Radiation Physics and Chemistry 95 (2014) 34–37

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Cross section calculations of photoabsorption and Compton scattering contributions to He single and double ionization via recoil momentum observable

Zoran Kaliman [a,*], Gordana Žauhar [b], Slaven Jurković [c]

[a] Department of Physics, University of Rijeka, Omladinska 14, Rijeka, Croatia
[b] Department of Physics, Faculty of Medicine, University of Rijeka, Braće Branchetta 20, Rijeka, Croatia
[c] University Hospital Rijeka, Radiotherapy Department, Physics Division, Krešimirova 42, Rijeka, Croatia

HIGHLIGHTS

- We calculate photoionization cross sections with respect to recoil-ion momenta.
- Recoil ions from photoabsorption on He are mainly distributed on near cut.
- Dominant contribution of recoil ions from Compton scattering is close to zero (few a.u.)
- Calculation is in accordance with experiment.
- Dipole pattern of the recoil ions due to the polarization of incoming radiation is seen.

ARTICLE INFO

Article history:
Received 30 September 2012
Accepted 11 January 2013
Available online 21 January 2013

Keywords:
Compton scattering
Photoabsorption
Photoionization
Recoil momentum

ABSTRACT

This paper presents a theoretical framework for the calculations of Compton scattering and photoabsorption on bound electrons for single and double ionization, based on recoil-ion observable. For the photoionization of helium (single or double) our calculations of cross sections for photon energy of 7 keV show that the recoil ions from photoabsorption are mainly distributed on a sphere in momentum space of 22 a.u. radius, while recoil ions from Compton scattering show a dominant contribution close to zero radius ($\lesssim 3$ a.u.). Our calculated cross sections are in agreement with the published experimental values.

1. Introduction

The ratio of double to single ionization determined by photoionization is an important quantity for understanding electron–electron correlation effects (Surić et al., 1994). In 1990s a new spectroscopic technique, cold target recoil-ion momentum spectroscopy (COLTRIMS), was developed. This technique allows final momentum measurements of recoiling target ion created in a photon–atom interaction process. Using COLTRIMS a separation of the contributions of photoabsorption and Compton scattering to the single and double ionization at photon energy of about 8 keV is obtained (Spielberger et al., 1995). Before COLTRIMS the photoionization of an atom was analyzed almost always in terms of the scattering photon (for Compton scattering) and/or ejected electron variables. Earlier, the validity of impulse approximation approach in single ionization via Compton scattering in terms of recoil momentum observable was discussed (Kaliman and Pisk, 2004).

In this paper we demonstrate a theoretical approach to distinguish mechanisms by cross section calculations in terms of recoil-momentum observable. We calculated contributions of photoabsorption and Compton scattering to He single and double ionization and compared our results with the published experimental results (Spielberger et al., 1995).

2. Cross sections

In the proposed model, the coordinate frame is fixed by incident photon putting the z-axis in the direction of propagation and the x-axis in the direction of photon polarization. Furthermore, the target

* Corresponding author. Tel.: +385 51582004.
E-mail addresses: kaliman@phy.uniri.hr, zoran.kaliman@gmail.com (Z. Kaliman), gordana.zauhar@medri.uniri.hr (G. Žauhar), slaven.jurkovic@medri.uniri.hr (S. Jurković).

0969-806X/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.radphyschem.2013.01.013

atom is at rest and kinetic energy of recoiling ion is neglected. All calculations are made in non-relativistic approximation with $c=\hbar=1$ units. Also, r_0 is the electron classical radius, m is the electron mass, α the fine structure constant.

In the following expressions for differential cross sections $|i\rangle$ is the initial electron state, $|\vec{p}\,\rangle$ is the final electron state with the momentum $\vec{p}$ for the single ionization, while in double ionization $|\vec{p}_1\vec{p}_2\rangle$ represents the final state of two electrons with the momenta $\vec{p}_1$ and $\vec{p}_2$.

2.1. Single ionization

In non-relativistic quantum mechanics the cross section for photoabsorption from bound electrons, in first order of perturbation theory, is given by "$\vec{p}\cdot\vec{A}$" term of the photon–atom interaction

$$d\sigma = r_0^2\frac{m}{2\alpha\omega}\left|\langle f|(\vec{p}\cdot\vec{\varepsilon})e^{i\vec{k}\cdot\vec{r}}|i\rangle\right|^2\delta(E_i+\omega-E_f))d^3p, \tag{1}$$

where $\vec{k}$, ω, and $\vec{\varepsilon}$ represent the photon momentum, energy and linear polarization, respectively. The initial and the final electron state $|i\rangle$ and $|f\rangle$ have energies E_i and E_f, respectively. Combining momentum conservation

$$\vec{p}=\vec{k}-\vec{P}, \tag{2}$$

(where $\vec{P}\equiv(P_x,P_y,P_z)$ represents a recoil-ion momentum), with energy conservation, we obtain the cross section in P_x, P_y variables

$$\frac{d\sigma}{dP_x\,dP_y}=\frac{r_0^2}{2\pi\alpha\omega}\left[\left(\frac{\left|\langle\vec{p}\left|(\vec{\varepsilon}\cdot\vec{p})e^{i\vec{k}\cdot\vec{r}}\right|i\rangle\right|^2}{|k_z-P_z|}\right)_{P_z=P_+}+\left(\frac{|\langle\vec{p}\left|(\vec{\varepsilon}\cdot\vec{p})e^{i\vec{k}\cdot\vec{r}}\right|i\rangle|^2}{|k_z-P_z|}\right)_{P_z=P_-}\right], \tag{3a}$$

where

$$P_\pm=k_z\pm\sqrt{A},\quad A=2m(\omega-E_i)-P_\perp^2,\quad \vec{P}_\perp\equiv(P_x,P_y,0). \tag{3b}$$

We calculated the cross section for Compton scattering from bound electrons, in first order of perturbation theory, by "A^2" term of the photon–atom interaction

$$d\sigma=\frac{r_0^2}{2}\frac{(\vec{\varepsilon}_1\cdot\vec{\varepsilon}_2)^2}{\omega_1\omega_2}|\langle f|e^{i\vec{k}\cdot\vec{r}}|i\rangle|^2\delta(E_i+\omega_1-E_f-\omega_2)\,d^3k_2\,d^3p, \tag{4}$$

where $\vec{k}=\vec{k}_1-\vec{k}_2$ is a momentum transfer, while $\omega_{1,2}$, $\vec{k}_{1,2}$, and $\vec{\varepsilon}_{1,2}$ represent, respectively, the energies, momenta and linear polarizations of incident and scattered photons. As in the photoabsorption case, from this cross section using momentum conservation

$$\vec{p}=\vec{k}_1-\vec{k}_2-\vec{P}, \tag{5}$$

we obtain the cross section in P_x, P_y variables (Kaliman and Pisk, 2004)

$$\frac{d\sigma}{dP_x\,dP_y}=\frac{r_0^2}{2\omega_1}\int d\omega_2\,d\Omega_2\,\omega_2(\vec{\varepsilon}_1\cdot\vec{\varepsilon}_2)^2\left[\left(\frac{|\langle\vec{p}|e^{i\vec{k}\cdot\vec{r}}|i\rangle|^2}{|k_z-P_z|}\right)_{P_z=P_+}+\left(\frac{|\langle\vec{p}|e^{i\vec{k}\cdot\vec{r}}|i\rangle|^2}{|k_z-P_z|}\right)_{P_z=P_-}\right], \tag{6a}$$

where

$$P_\pm=k_z\pm\sqrt{B},\quad B=2m(\omega_1-\omega_2-E_i)-(\vec{k}-\vec{P})_\perp^2. \tag{6b}$$

In contrast to earlier calculations (differential cross sections in scattered photon and/or ejected electron variables), we integrated over the scattering photon momenta.

2.2. Double ionization

Cross sections are calculated in shake off approximation (overlap integrals) (Pratt et al., 1998). The initial state is helium wave function $|i\rangle=\psi_{He}$, and the final is free electron states (in He nucleus field) $|f\rangle\equiv\left|\vec{p}_1\vec{p}_2\right\rangle$. We supposed that the first electron with momentum $\vec{p}_1$ was fast, and the second with the momentum $\vec{p}_2$ was slow.

Cross section for double ionization of He during photoabsorption reads as

$$d\sigma=r_0^2\frac{1}{(2\pi)^4\omega\alpha}\left|\langle f|(\vec{p}\cdot\vec{\varepsilon})e^{i\vec{k}\cdot\vec{r}}|i\rangle\right|^2\delta(E_i+\omega-E_1-E_2)\,d^3p_1\,d^3p_2. \tag{7}$$

In the same way as in the single ionization case, combining momentum conservation

$$\vec{p}_1=\vec{k}-\vec{p}_2-\vec{P},$$

with energy conservation we obtain a differential cross section with respect to the recoil momentum variable

$$\frac{d\sigma}{dP_x\,dP_y}=r_0^2\frac{m}{8\pi^4\alpha\omega}\sum_{P_z=P_\pm}\int\frac{\left|\left\langle\vec{p}_1\vec{p}_2\left|(\vec{p}_1\cdot\vec{\varepsilon})e^{i\vec{k}\cdot\vec{r}}\right|i\right\rangle\right|^2}{|q_z-P_z|}d^3p_2, \tag{8a}$$

where

$$P_\pm=q_z\pm\sqrt{A},\quad q\equiv\vec{k}-\vec{p}_2,\quad A=2m(\omega-E_i)-(\vec{P}_\perp-\vec{q}_\perp)^2-p_2^2. \tag{8b}$$

For Compton scattering we used "A^2" part of nonrelativistic photon–atom interaction Hamiltonian. In shake off approximation the cross section is

$$d\sigma=r_0^2\frac{1}{(2\pi)^6}\frac{(\vec{\varepsilon}_1\cdot\vec{\varepsilon}_2)^2}{\omega_1\omega_2}|\langle f|e^{i\vec{k}\cdot\vec{r}}|i\rangle|^2\,\delta(\omega+E_i-E_1-E_2)\,d^3k_2\,d^3p_1\,d^3p_2, \tag{9}$$

which after combining with momentum conservation

$$\vec{p}_1=\vec{k}-\vec{p}_2-\vec{P},$$

in terms of recoil momentum variables reads as

$$\frac{d\sigma}{dP_xdP_y}=r_0^2\frac{m}{(2\pi)^6}\sum_{P_z=P_\pm}\int\frac{\omega_2}{\omega_1}\frac{(\vec{\varepsilon}_1\cdot\vec{\varepsilon}_2)^2}{|q_z-P_z|}|\langle\vec{p}_1\vec{p}_2|e^{i\vec{k}\cdot\vec{r}}|i\rangle|^2\,d\omega_2\,d\Omega_2\,d^3p_2, \tag{10a}$$

where

$$P_\pm=q_z\pm\sqrt{B},\vec{q}\equiv\vec{k}-\vec{p}_2,\quad B=2m(\omega-E_i)-(\vec{P}_\perp-\vec{q}_\perp)^2-\vec{p}_2^{\,2}. \tag{10b}$$