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Relativistic effects in double ionization of helium via Compton scattering

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ABSTRACT

In this article we present the relativistic calculations, based on the QED theory, for double ionization of helium by the Compton scattering. In particular, we calculate the contribution of the spin–flip amplitude to the total cross section. Due to this amplitude the final triplet spin state of the ejected electrons is possible. In the calculations based on the non–relativistic A^2 term of the electron–photon interaction only the singlet spin state for the final electrons is allowed. We further assume the shake-off mechanism for process of double ionization. For the ground state of helium we use both the non–correlated and highly correlated wave function. We also discuss a degree of the scattered photon polarization in correlation with the formation of spin triplet state. Our calculations cover the photon impact energy range from 150 to 1000 keV.

1. Introduction

Simultaneous ejection of two bound electrons from an atom can be used to investigate the electron-electron correlation (McGuire et al., 2000). The helium atom is the simplest two–electron system and double ionization of helium via the Compton scattering became the prototype for these investigations. Of particular interest is the behaviour of the ratio of total cross section for double to single ionization Rat higher photon energies, e.g. above 100 keV. For these energies it is expected that R approaches an asymptotic constant limit as a result of an averaged correlation between two electrons in the initial state while the final state correlations become negligible.

However, the experimental findings of Spielberger et al. (1999) and Becker et al. (1999) in the energy range 40–120 keV exhibit a rather slow convergence to the asymptotic value $R \approx 0.8\%$ which is predicted in the various theoretical calculations (Spielberger et al., 1999; Andersson and Burgdörfer, 1994; Surić et al., 1994; Kornberg and Miraglia, 1996; Kaliman et al., 2007, 2010). The slow convergence is explained in the terms of final state correlations (Spielberger et al., 1999; Kaliman et al., 2007, 2010). In particular in Ref. Kaliman et al. (2010) the asymptotic value R = 0.8% within 4% is predicted at the impact energy of 200 keV. All quoted calculations are based on the A^2 term of the nonrelativistic electron-photon interaction.

In this work we extend the theoretical investigation of double ionization of helium to the energies where the relativistic effects are not negligible. In particular we calculate the contribution of spin-flip amplitude (SF) to the double ionization. Due to this amplitude the final spin triplet state of ionized electrons is possible, which is not the case in the non-relativistic calculation within the A^2 approximation. We discuss a degree of the scattered photon polarization in correlation with the formation of spin triplet state. The ratio of total cross section for double to single ionization is calculated for both the final singlet and triplet state. For the helium ground state we employ both the non-correlated and highly correlated wave function (Byron and Joachain, 1967; Kaliman et al., 2010).

2. Matrix element and cross sections

The relativistic matrix element M for high energy double ionization is graphically represented by the Feynman diagrams in Fig. 1. Diagrams are based on the QED Compton scattering amplitude for the fast ionized electron and shake amplitude for the slow ionized electron. Despite of relativistic considerations we neglect some less important contributions. In particular because of small Z for helium we neglect the relativistic effects in the ground state. Hence, we use constant 4-component spinor for the initially Compton interacting electron, and the 2-component Pauli spinors for both the ground and continuum energy state of the shaken electron.

With this simplifications the matrix element is written in the form $G(C) = \overrightarrow{C} (\overrightarrow{C}) (\overrightarrow{C$

$$\zeta_{S}^{(l,C_{2})} = \langle \vec{p}_{1} | \langle \vec{p}_{2} | H(\vec{r}_{1}) | \text{He} \rangle, \tag{1}$$

where $\vec{p_1}$, $\vec{p_2}$ are momenta of the Compton fast electron and slow shaken electron respectively, while subscript *S* denotes the spin state of these electrons. Also the superscripts C_1, C_2 denote the polarization state of incident and scattered photon, respectively.

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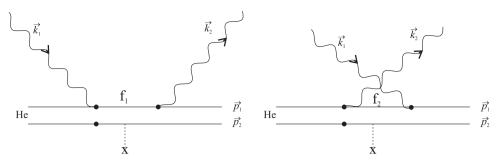


Fig. 1. Feynman diagrams for double ionization during Compton scattering via shake-off mechanism.

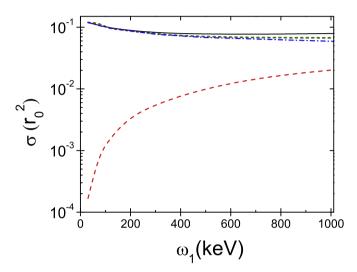


Fig. 2. Cross sections for the double ionization by Compton scattering as a function of incoming photon energy. Notation: short dashed green line shows calculations using only electrons' large components, blue dashed line is cross section without spin flip of electron, dash-dotted red line with spin flip, and black solid line is total SDCS. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

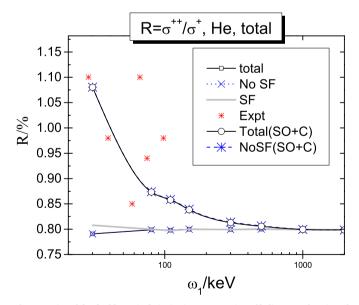


Fig. 3. Ratios of the double to single ionization cross section of helium as a function of incoming photon energy. NoSF (blue dashed line) is cross section without spin flip of electron, SF (dash-dotted red line) with spin flip, and total (black solid line) is total SDCS. Curves 'SO+C' are obtained by adding the Coulomb-interaction (non-relativistic) correction to the SO mechanism. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

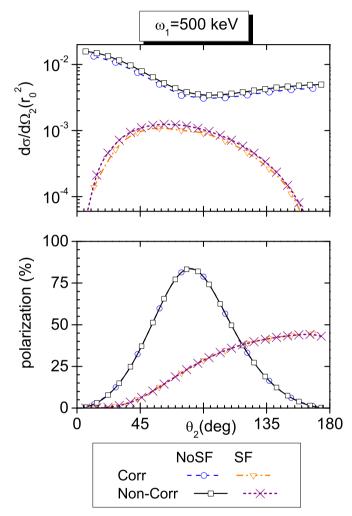


Fig. 4. SDCS for the double ionization by Compton scattering of photons with energy $\omega_1 = 500 \text{ keV}$ on helium as a function of scattering angle. Results obtained using correlated (uncorrelated) He wave function are denoted by *Corr (Non-Corr)*, and with (without) spin-flip by *SF (NoSF)*. On lower panel we show percentage of linear polarization of scattered photons, calculated using Eq. (8), when the incident photons are non-polarized.

In Eq. (1) the ground state helium wave function reads

$$|\text{HE}\rangle = \Psi_0(\vec{r_1}, \vec{r_2}) \begin{bmatrix} 1\\0\\0\\0\\0 \end{bmatrix}_1 \otimes \begin{bmatrix} 0\\1\\1 \end{bmatrix}_2$$
(2)

where indices 1,2 refer to the Compton interacting electron and shaken electron respectively.

In Eq. (1) the final two-electron wave function is represented by

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