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A SIMPLE AND EFFICIENT YET ACCURATE CALCULATION OF THE DOUBLE-DIFFERENTIAL COMPTON CROSS SECTION WITHIN THE IMPULSE APPROXIMATION

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It is shown that with proper values of the effective charge, the hydrogen-like (HL) wave functions are almost as good as the more sophisticated Hatree–Fock (HF) wave functions in calculations of the double-differential cross section of Compton scattering within the nonrelativistic impulse approximation (IA). Only a single value of the optimized effective charge for a given subshell of an atom is required for an accurate description of Compton spectra in a wide range of experimental conditions under which IA is a good approximation. That is demonstrated by results obtained for the K-shell of several atoms and for higher subshells in germanium. It has been found that a constant value of the optimal effective charge can be used as a criterion for the validity of IA, which is explained within the existing knowledge of IA. Simple analytical expressions for HL-Compton profiles have a compact form and are a much faster way to calculate the cross sections than using extensive tabulations of HF Compton profiles. These features can be useful in very extensive numerical calculations of Compton scattering in radiation physics, biomedicine, industry and in other practical applications.

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1. Introduction

In his article in 1929, DuMond [1] explained spectrum of Compton scattered photons by bound electrons. He intuitively assumed that electrons are free and connected their momentum distribution given by their initial state with the broadening of the Compton line. That connection, later called the impulse approximation (IA), has made the Compton scattering a valuable tool in studies of electron structures in atoms, molecules and solids. The double-differential cross section in the non-relativistic IA may be written as follows [2]

$$\frac{\mathrm{d}^2\sigma_{nl}}{\mathrm{d}E\mathrm{d}\Omega} = r_0^2\left(1+\cos^2\vartheta\right)\frac{E}{E_0}\frac{m_0}{\hbar k}J_{nl}(q), \tag{1}$$

where r_0 is the classical electron radius, ϑ is the scattering angle, E_0 and E are the energies of the incident and scattered photon, m_0 is the electron rest mass and $\hbar k$ is the photon momentum transfer. $J(q)$ is the Compton profile defined by

$$J_{nl}(q) = \int\int \mathrm{d}p_x \mathrm{d}p_y \rho(\vec{p}), \tag{2}$$

where $\vec{p}$ is the momentum of bound electrons in a given (n,l) subshell, $\rho(\vec{p})$ is electron distribution given by $\rho(\vec{p}) = |\Phi_{nl}(\vec{p})|^2$, where $\Phi_{nl}(\vec{p})$ is obtained by the Fourier transform of the spatial wave function of the bound electron $\Psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_l^m(\theta,\varphi)$ and $q = -\vec{k}\cdot\vec{p}/p$ is the projection of the electron momentum in the direction of the photon momentum transfer $\hbar\vec{k}$ (taken as z direction).

After DuMond's discovery, neither rigorous theoretical justification nor limits of validity of the IA were known for a long time. In 1970, Eisenberger and Platzman [2] derived the IA from first principles, justifying DuMond's assumptions. They also gave a criterion of its validity,

$$E_\mathrm{R}/E_\mathrm{B} \gg 1, \qquad \text{where} \qquad E_\mathrm{R} = \frac{\hbar^2 k^2}{2m_0} \tag{3}$$

is the kinetic energy of the recoil electron and E_B the electron binding energy. Later, some authors [3–5] have expressed the validity of IA in terms of the photon momentum transfer via dimensionless parameter ka as $ka \gg 1$, where a is the Bohr radius of the orbital of the scattered electron. These two criteria are similar within the hydrogenic model of atom, since the parameters $E_\mathrm{R}/E_\mathrm{B}$ and ka are connected via the relation

$$\frac{E_\mathrm{R}}{E_\mathrm{B}} = (ka)^2 \tag{4}$$

obtained using $E_\mathrm{B} = Ze^2/(2a)$ and $Ze^2 = \hbar^2/(am_0)$.

Many authors (Refs. [3–6] and references therein) experimentally checked the IA in the so-called intermediate momentum transfer regime where $ka \approx 1$. Surprisingly, they found reasonable agreement between the IA and experimental data. These results motivated Surić [7] to revise the criterion for the validity of the IA. Taking into account some qualitative arguments and comparing calculations of the relativistic IA with the exact (within the independent particle model) S-matrix calculation (Surić et al. [8], Bergstrom et al. [9]), he found that IA was good when

$$\frac{p_{\rm av}}{k} \leq 1, \tag{5}$$

where $p_{\rm av} = \sqrt{\langle p_x^2\rangle + \langle p_y^2\rangle + q^2}$, $\langle p_x^2\rangle$, $\langle p_y^2\rangle$ are expectation values of squares of electron momenta in the x and y directions, respectively, and q is given by the relativistic expression

$$q = \frac{(E_0 - E)m_0c^2 - E_0E(1-\cos\vartheta)}{\hbar ck}. \tag{6}$$

Kaliman et al. [10] have made a comparison of the relativistic IA with the S-matrix calculations and have shown that IA expressed by the triple differential cross section (additional differential with respect to outgoing-electron angle), which is directly proportional to the electron momentum distribution $\rho(\vec{p})$, is less accurate and in that case the criterion (4) takes a more strong form, $p_{\rm av}/k \ll 1$. Hence, when the cross section is proportional only to Compton profile, which is averaging of the electron momentum distribution over two dimensions, as in double-differential cross section, IA is much more accurate.

Most calculations of Compton scattering in radiation physics, technological and biomedical fields (Ref. [11] and references therein) and in studies of the detector response function [12,13] are based on modelling the electron–photon transport through matter. These applications demand both reliable and very high-speed computations of Compton scattering. Thus, until recently, only Klein–Nishina formula for Compton scattering on free electron at rest, and perhaps the incoherent scattering function, have been used in such computations. Compared to the simple Klein–Nishina analytical expression, IA is relatively inefficient and impractical even in its simplest form based on extensive tabulation of Compton profiles calculated by Hartree–Fock (HF) wave functions (Biggs et al. [14]). However, permanent growth of the computing power of personal computers has allowed the inclusion of IA in some sophisticated transport codes [15,16]. Nevertheless, many problems with complicated geometry, especially those involving multiple scattering, are hardly or not at all treated using the IA at present. Therefore, any simplification of IA would be helpful in accessing details of Compton scattering caused by the momentum distribution of bound electrons in numerically extensive applications.

Recently, Pašić and Ilakovac [17–20] have utilized the coincidence technique for the whole-atom Compton-scattering measurement using a germanium detector as the scatterer. This new type of experiment gave very clean and reliable results on Compton spectra on an absolute scale in a wide energy range. The agreement between the non-relativistic IA and data obtained for values of the incident-photon energies of 59.5, 86.3 and 105.3 keV, was excellent if relativistic value for q defined by Eq. (6) was taken and Hartree–Fock wave functions were used. Application of hydrogen-like (HL) wave functions gave worse results. As shown in Ref. [20], at the incident energy of 105 keV, IA using the HL wave functions agreed approximately as well with the experiment as IA with the HF wave functions, if adjusted values for the effective charges were used. To check the validity of the method, we apply the procedure for estimating the optimal values of the effective charge for variable incident photon energy E_0 and scattering angle ϑ, and for subshells of atoms from hydrogen to kripton ($Z = 36$) (for these atoms relativistic effects in the Compton profile can be neglected [14]). The aim is to investigate whether the simplification of the calculation of the Compton profiles, i.e. the calculation of the double-differential cross section within the IA, is possible by replacing relatively complicated HF with simple HL wave functions without loss of accuracy. Previously, Ribberfors [21] made a simplification of the calculation of the total Compton cross section, while Ribberfors and Berggren [22] made a simplification of the calculation of the cross section differential in scattering angle. A result of this investigation is the constancy of the effective charge with respect to the values of parameters ka and E_R/E_B for which the IA is a good approximation. An explanation of that result is given within the theory of the IA by Eisenberger and Platzman [2].

2. Procedure

The optimal value of the effective charge ($Z_{\rm eff}$) is derived from a comparison of the double-differential cross sections $\mathrm{d}^2\sigma/\mathrm{d}E\mathrm{d}\Omega$ for fixed values of E_0 and angle ϑ, calculated using the IA (Eq. (1)) with the HF and HL wave functions. These cross sections are only functions of the energy of scattered photons E. The first step is the calculation of the double-differential cross section $\mathrm{d}^2\sigma_{\rm HF}/\mathrm{d}E\mathrm{d}\Omega$ using IA with HF wave functions for a fixed pair of values (E_0, ϑ). The low (E_1) and high (E_2) energy limit of the data which will be considered is estimated from the conditions $\mathrm{d}^2\sigma_{\rm HF}(E_{1,2})/\mathrm{d}E\mathrm{d}\Omega = \varepsilon \cdot \mathrm{d}^2\sigma_{\rm HF}^{\rm max}/\mathrm{d}E\mathrm{d}\Omega$, where ε is an arbitrary number less than 0.1, and $\mathrm{d}^2\sigma_{\rm HF}^{\rm max}/\mathrm{d}E\mathrm{d}\Omega$ is the maximum value of the cross section for the chosen pair of values (E_0, ϑ). If the value of the cross section is higher than the one at the kinematic limit $E_0 - E_B$, then $E_2 = E_0 - E_B$.

The second step is fitting of the data set with the cross section function $\mathrm{d}^2\sigma_{\rm HL}(Z_{\rm eff}, E)/\mathrm{d}E\mathrm{d}\Omega$, obtained using the IA with HL wave function, and taking the effective charge as a free parameter. In other words, the optimal value of the effective charge is the value for which the function

$$F(Z_{\rm eff}) = \sum_{i=1}^{N} \left[\frac{\mathrm{d}^2\sigma_{\rm HL}(Z_{\rm eff}, E_i)}{\mathrm{d}E\mathrm{d}\Omega} - \frac{\mathrm{d}^2\sigma_{\rm HF}(E_i)}{\mathrm{d}E\mathrm{d}\Omega} \right]^2 \tag{7}$$

has a minimum. $E_i = E_1 + (i-1)\,(E_2 - E_1)/(N-1)$ and N is the number of points of the fit.

The presented procedure yields useful results if the function F is only a function of $Z_{\rm eff}$, for given E_0 and ϑ, but not a function of N, and ε. The calculation shows that the results for $Z_{\rm eff}$ are independent of ε when $\varepsilon \le 0.1$, and on N when $N \ge 10$. The calculations presented below were made with $\varepsilon = 5 \cdot 10^{-3}$ and $N = 100$.

Redefinitions of the function $F(Z_{\text{eff}})$, like using the differential cross section for the statistical weight (instead of 1 as used in Eq. (7)) have a small influence on the results.

3. Results

We show the key features of the results obtained by the calculations made for the K-shell electrons of ${}_{7}$N, ${}_{14}$Si, ${}_{22}$Ti, ${}_{29}$Cu, ${}_{32}$Ge and ${}_{36}$Kr and for the 2s, 2p, 3s, 3p, 3d and 4s subshells of Ge. The optimal values of Z_{eff} are shown as a function of incident photon energy E_0 and $\cos\vartheta$ in Fig. 1 for the Si, Cu, Ge and

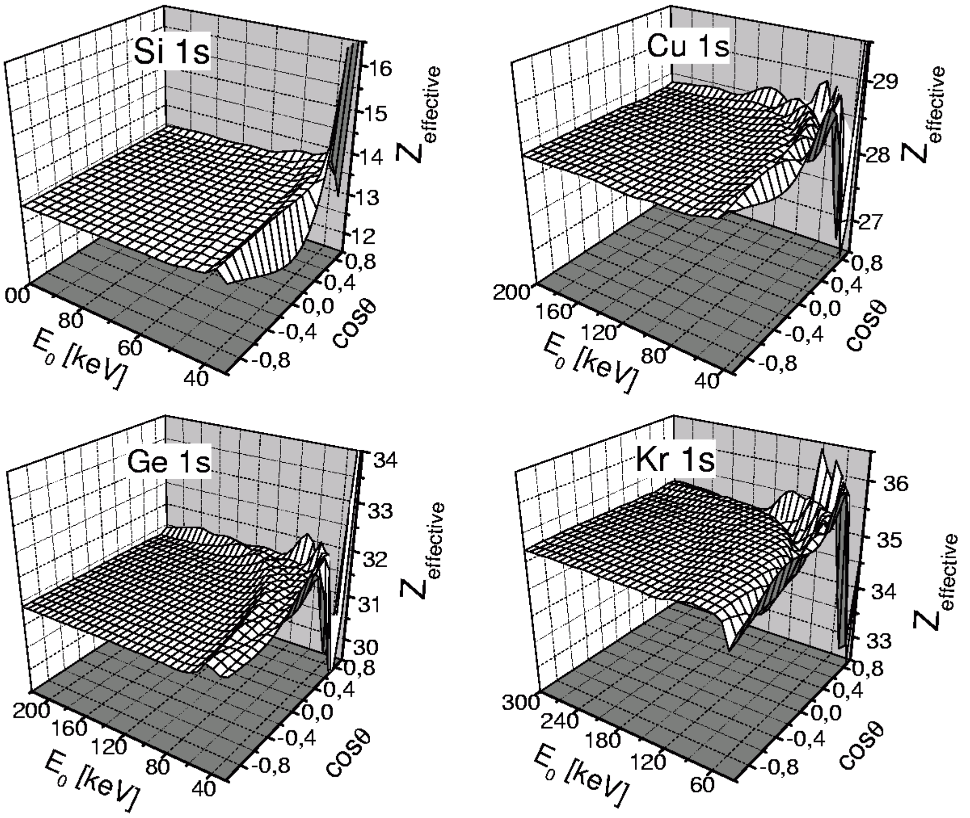

Fig. 1. Optimal values of Z_{eff} obtained for K*-shells of* Si, Cu, Ge *and* Kr *shown as a function of incident photon energy E_0 and ϑ. For every plot, about 1000 to 5000 data sets were fitted.*

Kr K-shell, as a function of the photon momentum transfer expressed as ka in Fig. 2, in which the results for N and Ti K-shell are included, and versus $E_{\text{R}}/E_{\text{B}}$

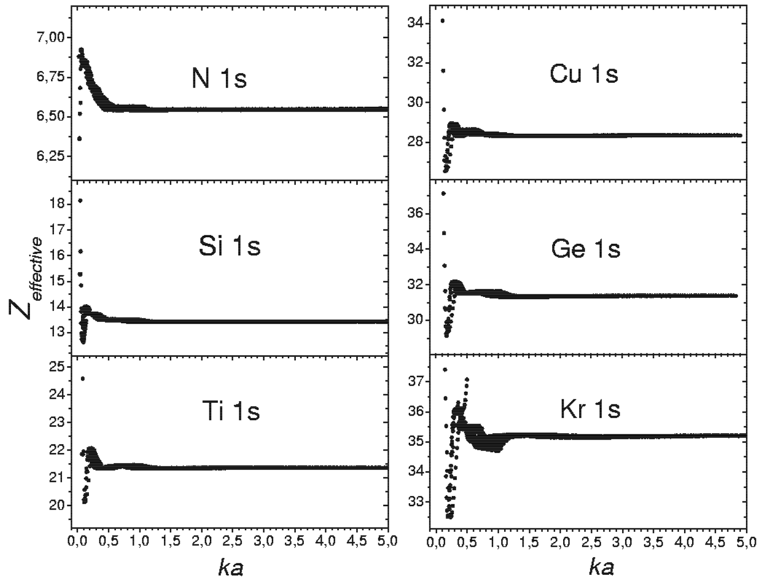

Fig. 2. Optimal values of $Z_{\rm eff}$ shown in Fig. 1, including the results for N *and* Ti *K-shells, shown as a function of ka. A value of ka corresponds to many different pairs (E_0, ϑ) in the 3D plot.*

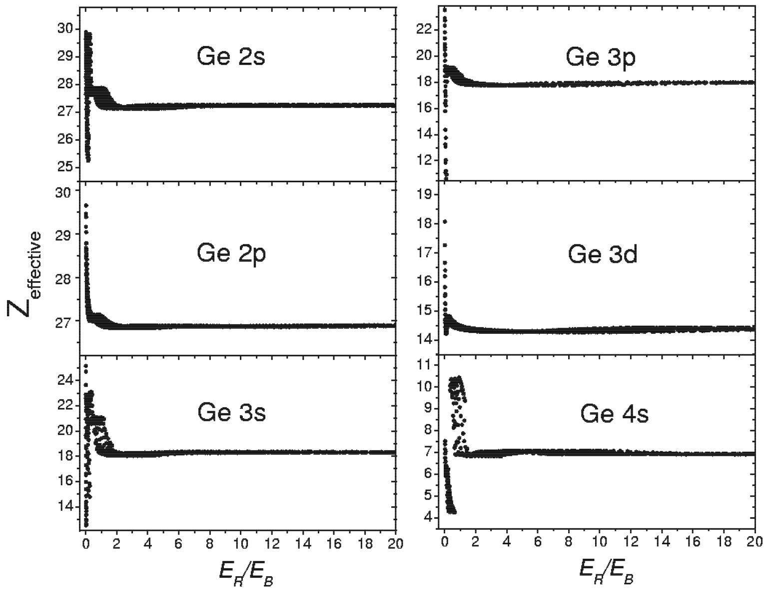

Fig. 3. Dependence of optimal values $Z_{\rm eff}$ for the 2s *to* 4s *subshells of* Ge *atom on* $E_{\rm R}/E_{\rm B}$.

for higher subshells of Ge atom in Fig. 3, where experimental values for $E_{\rm B}$ are taken. The validity of the IA is usually expressed via these parameters and that is the reason for their choice. The parameters are mutually related through Eq. (4) and $k = \sqrt{E_0^2 + \bar{E}^2 - 2E_0\bar{E}\cos\vartheta}$ ($\bar{E}$ is the average energy of scattered photon of a particular data set). The presentation of the results via different parameters reveals some details.

The results in Figs. 1 – 3 can be divided into tree regions:

1) the large photon momentum transfer, when $ka \gg 1$ and $E_{\rm R}/E_{\rm B} \gg 1$;

2) the intermediate photon momentum transfer, when $ka \approx 1$ and $E_{\rm R}/E_{\rm B} \approx 1$;

3) the small photon momentum transfer, when $ka \ll 1$ and $E_{\rm R}/E_{\rm B} \ll 1$.

One can clearly see that for large photon momentum transfers, the effective charge is very nearly a constant. These values are shown in Table 1. For the intermediate photon momentum transfers, variations of optimal values of $Z_{\rm eff}$ are seen, but they are not large, so that $Z_{\rm eff}$ can roughly be considered a constant. For small photon momentum transfers, the effective charge shows large deviations from the constant value, which grow as the photon momentum transfer is decreased. The criteria for the IA validity in the Introduction give a similar behaviour of the IA: it is a very good approximation in the momentum transfer region (1), can be accepted in the region (2), breakes down in the region (3). Therefore, the validity of the IA can be expressed via the constancy of the effective charge: the application of IA for Compton scattering is valid in a range of input parameters (E_0, ϑ) as long as the effective charge is a constant in that range.

TABLE 1. Constant values of the optimized effective charge obtained for the K-*shells of several elements and for higher subshels of* Ge.

K-shell

Element	N	Si	Ti	Cu	Ge	Kr
$Z_{\rm eff}$	6.55	13.43	21.36	28.31	31.38	35.18

Germanium atoms

Subshell	2s	2p	3s	3p	3d	4s
$Z_{\rm eff}$	27.23	26.68	18.36	17.98	14.39	6.92

Figure 4 demonstrates several examples of comparison of $\mathrm{d}^2\sigma_{\rm HF}(E)/\mathrm{d}E\mathrm{d}\Omega$ and $\mathrm{d}^2\sigma_{\rm HL}(Z_{\rm eff}, E)/\mathrm{d}E\mathrm{d}\Omega$ using the constant values of $Z_{\rm eff}$ given in Table 1. Comparison of many spectra for different subshells of elements at different scattering angles and incident energies (not shown in the present paper) has shown that the agreement between IA using the HF and HL wave functions is best for the s subshells, while it gets worse for small values of the cross section and larger values of angular momentum of the subshells. The agreement is very good in all cases where the cross

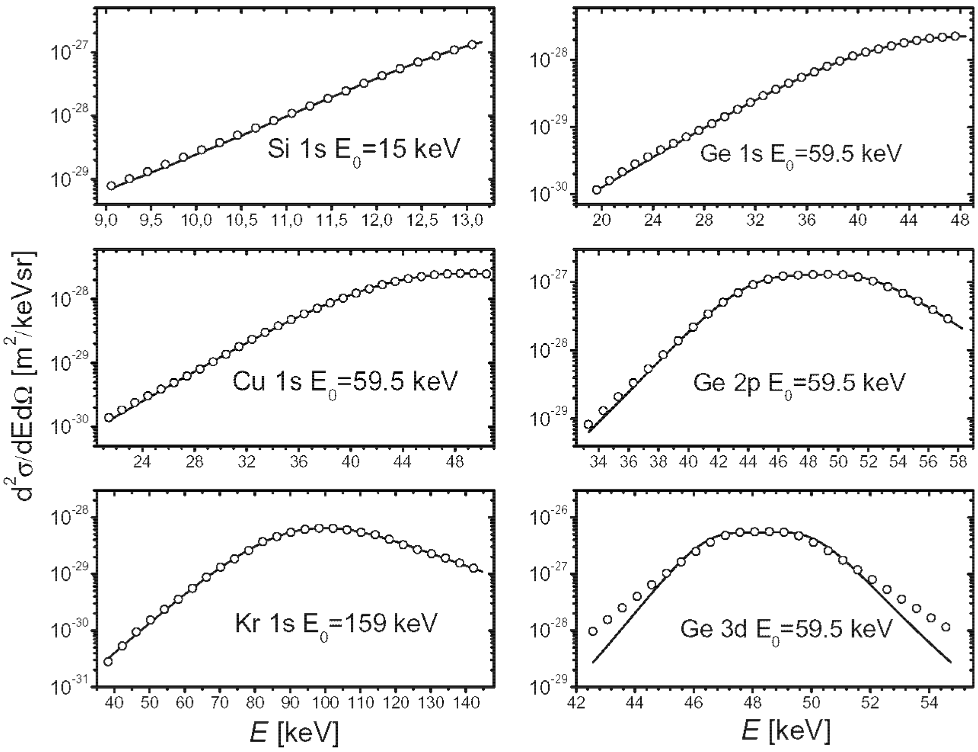

Fig. 4. Values of the double-differential cross section $\mathrm{d}^2\sigma/\mathrm{d}E\mathrm{d}\Omega$ *calculated using IA with HF-wave functions (open circles) and with HL wave functions (solid line) using the values of* Z_{eff} *from Table 1 for the* K*-shells of* Si, Cu, Kr *and* Ge*, and for the* 2s, 2p *and* 3d *subshells of* Ge *at several incident energies and scattering angle* $\vartheta = 180°$.

section can not be neglected, i.e. in the broad vicinity of the Compton peak, if the peak is kinematically allowed in the spectrum. That region of a spectrum is most important in practical application, especially for the calculations of whole-atom Compton scattering. Therefore, presented results lead to the following conclusion: *HL wave functions are almost as good as HF wave functions in the description of Compton scattering when conditions for the application of IA are fulfilled.* However, the optimal values of Z_{eff} obtained in the procedure do not make the HL wave functions the same or close to the HF wave functions. It means that these wave functions are not suitable for other physical situations. For instance, unlike the HF wave functions, the prediction of the binding energy in the hydrogen model atom using the values of Z_{eff} is not realistic except perhaps for the K-shell. What we actually obtained is that values of the HF and HL wave functions averaged over large values of the electron momentum are close to each other and they are closer as the region of the averaging is larger. That can be seen from the definition of the

Compton profile for spherically symmetric wave functions given by

$$J_{nl}(q) \quad = \quad 2\pi \int\limits_{q}^{\infty} p \left|\chi_{nl}(p)\right|^2 \mathrm{d}p, \tag{8}$$

where small values of q represent the energy region of large values of the spectrum, i.e. the vicinity of the Compton peak, which is given by $J_{nl}(q = 0)$. (In Eq. (8), $\chi_{nl}(p)$ is the Fourier transform of the radial wave function $R_{nl}(r)$).

IA with the HL wave functions using optimized values of the Z_{eff} is the simplest yet very realistic description of the double-differential Compton cross section in conditions of validity of IA. In comparison to the tabulated values of Compton profiles using the HF wave functions by Biggs et al. [14], the calculation of hydrogenic Compton profiles is more convenient for several reasons. A complete table of optimized values of Z_{eff} would be less than a fortieth of the size of the tables of HF-Compton profiles. Moreover, they give results for a broader range of values of q than the tabulated values. Finally, numerical calculations of a HL profile, i.e. the HL double-differential cross section within the IA, are considerable faster. Namely, an accurate estimation of the cross section using tabulated values of the HF-Compton profiles in the whole range of tabulated q values requires an application of the cubic spline interpolation or another accurate interpolation scheme in the log-log scale. On the other hand, HL-Compton profiles use simple analytical expressions [23]. For instance, the profile for K-electrons is given by $1/\left[3\left(1+(\eta q)^2\right)^3\right]$, where $\eta = 137/Z_{\text{eff}}$, which is considerable faster to calculate than any accurate interpolation scheme of the tabulated data. However, the efficiency of the calculations of HL-Compton profiles for higher shells decreases, unlike the interpolation scheme of tabulated data. Altogether, the benefit is still considerable. For example, without a loss of accuracy, we accelerate the calculation of double Compton scattering in germanium by about the factor of three when using the IA with HL wave functions and new values of the effective charge, instead of the cubic spline interpolation of HF-Compton profile data. Therefore, the new scheme can be very useful in applications of the IA with HL wave functions for practical and numerically very extensive calculations of single and multiple Compton scattering, which require enormous number evaluations of the cross sections. These applications are important in radiation physics, medicine, studies of environment, diagnostics, radiation detector investigations, engineering, etc.

We consider now the constancy of optimal values Z_{eff} with respect to the parameters ka, $E_{\text{R}}/E_{\text{B}}$, when IA is valid. But first, we give a short review of IA following Eisenberger and Platzman paper [2].

In the regime of the validity of IA, the photon energy transfer $\omega = E_0 - E$ is large compared to the energy characteristics of an electron in an atom. That results in a very short time of the photon-electron interaction, $t \approx \hbar/\omega$, which causes that the electron feels the same potential immediately before and after the interaction. In this way, the potential a constant, which is canceled in the energy conservation equation, i.e. the electron energies in the initial and final state are measured relative to that constant potential. The connection between the relatively large ω and the cancellation of the potential of the atomic electron is expressed by the operator equation [2]

$$\exp\left(-\frac{1}{2}\left[H_0, V\right] t^2\right) \quad = \quad 1, \tag{9}$$

where H_0 is Hamiltonian operator of a free electron and V the atomic potential of the electron.

The double-differential Compton cross section in IA is only given by the state of the electron in the atom before its interaction with the photon. The initial state of the electron is represented by the HL or HF wave functions depending on the assumption of the atomic potential V. HL wave functions are determined by $V = Z_{\mathrm{eff}} e^2/r$, where the Z_{eff} incorporates interactions of the electron with the nucleus and other electrons in the atom, assuming averaged Coulomb interaction. A single value of the effective charge determines the initial electron state for a given subshell. There are several ways to determine that value. We did it by the requirement that differences between HL and HF Compton profiles are minimal.

The parameters ka, $E_{\mathrm{R}}/E_{\mathrm{B}}$ and p_{av}/k are in fact a ratio of the kinematic quantity k and one of structure factors $(1/a, E_{\mathrm{B}}, p_{\mathrm{av}})$ (see Eq. (3)). When these parameters express the validity of IA, each of them tells the same: the photon energy transfer ω is large compared to an energy characteristic of the electron in the atom, which is represented by a structure factor for a particular parameter (ω and k are proportional which follows from $\omega = E_{\mathrm{R}}$ and Eq. (3)). That means a short time of the photon–electron interaction, which leads to cancellation of the potential of the electron. Therefore, the description of the Compton scattering by a single value of Z_{eff} for a subshell within the IA is possible, i.e., Z_{eff} is independent of the values of the parameters.

4. *Conclusions*

Values of the parameters ka, $E_{\mathrm{R}}/E_{\mathrm{B}}$ and p_{av}/k for which IA is good characterise the experimental conditions of very short photon–electron interaction in the Compton scattering. That physical situation leads to the cancellation of the electron potential in the calculation of the cross sections. Then, the double-differential Compton cross section is determined only by the initial state of the electron. Assuming the screened Coulomb potential, it is given by a single value of the effective charge for a given subbshell of an atom. Our procedure shows that the double-differential cross section can be equally well described by the HL and HF Compton profiles in the regime of validity of IA using one value for the effective charge. In other words, the description of the electron atomic states by HL-wave functions is good for the purpose of the calculation of a spectrum of Compton scattered photons within the IA. Calculations of HL-Compton profiles using the new scheme for arbitrary values of input parameters are easier and faster than the calculations of

HF-Compton profiles using tabulated values of Biggs et al. [14]. That can be useful in practical applications, which require a large number of calculations of the cross section.

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JEDNOSTAVNO I UČINKOVITO A IPAK TOČNO RAČUNANJE DVOSTRUKIH DIFERENCIJALNIH COMPTONOVIH UDARNIH PRESJEKA U IMPULSNOJ APROKSIMACIJI

Pokazuje se kako se s određenim vrijednostima efektivnog naboja i vodikovih (H) valnih funkcija postižu dvostruko-diferencijalni presjeci za Comptonovo raspršenje u nerelativističkoj impulsnoj aproksimaciji (IA) koji su gotovo jednako dobri kao s profinjenim Hartree-Fockovim (HF) valnim funkcijama. Potrebna je samo jedna povoljna vrijednost efektivnog naboja za danu podljusku za točan opis Comptonovih spektara u širokom području eksperimentalnih uvjeta za koje vrijedi IA. To se prikazuje rezultatima za K-ljuske više atoma i za više podljuske germanija. Rezultati pokazuju da se stalnost povoljnog efektivnog naboja može uzeti kao uvjet punovažnosti IA, što se obrazlaže na osnovi poznavanja IA. Jednostavni analitički izrazi za H-Comptonove profile su sažeti i brži su način računanja udarnih presjeka nego upotreba velikih tablica za HF-Comptonove profile u tablicama F. Biggsa i dr., a dobivaju se pouzdani rezultati. Te su odlike pogodne u opsežnim numeričkim računima Comptonovog raspršenja.