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Compton ionization of hydrogen atom near threshold by photons in the energy range of a few keV: nonrelativistic approach

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Abstract. Recently, there have been published the results of unique experiments on measuring the fully differential cross sections of the Compton single ionization of the helium atom near the ionization threshold at a photon energy of a few keV. This opens up a possibility of using Compton ionization along with the ionization of atoms/molecules by fast charged particles to study characteristics of the ionization processes in more detail, since photons are neutral particles. In this regard, the paper deals with the ionization cross sections of the reaction $(\gamma, \gamma e)$ at the hydrogen atom, because the theoretical description of this reaction at the hydrogen atom does not need to consider a number of additional assumptions and approximations inherent in heavier atoms. Special attention is paid to the study of the kinematic region of the reaction near threshold, where it is expected to obtain a valuable information about the initial and final states of the target. The contribution of corrections to the first Born approximation due to the electron boundness is also discussed.

1 Introduction

Scattering of light by bound electrons has been extensively studied both experimentally and theoretically for a long time already. As a result of the light scattering process, an atom (or molecule) can remain in the ground state (Rayleigh scattering), go into an excited state (Raman scattering) or be ionized (scattering with ionization). In the latter case, if only one electron is ejected, the scattering process is called Compton scattering by bound electrons. Unlike the first two types of scattering processes, Compton scattering can also take place at free electrons.

A theoretical quantum description of Compton scattering by free electrons was given almost 100 years ago [1] and was based on the idea of the corpuscular nature of light. A quantum of light (photon) is considered as a particle with a specific relativistic energy-momentum relation due to the zero mass of the photon. When a photon is scattered by a free electron, the kinetic energy of the latter can vary widely depending on the momentum transfer and be comparable to the energy of the photon. In principle, the same applies to a weakly bound electron of the outer shells of an atom, if the energy of the photon is large enough.

However, strictly speaking, Compton scattering of a photon by a bound electron is a three-body problem involving the residual ion of an atom. If the photon energy is of the order of a few keV, the energy that can be transferred to the ion is comparable with the energy of the photon, but incomparably smaller than the mass of the ion. Thus, the ion will remain actually stationary during the collision, and the ion recoil momentum will determine the momentum distribution of the electrons in the atom. In this case the ion can be approximately considered as an external field source, and the problem is reduced to a two-body problem in an external field.

In this approximation, the description of Compton scattering is usually carried out in the framework of quantum electrodynamics (QED) (see any textbook, for example [2], where the two corresponding Feynman diagrams of the second order are presented), and the interaction of bound electrons is considered in the Furry picture. A virtual electron between two (e, γ) interactions is described by relativistic Green's function in an external field, which cannot be found exactly and whose reasonable interpretation, in contrast to free Green's function, requires the involvement of approximations.

Photon energies of a few keV are interesting also because they allow one to consider Compton scattering by bound electrons in the non-relativistic limit. Kramers and Heisenberg [3], as well as Waller and Hartree [4] wrote out the corresponding matrix elements in the 20s of the last century (their modern form is presented in [5]). These

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matrix elements can also be obtained from their relativistic expressions (see again [2] or any other textbooks). However, this non-relativistic limit has an "inheritance" of the relativistic treatment, namely, the absence of momentum conservation. It is also impossible to use advanced models of atoms without loss of logic, in particular, to take into account the correlations of electrons in a complex atom.

Over the last hundred years, a large volume of theoretical calculations of various Compton scattering characteristics, mainly total cross section (TCS) and single differential cross sections (SDCS), has been accumulated. The fact is that the measurement of multiple differential cross sections required coincidence experiments. However, the experiments lagged far behind the theory. A rather detailed review of theoretical approaches to Compton scattering was made in paper [5]. Some relatively recent experimental and theoretical results can be found, for example, in [6–8].

The situation changed with the invention of COLd Target Recoil Ion Momentum Spectroscopy (COLTRIMS) [9], which was a significant progress in the experimental technique. Recently, there have been published the results of experiments on Compton ionization of helium atoms by 2 keV photons producing electrons with energy of several eV using such a setup [10]. Furthermore, the problem of a very small Compton ionization cross section in this energy range, which is about 6 orders of magnitude smaller than the typical photoabsorption cross section, has been overcome. This opens up a possibility of using Compton scattering as one more tool in the study of the angular and energy spectra of emitted electrons and scattered photons, along with such powerful methods of studying atoms and molecules as $(e, 2e)$, (ion, ion e) and the others.

However, here it is worth paying attention to a logic discrepancy between the relativistic theoretical description and the use of COLTRIMS. In such experiments the ion is guided by electric and magnetic fields on its way to a detector. In so doing, it behaves like a particle. Of course, in fact, during the collision of an energetic photon with a bound electron, the ion practically does not move due to its huge mass, but it acquires a momentum. However, there is no ion in the QED description, but a source of the external Coulomb field. In such a situation it is more convenient to consider the non-relativistic time-dependent Schrödinger equation (TDSE).

In the theoretical study of the ionization of atoms and molecules heavier than hydrogen one has to make a number of additional assumptions and approximations. Among these are a trial model of the wave function of an atom (molecule), including a single-electron (very primitive) model, and the need for an artificial orthogonalization of the initial and final states of the atom, and the summation over the infinite set of the excited states of the final ion, etc. All these problems are absent in the case of the hydrogen atom, which allows one to understand better the actual precision and the applicability range of various approximations used in the theoretical description of Compton scattering. Of course, scattering experiments on a hydrogen target are quite complicated because of the ability of hydrogen atoms to quickly combine to form molecules, but still $(e, 2e)$ experiments on hydrogen are known [11]. Thus, it is necessary to wait and, in the meantime, to continue theoretical studies of the characteristics of Compton scattering from hydrogen atoms in more detail. In this context we would like to accentuate paper [12], which describes the non-relativistic Compton scattering by a hydrogen-like ion and whose approach is close to ours.

In the present paper, we use a non-relativistic approach with the accuracy up to the second order in the photon interaction. The purpose of the study is to determine the kinematic region of the initial photon frequencies, transferred momenta and electron momenta, where it is theoretically possible to accurately extract the momentum distribution of the active electron in the target; also, in relation to the hydrogen atom, to determine the advantages (or disadvantages) of Compton scattering as a method of direct measurement of such a distribution in comparison with other known methods.

The paper uses atomic units: $\hbar = e = m_e = 1$. In these units, $c = 137$, $\alpha = 1/c = 1/137$, $E(\text{a.u.}) = E(\text{eV})/27.2$, $\omega(\text{a.u.}) = 10^2\ \omega(\text{keV})/2.72$. For example, the binding energy of the hydrogen atom is $\varepsilon_0 = -0.5$ a.u.

2 Theoretical method

The formulas below repeat in some sense those from paper [12]. Let us consider the non-relativistic TDSE, which describes the atom-light interaction:

$$i\frac{\partial}{\partial t}\Psi(\vec{r}_e, \vec{r}_p, t) = \left[\frac{1}{2}\left(-i\vec{\nabla}_{r_e} - \frac{1}{c}\vec{A}(\vec{r}_e, t)\right)^2 + \frac{1}{2M}\left(-i\vec{\nabla}_{r_p} + \frac{1}{c}\vec{A}(\vec{r}_p, t)\right)^2 - \frac{1}{|\vec{r}_p - \vec{r}_e|}\right]\Psi(\vec{r}_e, \vec{r}_p, t). \quad (1)$$

In equation (1) $M = 1836$ a.u. is the mass of the proton, $\vec{r}_p$ is its coordinate and $\vec{r}_e$ is the coordinate of the electron. The vector potential is defined as follows

$$\frac{1}{c}\vec{A}(\vec{r}, t) = \sqrt{\frac{2\pi}{\omega}}\ \vec{e}\ e^{i(\vec{k}\vec{r} - \omega t)} + \sqrt{\frac{2\pi}{\omega_1}}\ \vec{e}_1\ e^{-i(\vec{k}_1\vec{r} - \omega_1 t)}. \quad (2)$$

Here $\vec{e}(\vec{e}_1)$ are linear polarizations of the initial (final) photons, $\vec{k}(\vec{k}_1)$ are their momenta, and the frequency (energy of photon) is $\omega = kc$. We remind that $(\vec{k} \cdot \vec{e}) = 0$. This choice of the vector potential corresponds to single incident and single outgoing photon. It is easy to see that $\text{div}\vec{A}(\vec{r}, t) = 0$ (the Coulomb gauge).

Here it is convenient to go to the system of the center of mass of the proton and electron $\vec{r} = \vec{r}_e - \vec{r}_p$, $\vec{R} = (\vec{r}_e + M\vec{r}_p)/(M+1)$. Integration with respect to the coordinate $\vec{R}$ in the matrix element gives the δ-function of momentum conservation, and the huge mass of the proton allows one to put $\vec{r}_e \approx \vec{r}$ and to neglect all the terms of the order $\sim 1/M$. The result is an equation for the motion of the electron that is the same as the one for the motion in

the central external Coulomb field, which is essentially exploited in relativistic physics, but now we have found the law of momentum conservation and other advantages of the non-relativistic approach, mentioned above. Besides that, in such a way we consider the nucleus as a particle that can move after the interaction in the experiments of COLTRIMS type. The final equation in our case can be obtained, if we put in (1) $\vec{r}_p = 0$ and neglect the second term in the square brackets. This is the equation used in [12]. However, for example, for the decay of positronium in the process of Compton scattering, such a non-relativistic equation is no longer suitable.

The interaction term of the electron and the photons is written as

$$\begin{aligned} V_{\rm int} &= i\frac{1}{c}\,(\vec{A}(\vec{r},t)\cdot\vec{\nabla}_r) + \frac{1}{2c^2}A^2(\vec{r},t) \\ &= i\left(\sqrt{\frac{2\pi}{\omega}}\; e^{i(\vec{k}\vec{r}-\omega t)}(\vec{e}\cdot\vec{\nabla}_r)\right. \\ &\quad \left. + \sqrt{\frac{2\pi}{\omega_1}}\; e^{-i(\vec{k}_1\vec{r}-\omega_1 t)}(\vec{e}_1\cdot\vec{\nabla}_r)\right) \\ &\quad + \left(\frac{\pi}{\omega}\; e^{2i(\vec{k}\vec{r}-\omega t)} + \frac{\pi}{\omega_1}\; e^{-2i(\vec{k}_1\vec{r}-\omega_1 t)}\right. \\ &\quad \left. + \frac{2\pi}{\sqrt{\omega\omega_1}}\;(\vec{e}\cdot\vec{e}_1)\; e^{i[(\vec{k}-\vec{k}_1]\vec{r}-(\omega-\omega_1)t]}\right). \end{aligned} \tag{3}$$

Choosing in equation (3) only the terms that correspond to Compton scattering, we obtain the second order matrix element [3,4]

$$\begin{aligned} M(\vec{p},\vec{e},\vec{e}_1) &= (\vec{e}\cdot\vec{e}_1)\langle\varphi^-(\vec{p})|e^{i(\vec{k}-\vec{k}_1)\cdot\vec{r}}|\varphi_0\rangle \\ &- \sum_\beta \frac{\langle\varphi^-(\vec{p})|e^{-i\vec{k}_1\vec{r}_2}(\vec{e}_1\cdot\vec{\nabla}_2)|\varphi^-_\beta\rangle\langle\varphi^-_\beta|e^{i\vec{k}\vec{r}_1}(\vec{e}\cdot\vec{\nabla}_1)|\varphi_0\rangle}{\omega+\varepsilon_0-\varepsilon_\beta+i0} \\ &- \sum_\beta \frac{\langle\varphi^-(\vec{p})|e^{i\vec{k}\vec{r}_2}(\vec{e}\cdot\vec{\nabla}_2)|\varphi^-_\beta\rangle\langle\varphi^-_\beta|e^{-i\vec{k}_1\vec{r}_1}(\vec{e}_1\cdot\vec{\nabla}_1)|\varphi_0\rangle}{-\omega_1+\varepsilon_0-\varepsilon_\beta}. \end{aligned} \tag{4}$$

This matrix element completely coincides with the one obtained from the second-order relativistic matrix element in the non-relativistic limit (see e.g. [2]). In (4) $|\varphi_0\rangle$ denotes the wave function of the ground state of the hydrogen atom and $|\varphi^-_\beta\rangle$ are the eigenfunctions of the Coulomb problem, including both discrete and continuous spectra, and ε_β stands for the energy eigenvalues. The first term is very similar to the first Born term in the description of the ordinary target ionization by a fast particle. However, there is different physics behind these terms. In every interaction of a photon with a charged particle the photon is absorbed. The nonlinear term A^2 in (3) has no analogues in the scattering theory of ordinary particles, and in our case it describes an "instantaneous" absorption/emission of a photon without an excitation of the intermediate states of the target. Formally, such an interaction can be described by an intermediate δ-function.

The physical meaning of the other two terms corresponds rather to the second Born approximation (SBA), which takes into account the excitations of the intermediate states (Green's function), including the continuous spectrum. These terms were calculated analytically for a hydrogen-like atom by Gavrila [13,14], but his results are very complicated and difficult for applications, and in his papers he mainly analysed the low momentum limit $\vec{k}_1 \to 0$. In our case of relatively high photon energies the closure approximation turns out to be more convenient for calculating the matrix elements (see below Eqs. (8)–(10)).

Now the fully differential cross section (FDCS) takes the form:

$$\begin{aligned} d^3\sigma = \frac{(2\pi)^2\alpha}{\omega\omega_1}|M|^2\;(2\pi)^4\delta\left(\omega+\varepsilon_0-\omega_1-p^2/2-E_{\rm ion}\right) \\ \times\,\delta^3\left(\vec{k}-\vec{k}_1-\vec{p}-\vec{K}\right)\;\frac{d^3p}{(2\pi)^3}\frac{d^3k_1}{(2\pi)^3}\frac{d^3K}{(2\pi)^3}. \end{aligned} \tag{5}$$

Here $E_{\rm ion} = \vec{K}^{\,2}/2M$ and $\vec{K}$ stand for the ion kinetic energy and momentum (proton in our case). Also, in atomic units $\alpha^2 = r_0$ is the classical radius of the electron. Integrating with respect to this momentum and dropping the ion kinetic energy, which is negligibly small, we get

$$\begin{aligned} d^3\sigma = \frac{(2\pi)^2\alpha}{\omega\omega_1}|M|^2\;(2\pi)\delta(\omega+\varepsilon_0-\omega_1-p^2/2) \\ \times\,\frac{d^3p}{(2\pi)^3}\frac{d^3k_1}{(2\pi)^3}. \end{aligned} \tag{6}$$

The photon volume element can be represented as $d^3k_1 = \omega_1^2 d\omega_1 d\Omega_1/c^3$. Integrating (1) with respect to ω_1 we finally obtain

$$\frac{d^3\sigma}{dE_e d\Omega_e d\Omega_1} = \frac{\alpha^4}{(2\pi)^3}\;p\;\left(1-\frac{p^2/2-\varepsilon_0}{\omega}\right)|M|^2. \tag{7}$$

We note once again that these formulas are completely identical to those obtained in the non-relativistic limit from the relativistic formulas, but they have the logic of three-particle scattering, including the photon, and not of the two-particle scattering.

In equation (4) we have summation/integration over the Coulomb spectrum. To perform it explicitly, we can use the following trick. We write

$$\begin{aligned} M(\vec{p},\vec{e},\vec{e}_1) &= (\vec{e}\cdot\vec{e}_1)\langle\varphi^-(\vec{p})|e^{i(\vec{k}-\vec{k}_1)\cdot\vec{r}}|\varphi_0\rangle \\ &- \sum_s \frac{\langle\varphi^-(\vec{p})|e^{-i\vec{k}_1\vec{r}_2}(\vec{e}_1\cdot\vec{\nabla}_2)|\varphi_s\rangle\langle\varphi_s|e^{i\vec{k}\vec{r}_1}(\vec{e}\cdot\vec{\nabla}_1)|\varphi_0\rangle}{\omega+\varepsilon_0-\varepsilon_s+i0} \\ &- \int\frac{d^3q}{(2\pi)^3} \\ &\times \frac{\langle\varphi^-(\vec{p})|e^{-i\vec{k}_1\vec{r}_2}(\vec{e}_1\cdot\vec{\nabla}_2)|\varphi^-(\vec{q})\rangle\langle\varphi^-(\vec{q})|e^{i\vec{k}\vec{r}_1}(\vec{e}\cdot\vec{\nabla}_1)|\varphi_0\rangle}{\omega+\varepsilon_0-q^2/2+i0} \\ &- \sum_s \frac{\langle\varphi^-(\vec{p})|e^{i\vec{k}\vec{r}_2}(\vec{e}\cdot\vec{\nabla}_2)|\varphi_s\rangle\langle\varphi_s|e^{-i\vec{k}_1\vec{r}_1}(\vec{e}_1\cdot\vec{\nabla}_1)|\varphi_0\rangle}{-\omega_1+\varepsilon_0-\varepsilon_s} \\ &- \int\frac{d^3q}{(2\pi)^3} \\ &\times \frac{\langle\varphi^-(\vec{p})|e^{i\vec{k}\vec{r}_2}(\vec{e}\cdot\vec{\nabla}_2)|\varphi^-(\vec{q})\rangle\langle\varphi^-(\vec{q})|e^{-i\vec{k}_1\vec{r}_1}(\vec{e}_1\cdot\vec{\nabla}_1)|\varphi_0\rangle}{-\omega_1+\varepsilon_0-q^2/2}, \end{aligned} \tag{8}$$

where s stands for the quantum numbers of the Coulomb problem, $s = (n, l, m)$. For $\omega \gg |\varepsilon_0|$ we can apply the so-called "closure approximation" to the sums over the bound states, i.e. we can replace $\varepsilon_s \to \bar{\varepsilon}$, where $0 < |\bar{\varepsilon}| < |\varepsilon_0|$. We also take into account the completeness of the Coulomb spectrum:

$$\sum_s |\varphi_s\rangle\langle\varphi_s| = I - \int \frac{d^3q}{(2\pi)^3} |\varphi^-(\vec{q})\rangle\langle\varphi^-(\vec{q})| \qquad (9)$$

and obtain

$$\begin{aligned} M(\vec{p},\vec{e},\vec{e}_1) &= (\vec{e}\cdot\vec{e}_1)\langle\varphi^-(\vec{p})|e^{i\vec{Q}\cdot\vec{r}}|\varphi_0\rangle \\ &- \frac{\langle\varphi^-(\vec{p})|(\vec{e}_1\cdot\vec{\nabla})e^{i\vec{Q}\vec{r}}(\vec{e}\cdot\vec{\nabla})|\varphi_0\rangle}{\omega+\varepsilon_0-\bar{\varepsilon}} \\ &- \frac{\langle\varphi^-(\vec{p})|(\vec{e}\cdot\vec{\nabla})e^{i\vec{Q}\vec{r}}(\vec{e}_1\cdot\vec{\nabla})|\varphi_0\rangle}{-\omega_1+\varepsilon_0-\bar{\varepsilon}} \\ &- \int \frac{d^3q}{(2\pi)^3} \langle\varphi^-(\vec{p})|e^{-i\vec{k}_1\vec{r}_2}(\vec{e}_1\cdot\vec{\nabla}_2)|\varphi^-(\vec{q})\rangle \\ &\times \langle\varphi^-(\vec{q})|e^{i\vec{k}\vec{r}_1}(\vec{e}\cdot\vec{\nabla}_1)|\varphi_0\rangle \\ &\times \left[\frac{q^2/2-\bar{\varepsilon}}{(\omega+\varepsilon_0-q^2/2+i0)(\omega+\varepsilon_0-\bar{\varepsilon})}\right] \\ &- \int \frac{d^3q}{(2\pi)^3} \langle\varphi^-(\vec{p})|e^{i\vec{k}\vec{r}_2}(\vec{e}\cdot\vec{\nabla}_2)|\varphi^-(\vec{q})\rangle \\ &\times \langle\varphi^-(\vec{q})|e^{-i\vec{k}_1\vec{r}_1}(\vec{e}_1\cdot\vec{\nabla}_1)|\varphi_0\rangle \\ &\times \left[\frac{q^2/2-\bar{\varepsilon}}{(-\omega_1+\varepsilon_0-q^2/2)(-\omega_1+\varepsilon_0-\bar{\varepsilon})}\right]. \end{aligned} \qquad (10)$$

In equation (10) $\vec{Q} = \vec{k} - \vec{k}_1$ is the momentum transfer, and $\omega_1 = \omega + \varepsilon_0 - p^2/2$. For the sake of convenience, we introduce a new variable

$$t = \frac{\omega_1}{\omega} = 1 - \frac{E_e + |\varepsilon_0|}{\omega} \geq 0.$$

In terms of this variable the momentum transfer is written as $Q = \frac{\omega}{c}\sqrt{1+t^2-2t\cos\theta}$, but for relatively small electron energies $\omega \approx \omega_1$, and $Q \approx 2\alpha\omega\sin(\theta/2)$ with θ being the photon scattering angle.

Now we discuss equation (10) in more detail. The first term in this equation is just the A^2 approximation, so called seagull matrix-element. Formally it is a term of the second order, but it looks like the first Born approximation (FBA) in the scattering processes of ordinary projectiles: electrons, ions. However, the evaluation of the integral terms looks quite problematic because of the matrix element

$$\langle\varphi^-(\vec{p})|e^{-i\vec{k}_1\vec{r}_2}(\vec{e}_1\cdot\vec{\nabla}_2)|\varphi^-(\vec{q})\rangle.$$

This term describes continuum–continuum dipole transition, its analytic form is known, but not practically tractable because of the singularities. On the other hand, if $q^2/2 \sim \omega$, the integral terms in equation (10) should be rather small. These two terms are of the order $1/\omega^2$ and we omit them for a moment. Thus, the energy of the intermediate electron should not be too large and be comparable to E_e.

Then we can approximately write up to the order $\mathcal{O}(1/\omega)$

$$\begin{aligned} M(\vec{p},\vec{e},\vec{e}_1) \approx{}& (\vec{e}\cdot\vec{e}_1)\langle\varphi^-(\vec{p})|e^{i\vec{Q}\cdot\vec{r}}|\varphi_0\rangle \\ &- \frac{1}{\omega}\left[\langle\varphi^-(\vec{p})|\left(\vec{e}_1\cdot\vec{\nabla}\right)e^{i\vec{Q}\vec{r}}\left(\vec{e}\cdot\vec{\nabla}\right)|\varphi_0\rangle\right. \\ &\left.- \langle\varphi^-(\vec{p})|\left(\vec{e}\cdot\vec{\nabla}\right)e^{i\vec{Q}\vec{r}}\left(\vec{e}_1\cdot\vec{\nabla}\right)|\varphi_0\rangle\right]. \end{aligned} \qquad (11)$$

Taking into account the explicit form of the hydrogen ground state wave function φ_0, after a little algebra we obtain

$$\begin{aligned} M(\vec{p},\vec{e},\vec{e}_1) &= (\vec{e}\cdot\vec{e}_1)\,J_0\left(\vec{Q},\vec{p}\right) - \frac{\sqrt{2|\varepsilon_0|}}{\omega} \\ &\times\left[\left(\vec{e}_1\cdot\vec{Q}\right)\left(\vec{e}\cdot\vec{\nabla}_Q\right)\right. \\ &\left.-\left(\vec{e}\cdot\vec{Q}\right)\left(\vec{e}_1\cdot\vec{\nabla}_Q\right)\right]J_1\left(\vec{Q},\vec{p}\right), \end{aligned} \qquad (12)$$

$$\begin{aligned} J_0\left(\vec{Q},\vec{p}\right) &= \langle\varphi^-(\vec{p})\,|e^{i\vec{Q}\vec{r}}|\varphi_0\rangle = -16\pi\sqrt{\frac{Z^5}{\pi}}e^{-\pi\zeta/2} \\ &\times\Gamma(1+i\zeta)\,\frac{\left[Q^2-(p+iZ)^2\right]^{-1+i\zeta}}{\left[(\vec{Q}-\vec{p})^2+Z^2\right]^{2+i\zeta}} \\ &\times Q\left[Q-(p+iZ)\cos\chi\right] \end{aligned}$$

and

$$\begin{aligned} J_1(\vec{Q},\vec{p}) &= \left\langle\varphi^-(\vec{p})\left|\frac{1}{r}e^{i\vec{Q}\vec{r}}\right|\varphi_0\right\rangle = 4\pi\sqrt{\frac{Z^3}{\pi}}\,e^{-\pi\zeta/2} \\ &\times\Gamma(1+i\zeta)\frac{\left[Q^2-(p+iZ)^2\right]^{i\zeta}}{\left[(\vec{Q}-\vec{p})^2+Z^2\right]^{1+i\zeta}}. \end{aligned}$$

Here $p\zeta = -Z$, $\quad Z = \sqrt{2|\varepsilon_0|} = 1$, and

$$\cos\chi = \frac{\cos\phi_e(1-t\cos\theta) - t\sin\phi_e\sin\theta\cos\Phi}{\sqrt{1+t^2-2t\cos\theta}}$$

with χ being the angle between vectors $\vec{p}$ and $\vec{k}_1$. Vector $\vec{k}$ is the z-axis, ϕ_e is the angle between vectors $\vec{k}$ and $\vec{p}$, and Φ is the angle between the plane formed by vectors $\vec{k}, \vec{k}_1$ and the plane formed by vectors $\vec{k}, \vec{p}$.

It follows from equation (12) that $\vec{\nabla}_Q J_1(\vec{Q},\vec{p}) = A\vec{Q} + B\vec{p}$. Thus,

$$\begin{aligned} &\left[\left(\vec{e}_1\cdot\vec{Q}\right)\left(\vec{e}\cdot\vec{\nabla}_Q\right) - \left(\vec{e}\cdot\vec{Q}\right)\left(\vec{e}_1\cdot\vec{\nabla}_Q\right)\right]J_1\left(\vec{Q},\vec{p}\right) \\ &= \left[\left(\vec{e}_1\cdot\vec{Q}\right)(\vec{e}\cdot\vec{p}) - \left(\vec{e}\cdot\vec{Q}\right)(\vec{e}_1\cdot\vec{p})\right]B, \end{aligned}$$

and

$$B\left(\vec{Q},\vec{p}\right) = 8\pi\sqrt{\frac{Z^3}{\pi}}\,e^{-\pi\zeta/2}\Gamma(2+i\zeta)\frac{\left[Q^2-(p+iZ)^2\right]^{i\zeta}}{\left[(\vec{Q}-\vec{p})^2+Z^2\right]^{2+i\zeta}}.$$

The calculation of FDCS demands averaging over the initial photon polarizations and the summation over the final photon polarizations. For averaging over the initial photon polarizations we have the following formula

$$\frac{1}{2}\sum_{e}|(\vec{a}\cdot\vec{e})|^2=\frac{a^2k^2-\left(\vec{a}\cdot\vec{k}\right)^2}{2k^2},$$

and a similar formula for the summation over the final photon polarizations

$$\sum_{e_1}|(\vec{b}\cdot\vec{e}_1)|^2=\frac{b^2k_1^2-\left(\vec{b}\cdot\vec{k}_1\right)^2}{k_1^2}.$$

In the general case

$$\sum_{e}\left(\vec{a}\cdot\vec{e}\right)\left(\vec{b}\cdot\vec{e}^{*}\right)=\left(\vec{a}\cdot\vec{b}\right)-\frac{\left(\vec{a}\cdot\vec{k}\right)\left(\vec{b}\cdot\vec{k}\right)}{k^2}.$$

Up to the order $\mathcal{O}(1/\omega)$, we get:

$$\begin{aligned}|M|^2\to|\bar{M}|^2=\frac{1}{2}\sum_{e1,e2}|M|^2=\frac{1}{2}|J_0|^2\left(1+\cos^2\theta\right)\\-\frac{\sqrt{2|\varepsilon_0|}}{2\omega}\cos\theta\left(J_0^{*}B+J_0B^{*}\right)\\\times\left[\frac{\left(\vec{k}\cdot\vec{Q}\right)\left(\vec{k}_1\cdot\vec{p}\right)}{kk_1}-\frac{\left(\vec{k}\cdot\vec{p}\right)\left(\vec{k}_1\cdot\vec{Q}\right)}{kk_1}\right].\end{aligned}\tag{13}$$

In this formula, the first term is just the standard FBA. The second term is a correction due to the electron boundness, which can be written as

$$\begin{aligned}\Delta M=-\frac{\sqrt{2|\varepsilon_0|}}{2\omega}\cos\theta\ \left(J_0^{*}B+J_0B^{*}\right)\\\times\left[\frac{\left(\vec{k}\cdot\vec{Q}\right)\left(\vec{k}_1\cdot\vec{p}\right)}{kk_1}-\frac{\left(\vec{k}\cdot\vec{p}\right)\left(\vec{k}_1\cdot\vec{Q}\right)}{kk_1}\right]\\\approx-p\frac{\sqrt{2|\varepsilon_0|}}{2c}\ \mathrm{Re}\left(J_0^{*}B\right)\sin2\theta\\\times\left[t\cos\phi_e\sin\theta+(1-t\cos\theta)\sin\phi_e\cos\Phi\right].\end{aligned}$$

We see that for $\omega\sim c$ or $k,k_1,Q\sim1$ the ratio $|\varepsilon_0|/\omega\ll1$ for the light atoms, and the correction is expected to be rather small.

3 Results and discussion

The most of the calculations are carried out for $\omega=2.06\,\mathrm{keV}$. In atomic units the fully differential cross section looks like

$$\mathrm{FDCS}=\frac{d^3\sigma}{dE_ed\Omega_ed\Omega_1}=\frac{\alpha^4}{(2\pi)^3}\ p\ t|\bar{M}|^2.\tag{14}$$

To get the FDCS in $\mathrm{cm}^2/\mathrm{eV}\cdot\mathrm{Sr}^2$, we have to multiply equation (14) by the factor 1.03×10^{-18}. If we multiply this factor by α^4, we obtain the total factor $F=0.29\times10^{-26}$ $\mathrm{cm}^2/\mathrm{eV}\cdot\mathrm{Sr}^2=0.29\times10^{-2}\mathrm{barn}/\mathrm{eV}\cdot\mathrm{Sr}^2$. Thus,

$$\frac{d^3\sigma}{dE_ed\Omega_ed\Omega_1}=\frac{F}{(2\pi)^3}\ p\ t|\bar{M}|^2.\tag{15}$$

Since the ionization potential $I_p=|\varepsilon_0|=0.5$ and the kinetic energy of the ejected electron is of the same order, in calculating the correction we can put $t=1$. Then we obtain

$$|\bar{M}|^2=|\bar{M}_0|^2+\Delta M,\tag{16}$$

where

$$|\bar{M}_0|^2=\frac{1}{2}|J_0|^2(1+\cos^2\theta)$$

and

$$\begin{aligned}\Delta M=-2p\ \alpha\ \mathrm{Re}(J_0^{*}B)\sin(2\theta)\sin\frac{\theta}{2}\\\times\left[\cos\phi_e\cos\frac{\theta}{2}+\sin\phi_e\sin\frac{\theta}{2}\cos\Phi\right].\end{aligned}$$

The angular spectrum of the scattered photons as a function of θ is given by

$$\begin{aligned}\frac{d\sigma}{d\Omega_{\vec{k}_2}}=(27.2\ \mathrm{eV})\int_0^{p_{\max}}xdx\int_0^{2\pi}d\Phi\int_0^{\pi}\sin\phi_ed\phi_e\\\times\frac{d^3\sigma}{d\Omega_{\vec{k}_2}d\Omega_ed\Omega_e}.\end{aligned}\tag{17}$$

Here $p_{\max}=\sqrt{2(\omega-|\varepsilon_0|)}$, but for the actual calculations $p_{\max}$ is much smaller.

The energy spectrum of the emitted electrons looks like:

$$\frac{d\sigma}{dE_e}=(2\pi)\int_0^{2\pi}d\Phi\int_0^{\pi}\sin\theta d\theta\int_0^{\pi}\sin\phi_ed\phi_e\ \frac{d^3\sigma}{d\Omega_{\vec{k}_2}d\Omega_ed\Omega_e}.\tag{18}$$

Finally, we have to calculate the TCS

$$\begin{aligned}\mathrm{TCS}=\sigma(\mathrm{barn})=(2\pi)(27.2\ \mathrm{eV})\int_0^{2\pi}d\Phi\int_0^{\pi}\sin\theta d\theta\\\times\int_0^{\pi}\sin\phi_ed\phi_e\int_0^{p_{\max}}kdk\ \frac{d^3\sigma}{d\Omega_{\vec{k}_2}d\Omega_ed\Omega_e}.\end{aligned}\tag{19}$$

It is also necessary to note that the following relations are valid:

$$\int_0^{2\pi}d\Phi\int_0^{\pi}\sin\phi_ed\phi_e\ f(\cos\chi)=(2\pi)\int_{-1}^{1}dy\ f(y)$$

and

$$\int_0^{2\pi}d\Phi\int_0^{\pi}\sin\phi_ed\phi_e\ \Delta M=0.$$

Both these mathematical statements can be rigorously proved. The last formula shows that the first correction

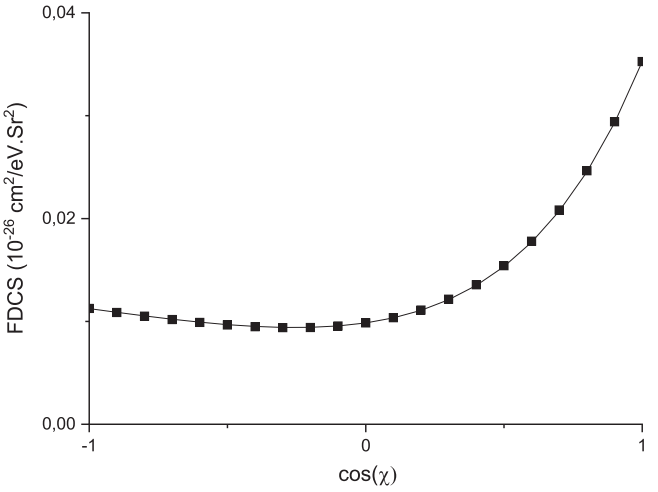

Fig. 1. FDCS equation (15) versus $\cos\chi$. Coplanar geometry: angle $\Phi = 0°$, $\theta = 150°$, $E_e = 0.5$ eV. Solid line: $|M|^2 = |M_0|^2$, squares: equation (16).

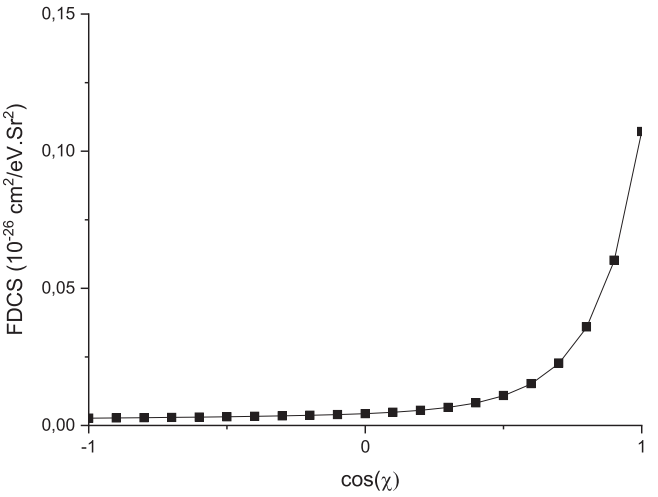

Fig. 2. The same like in Figure 1, but $E_e = 6$ eV.

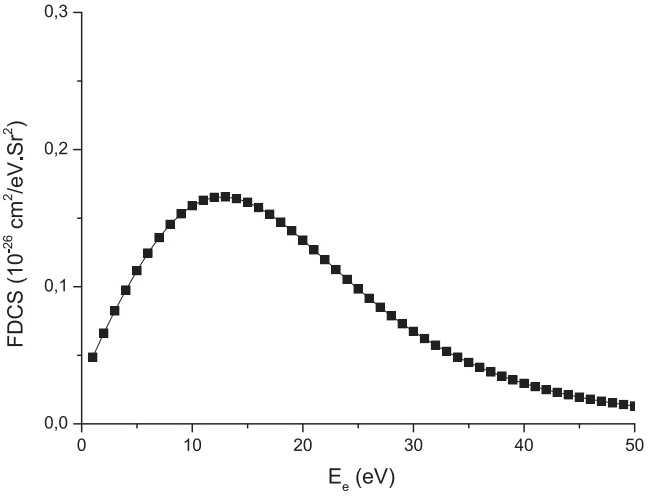

Fig. 3. FDCS equation (15) versus the energy of escaped electron. Coplanar geometry: angle $\Phi = 0°$, $\theta = 180°$ (backward scattering), $\phi_e = 0°$ (forward scattering). Solid line: $|M|^2 = |M_0|^2$, squares: equation (16).

due to the electron boundness (13) vanishes to all integral cross sections (17)–(19).

In what follows, we consider the energy range 2 keV $\leq \omega \leq$ 10 keV. First of all, we pay attention to the small contribution of the term ΔM due to the electron boundness, as predicted. In this energy range, the FBA dominates overwhelmingly. This makes it possible to study this term in detail in contrast to the ionization reactions with charged particles (electrons, protons, bar ions), where the contributions of the higher Born terms and corrections can be noticeable.

We also note that the cross section taking into account only the FBA equals to zero at $Q = 0$. This significantly distinguishes Compton scattering by bound electrons from that by free electrons, because in the latter case the maximum cross section is achieved at $Q = 0$. If we consider the ionization of a more complex atom (molecule) than hydrogen, it becomes necessary to orthogonalize the initial and final states of the atom. This operation is in a sense artificial, and the experiments on measuring the differential cross section can allow one to estimate the accuracy of such a procedure.

Let us consider Figures 1 and 2. Here the cross sections depend on the angle χ between the momentum transfer and the electron momentum. These angular distributions differ little from the similar distributions in the case of the ionization of an atom by fast protons or electrons: there are also a binary peak at $\chi = 0$ and a much less pronounced recoil peak at $\chi = \pi$. In this case, the ratio of the values of the peaks increases with increasing electron energy (see e.g. [15]). Here it is necessary to note that in the case under consideration, since the photon is a neutral particle, one does not need to include into the calculations the states of tree-body Coulomb post-interactions of 3C type.

From Figures 3–5 it follows that the largest cross section is observed in the backscattering of the photon, which is well known. For this geometry, the momentum transfer Q is maximal, and the orthogonality does not play a special role here. In terms of the process dynamics, in this area we are most close to the symmetric high energy $(e, 2e)$ reactions, which are the best ones to study the single electron density in the target [11,16]. In accordance with physical considerations, it is natural that, when the projectile recoils backwards, the electron flies forward with a much greater probability than backwards, which we observe in these figures. In Compton scattering by a free electron at rest, it follows from the law of momentum conservation that $p = Q$ or $E_e(\text{eV}) = 13.6(2\omega/c)^2$. From the series of curves in Figure 4 it is seen that this energy corresponds to the position of the maximum of the energy distribution, when the photon is scattered backwards, which, however, was expected. We also note that for $E_e \to 0$ the cross section does not go to zero, but tends to a constant. This is a characteristic feature of the ejected electron description by the Coulomb wave function. In the case of the

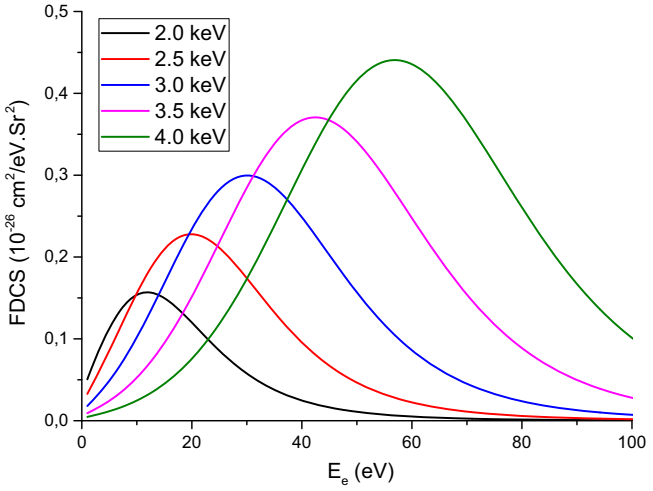

Fig. 4. FDCS equation (15) versus the energy of escaped electron for different photon energies. Coplanar geometry: angle $\Phi = 0°$, $\theta = 180°$ (backward scattering), $\phi_e = 0°$ (forward scattering). $|M|^2 = |M_0|^2$.

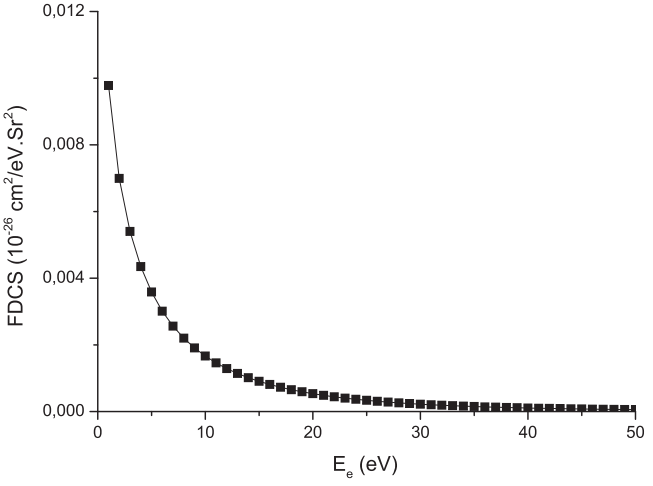

Fig. 5. The same like in Figure 3, but $\phi_e = 180°$ (backward scattering).

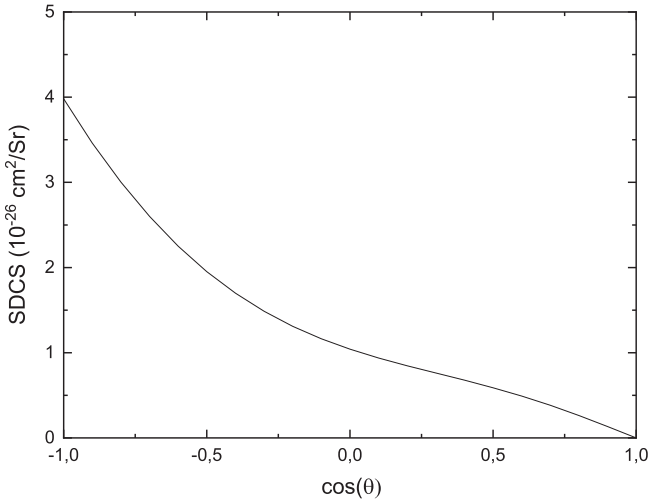

Fig. 6. SDCS equation (17) versus the photon scattering angle. Solid line: $|M|^2 = |M_0|^2$.

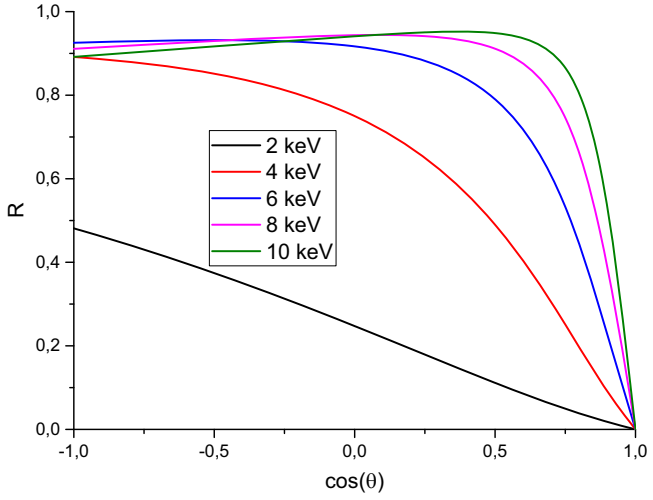

Fig. 7. The ratio $R(\theta,\omega) = \frac{d\sigma}{d\Omega_{\vec{k}_2}} / \frac{d\sigma^{KN}}{d\Omega_{\vec{k}_2}}$ versus the photon scattering angle for different photon energies. Here $|M|^2 = |M_0|^2$.

ejected electron description by a plane wave as in impulse approximation [12], it is not so.

In Figures 6–9 the angular spectra of the scattered photon, the energy spectrum of the ionized electron (SDCS), and the total ionization cross section (TCS) are given. We attract attention to the emerging peak at $\cos\theta \approx 0.5$ in Figure 6. If one increases the energy of the photon, the peak will more and more manifest itself. This is clearly seen in Figure 7, where the ratio of SDCS (17) and the classical Klein–Nishina cross section is given in the approximation $\omega_1/\omega \sim 1$

$$\frac{d\sigma^{KN}}{d\Omega_{\vec{k}_2}} = (27.2\text{ eV})\frac{F}{2}\left(1+\cos^2\theta\right). \qquad (20)$$

In fact, expression (20) follows from equation (17), if we put $t = 1$ in it and replace the Coulomb wave with a plane wave. In this case, replacing in equation (17) the integration with respect to $\vec{p}$ by the integration with respect to $\vec{q}$, where $\vec{q} = \vec{p} - \vec{Q}$, we get unity as a result of this integration, since it is the normalization of the initial state. Taking into account the factor t will complicate the integration, but it will not change anything fundamentally.

With increasing photon energy, the ratio $R(\theta,\omega)$ approaches unity in an increasing range of angles θ except the small ones (orthogonality!). A small deviation of the plateau from unity is due to the factor t taken into account in the calculations in equation (17) and its omission in equation (20). If we put the factor $t = 1$ in equation (17), we get a plateau exactly equal to unity. The effect of the angular spectrum of photons scattered by bound electrons coming close to the free electron scattering spectrum at high angles and photon energies has been noted by a number of authors (see e.g. [17]).

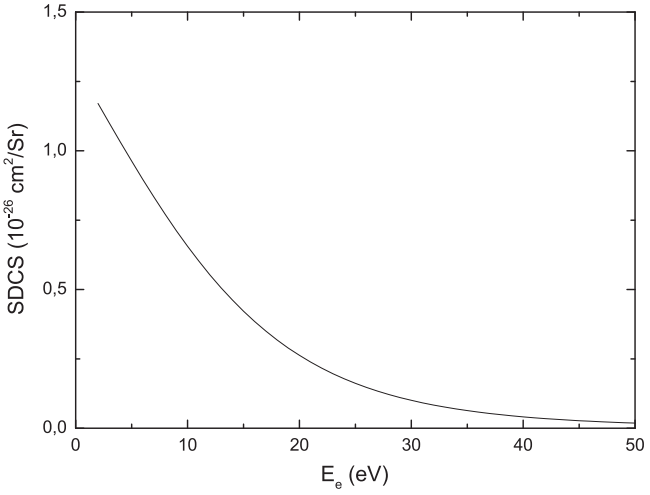

Fig. 8. SDCS equation (18) versus the electron energy. Solid line: $|M|^2 = |M_0|^2$.

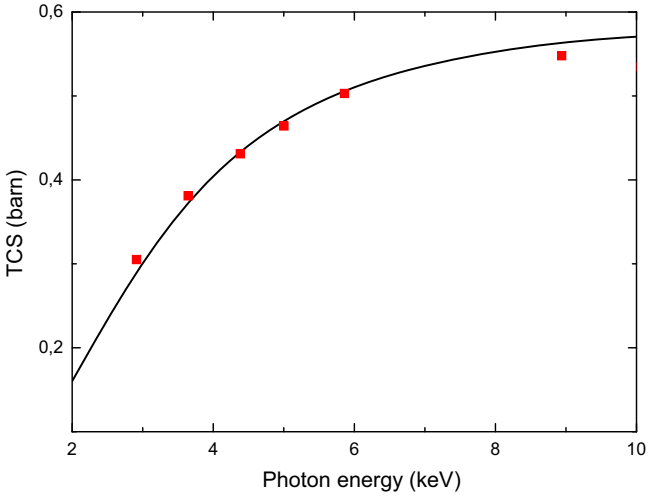

Fig. 9. TCS equation (19) versus the photon energy. Solid line: $|M|^2 = |M_0|^2$; squares: the points extracted from Figure 29 in paper [5].

It should also be noted that the dynamics of the processes presented in Figures 4 and 7 is linked. With the growth of the photon energy, the energy of the ejected electron sharply increases, which results in its Coulomb wave function approaching the corresponding plane wave. Thus, the angular spectrum at the backward scattering angles of the photon increasingly approaches the Klein–Nishina spectrum.

In Figure 8 one should note that the SDCS tends to a nonzero constant as $E_e \to 0$. This is a direct consequence of the description of the final electron by the Coulomb wave instead of the plane wave. In the latter case, the SDCS is equal to zero at $E_e = 0$. When the electron energy increases, the difference in the course of the curves is levelled, which is quite expected.

Finally, we discuss the TCS presented in Figure 9. The corresponding calculation in a much wider range of photon energies is presented in Figure 29 in paper [5]. We compared our calculation results in the photon energy range of $2 \div 10$ keV with those presented in that figure, despite the difficulties of extracting the data from the figure drawn in the double logarithmic scale along the X and Y axes. The agreement is quite satisfactory as it should be, taking into account a rather rough accuracy of the data extraction.

4 Conclusions

Taking the hydrogen atom as a benchmark example, we consider the problem of extracting useful information about the orbital structure of a light atomic/molecular target by exploring the fully differential and integral cross sections of the Compton single ionization near threshold. It is shown that in the energy range of the incoming photons of a few keV and the energies of the ejected electron not larger than 20–30 eV the information obtained in this process is comparable to the one that follows from the reactions $(e, 2e)$, (p, pe), etc.

In the specified kinematic region a non-relativistic treatment of Compton scattering in the framework of the Schrödinger equation is possible, which puts this reaction in one row with other reactions of the target ionization by fast particles.

Of course, the measurement of the fully differential cross section of Compton ionization in coincidence experiments is still very complicated (though implemented), but it has a number of advantages compared to the ionization of a light atomic target by fast particles. These are small corrections from higher Born approximations, the possibility to vary the momentum transfer within wide limits, as well as the comparatively simple description of the initial and final states.

We see that with increasing energy and the scattering angle of the photon, the single angular cross sections (17) increasingly approach the Klein–Nishina scattering cross section by a free electron. The energy of the electron giving the maximum of the differential cross section (15) also corresponds to that of the scattering by a free electron at rest and grows rapidly with the growth of the photon energy. All this suggests that the interesting information about both the single electron momentum profile of a light atom (molecule) target and the final state of the ion + outgoing electron should be sought at relatively small photon energies of 1–3 keV, where the contribution of the SBA is still small, and the quantum effects still dominate the classical ones.

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Author contribution statement

All authors contributed equally to the paper.

References

1. A.H. Compton, Phys. Rev. **21**, 484 (1923)
2. A.I. Akhiezer, V.B. Berestetskii, *Quantum Electrodynamics* (John Wiley and Sons, 1965)
3. H.A. Kramers, W. Heisenberg, Z. Phys. **31**, 681 (1925)
4. I. Waller, D.R. Hartree, Proc. R. Soc. (London) A **124** 119 (1929)
5. P.M. Bergstrom Jr., T. Surić, K. Pisk, R.H. Pratt, Phys. Rev. A **48**, 1134 (1993)
6. J.H. Hubbell, W.J. Veigele, E.A. Briggs, R.T. Brown, D.T. Cromer, R.J. Howerton, J. Phys. Chem. Ref. Data **4**, 471 (1975)
7. J.A.R. Samson, Z.X. He, R.J. Bartlett, M. Sagurton, Phys. Rev. Lett. **72**, 3329 (1994)
8. Z. Kaliman, T. Surić, K. Pisk, R.H. Pratt, Phys. Rev. A **57**, 2683 (1998)
9. J. Ullrich, R. Moshammer, A. Dorn, R. Dörner, L.P.H. Schmidt, H. Schmidt-Böcking, Rep. Prog. Phys. **66**, 1463 (2003)
10. M. Kircher, F. Trinter, S. Grundmann, I. Vela-Perez, S. Brennecke, N. Eicke, J. Rist, S. Eckart, S. Houamer, O. Chuluunbaatar, Y.V. Popov, I.P. Volobuev, K. Bagschick, M.N. Piancastelli, M. Lein, T. Jahnke, M.S. Schöffler, R. Dörner, arXiv:1911.04780v1 [physics.atom-ph] (2019) (accepted to Nature physics)
11. E. Weigold, I.E. McCarthy, *Electron Momentum Spectroscopy* (Kluwer, New York, 1999)
12. P. Eisenberger, P.M. Platzman, Phys. Rev. A **2**, 415 (1970)
13. M. Gavrila, Phys. Rev. A **6**, 1348 (1970)
14. M. Gavrila, Phys. Rev. A **6**, 1360 (1970)
15. O. Chuluunbaatar, K.A. Kouzakov, S.A. Zaytsev, A.S. Zaytsev, V.L. Shablov, Y.V. Popov, H. Gassert, M. Waitz, H.-K. Kim, T. Bauer, A. Laucke, C. Muller, J. Voigtsberger, M. Weller, J. Rist, K. Pahl, M. Honig, M. Pitzer, S. Zeller, T. Jahnke, L.P.H. Schmidt, H. Schmidt-Boecking, R. Doerner, M.S. Schoeffler, Phys. Rev. A **99**, 062711 (2019)
16. V.G. Neudachin, Y.V. Popov, Y.F. Smirnov, Phys. Usp. **42**, 1017 (1999)
17. A.M. Dykhne, G.L. Yudin, Sov. Phys. Usp. **21**, 549 (1978)