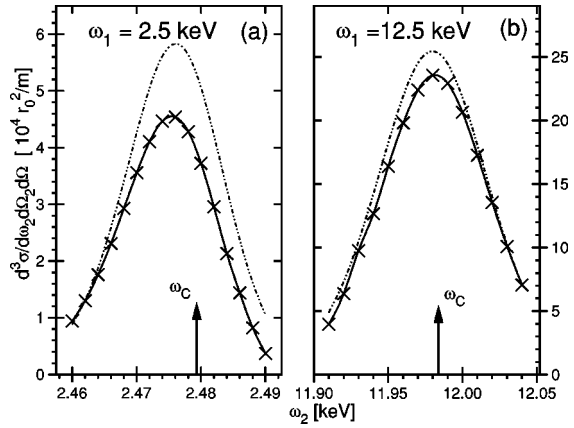

FIG. 6. Triply differential cross section per electron for the scattering of linearly polarized 2.5- and 12.5-keV photons from an $N1$-shell electron of copper. Incident photon polarization is in the scattering plane ($\phi=0°$), the photon scattering angle $\theta=140°$ and outgoing electron angles are $\vartheta=19°$ and $\varphi=180°$. The cross sections are obtained from the impulse approximation (dashed-dotted line) and present S-matrix IPA calculations ($\times$).

In Fig. 2 we show the TDCS for the scattering of 2.94-keV photons from the K-shell electrons of carbon for a photon scattering angle of 60°. The angles of the outgoing electron are chosen to be $\vartheta=60°$ and $\varphi=180°$, which correspond to the outgoing electron angles for free kinematics (as defined in the Introduction). The incident energy is large compared to the binding energy, but the Compton peak is outside the kinematically allowed region for all scattering angles. The figure represents an example in which both the ''$\mathbf{p}\cdot\mathbf{A}$'' and ''$\mathbf{A}^2$'' terms of the interaction Hamiltonian contribute significantly through most of the spectrum. It illustrates our findings, in agreement with the DDCS study in [5],

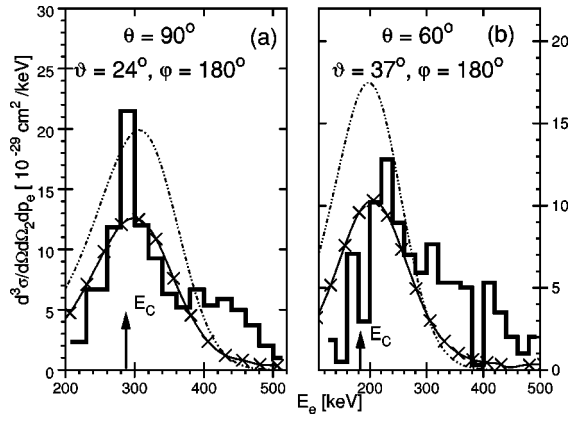

FIG. 7. Triply differential cross section for the scattering of 662-keV photons from a K-shell electron of gold as a function of outgoing electron kinetic energy. The cross sections are obtained from the impulse approximation (dashed-dotted line) and present S-matrix IPA calculations ($\times$). The histogram represents the experimental results of [15].

that the low photon energy part of the spectrum (infrared divergence) is well described by the low-energy theorem, and that for a low-Z element and low incident photon momentum ($|\mathbf{k}_1| \ll p_{\mathrm{av}}$, where a relatively small number of partial waves contributes) the ''$\mathbf{p}\cdot\mathbf{A}$'' dipole approximation gives a good description of the soft photon part of the spectrum (as it is adequate for the total cross section for the photoeffect, integrated over angles [41]). While, in general, when the electron can be considered nonrelativistic, the ''$\mathbf{A}^2$'' term will describe well the high-energy part of the spectrum, in this case the contribution of the ''$\mathbf{p}\cdot\mathbf{A}$'' term is not negligible. From the figure it can be observed that IA gives a poor description of the high-energy part of the spectrum, which is to be expected since in this case $p_{\mathrm{av}}/|\mathbf{k}_1| \gg 1$.

Our results in the infrared divergent region and now also in the peak region are further illustrated in Figs. 3 and 4. In Fig. 3 we show the scattering of 279-keV photons from a K-shell electron in lead. The Compton peak is visible for the backscattering angles (the outgoing electron angles are chosen according to free kinematics). In the case of $\theta = 120°$ we have $p_{\mathrm{av}}/|\mathbf{K}| \sim 1$ near the peak. The IA gives predictions that are higher than the SM results by more than factor of 2.5, as can be seen from Fig. 3(a). The nonrelativistic ''$\mathbf{A}^2$'' approximation agrees reasonably well with the SM results at these relatively large photon energies. The soft photon region is well described by LET (which includes retardation), differing much from the results obtained in the dipole ''$\mathbf{p}\cdot\mathbf{A}$'' approximation, as is illustrated for forward photon scattering angles in Fig. 3(b).

In order to illuminate further the differences between SM results and more approximate approaches, we study the TDCS (for the same case as in Fig. 3) as a function of outgoing electron angle ϑ for a fixed outgoing photon energy and angle. We show results for outgoing photon energies of 25 keV (soft photon region) in Fig. 4(a) and for 150 keV (near the Compton peak region) in Fig. 4(b). In the soft photon region (region of infrared divergence) the dipole approximation predicts that most electrons are ejected in the direction perpendicular to the direction of the incident photon, with a distribution symmetrical about $\vartheta = 90°$, as can be seen from Fig. 4(a). However, at these large energies the retardation effects (higher multipole effects) cause peaking in the forward direction, in accord with a similar effect in the photoeffect for large photon energies [41]. We observe that LET predictions (which are obtained, using the low-energy theorem, from the photoeffect differential cross section calculated within a full IPA approach), unlike dipole predictions, are in good agreement with SM results. At scattered photon energies near the Compton peak the TDCS is fairly well described by the ''$\mathbf{A}^2$'' approximation, while IA (for the chosen electron angle φ) overestimates the TDCS for all electron angles ϑ. However, for some other electron angles φ IA underestimates TDCS. By integrating the IA result for TDCS over outgoing electron angles the DDCS in IA is obtained, and it fairly well describes the behavior of DDCS near the Compton peak for this case, as was shown in [5].

We now turn to comparison with experiment. Recently, an absolute measurement of DDCS on K-shell electrons of copper [36] 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 Eq. (2), $p_{\mathrm{av}}/|\mathbf{K}| \sim 0.7$. 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 $p_{\mathrm{av}}/|\mathbf{K}| \sim 1$, as we illustrate in Fig. 5(a) 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. 5(b). We show results for two choices of outgoing electron angles, one choice being made according to free kinematics for an electron at rest ($\vartheta = 18°$). We find that, in general, for angles close to those corresponding to free kinematics for scattering from free electrons at rest, the IA overestimates TDCS in the peak region, while for angles differing much from free kinematics it underestimates the TDCS. By integrating the IA TDCS over outgoing electron angles these discrepancies average, resulting in a quite accurate IA description of DDCS.

Recently experiments [13,14] measuring TDCS were performed by scattering high-energy photons ($\omega_1 > 100$ keV) from weakly bound electrons in solid state targets. This was not a scattering from a specified subshell. The main contributions to the differential cross section were from valence electrons, but the contribution of some inner shells, because of the finite energy resolution (typically several hundred eV [13]), was also included. The purpose of such experimental studies is to obtain information about EMD directly from TDCS measurements through employment of IA, as discussed in the Introduction. The employment of such high photon energies (much higher than one would need for IA to be valid, for Compton profile measurements) 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 with higher photon energies yielding higher-energy electrons and less multiple scattering. Our study here confirms that for these relatively high photon energies one has achieved validity of IA for TDCS. Although we cannot run such a high-energy case for so weakly bound electrons (because we need too many multipoles for convergence), we may demonstrate, performing calculations at lower photon energies, that agreement with IA is already achieved. Our investigation indicates that we can use IA for TDCS, near the peak region, with an error less than about 5%, if the ratio $p_{\mathrm{av}}/|\mathbf{K}|$ is less than about 0.1.

We illustrate this in Fig. 6, where we show the cross sections for scattering of 2.5- and 12.5-keV photons (polarized in the scattering plane) from the $N1$ shell electron of copper, calculated using IA and our code. For the bound state wave function we use the same self-consistent wave function in both IA and in the code calculations. The electron angles are chosen according to free kinematics. The differences between IA and code calculations are smaller as photon energy increases, and for the highest shown energy they are around 7%. For this particular shell the binding energy is several eV (in the self-consistent model) and the criterion $p_{\mathrm{av}}/|\mathbf{K}| \lesssim 0.1$ is fulfilled at about 15 keV for this case. However, if M-shell electrons, with binding energies of some hundred eV, are included, as would be required if an energy

resolution of several hundred eV is assumed, higher photon energies (60–70 keV) are required in order to achieve the same accuracy of IA. We conclude that for hard incident photons (as used in [13]) the IA is reliable.

We have mentioned the earliest experiment measuring TDCS for Compton scattering of which we are aware [15]. Photons of 662 keV were scattered from the K shell of gold, and results of an absolute measurement were reported for photon scattering angles of 90° and 60°. The outgoing electron angles were chosen from free kinematics in scattering from an electron at rest. The ratio of $p_{\rm av}/|\mathbf{K}|$ for these cases is 0.35 (for 90°) and 0.45 (for 60°) for outgoing photon energies near the peak. This is a situation in which IA works very well for DDCS and poorly for TDCS, as discussed above. We present results for TDCS for this case as a function of outgoing electron energy in Fig. 7, both in IA and in our S-matrix calculation. Although the discrepancies between IA and our S-matrix calculations are 50%–70% near the peak, both results are consistent with the experimental data because of the large experimental uncertainties [42].

The development of experimental techniques in the last 30 years, since the experiment [15] was performed, should make it possible to measure TDCS more accurately for cases where $p_{\rm av}/|\mathbf{K}|$ is not very small. Such experiments should involve relatively large photon energies (in order to have large electron energies and so avoid large contributions of multiple electron scattering) and large Z (in order to have $p_{\rm av}/|\mathbf{K}|\sim 1$). In such circumstances IA is poor for calculating TDCS, although it predicts DDCS very well, and a more accurate approach (such as our SM approach) is required.

The dipole ''$\mathbf{p}\cdot\mathbf{A}$'' approximation shows noticeable disagreement with SM calculation of TDCS in the infrared divergent and resonant regions, as we have already illustrated for the infrared divergent region. This discrepancy strongly depends on outgoing electron angles. This behavior for soft final photons can be explained by observing that in dipole approximation the electrons are then described as ejected dominantly in the direction of incident photon polarization (orthogonal to the direction of the incident photon, as in the description of photoeffect in dipole approximation). However, for high photon energies (and for all Z) higher multipoles (and retardation) contribute significantly, so as to give forward peaking. We observe a similar failure of the ''$\mathbf{p}\cdot\mathbf{A}$'' dipole approximation in the resonant region of TDCS. However, we should remember that resonant Compton scattering is pronounced when the incident photon energy is close to the K-shell binding energy, and therefore relatively large deviations from the dipole approximation may be expected only for high-Z atoms. (In our SM approach the widths of the bound states are zero, and so in our model the resonances appear as singularities, behaving as $[\omega_2-(E_1-E_2)]^{-2}$, where E_1 and E_2 are electron binding energies). The dipole approximation predicts that electrons are ejected dominantly in the direction perpendicular to the incident photon beam. Our calculations for the resonant region show this direction is shifted somewhat toward forward angles. For example, studying the K-L resonance in the case of lead, using photons of 100–120 keV, we find that electrons are ejected dominantly into angles of about 77°.

It is interesting to note that we may apply our conclusions about the validity of IA in TDCS to clarify the probable validity of IA in treating another Compton scattering observable that is also less averaged than single ionization DDCS. IA has also been employed for calculating cross sections for double ionization in Compton scattering [16], a subject of considerable recent experimental and theoretical investigation [43], particularly of the ratio of double to single ionization in helium. There, as in the case of TDCS for single ionization treated here, it had been hoped that a similar region of validity would apply as in DDCS. But, again, the comparison of IA calculations with experiments [44,45] and other calculations [46] 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. We may understand this from our TDCS considerations. In the derivation of IA for double ionization explicit use of the plane-wave approximation for the fast outgoing electrons is made, similar to TDCS, and unlike in DDCS. We may, evidently, view the double ionization Compton total cross section as a more differential observable than DDCS for single ionization, as is also TDCS. Although IA is fairly accurate in calculating the total cross section for single-ionization Compton scattering for He even at lower energies [47], it is adequate for single ionization DDCS at about 5–6 keV (except for forward angles where the contribution to the total cross section is small). In estimating the accuracy of IA for calculating the double ionization total cross section, we require that the criteria for TDCS be satisfied for most angles. Assuming that the contribution of forward angles to the double ionization total cross section is as important as in the single ionization case leads to the expectation that IA for the total cross section for double ionization in Compton scattering from helium is adequate above about 50 keV.

V. CONCLUSIONS

The theory of the triply differential cross section for Compton scattering has been developed in the framework of a relativistic second-order S-matrix element calculation, assuming IPA for the atomic electrons. The theory is based on the general framework of [5], and the calculation is developed as an extension of the previous DDCS code. The triply differential cross sections have been obtained and compared with the results of widely used simpler approximate methods and with existing experimental data. We confirm most conclusions that followed from the analysis of the DDCS [5]. However, there are important circumstances of considerable disagreement with more approximate methods, in particular with IA, which are not seen in the DDCS. Here we found: (1) much larger disagreement between SM calculation and dipole ''$\mathbf{p}\cdot\mathbf{A}$'' approximation in the infrared divergent region of the TDCS for relatively large incident photon energies and in the resonant region for large Z, and (2) large discrepancies between the IA approach and SM results in the region where $p_{\rm av}/|\mathbf{K}|\lesssim 1$ (but not yet $\ll 1$). We find that for TDCS the criterion for the validity of IA is an order of magnitude greater than for DDCS. This stronger criterion agrees with the fundamental assumptions in deriving IA. From the experimental point of view this means that, for a given photon energy and for a particular atomic system, we can expect validity in TDCS of IA for valence electrons, in situations

when it will not be valid for core electrons, even when it is valid for both valence and core electrons in DDCS. The EMD determination through the Compton profile (which is obtained from Compton DDCS) is more accurate at lower energies than direct determination through measurement of the TDCS at the same energy.

We have discussed the existing experimental work in TDCS. There is one experimental situation, which has been studied in the past and which could now be studied with much higher experimental accuracy, for which our calculations show the validity of IA for the DDCS, but considerable difference from IA for the TDCS.

We have also discussed the adequacy of IA in treating the double ionization Compton scattering total cross section. Viewing this as another observable less averaged than the DDCS, based on our single ionization TDCS study we estimate that the IA total cross section for double ionization in Compton scattering from helium is adequate above about 50 keV.

ACKNOWLEDGMENTS

This work was supported by the Croatian Ministry of Science under Grant No. 00980204, and by the National Science Foundation under Grant No. PHY-9506853. K.P. is grateful for the hospitality of the Department of Physics and Astronomy at the University of Pittsburgh during his visit. We also wish to acknowledge helpful discussions with Dr. P. M. Bergstrom.

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