Analytical evaluation of cross sections for double ionization of heliumlike ions by high-energy-photon scattering

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Double K-shell ionization of two-electron ions in Compton scattering of high-energy photons is investigated. The problem is treated analytically within the framework of nonrelativistic perturbation theory with respect to the interelectron interaction, using the Coulomb Green's and wave functions. The energy distribution of ejected electrons and the double-to-single cross section ratio are cast in the form of the universal scalings. The approximations made in previous theoretical works are discussed. Atomic targets are assumed to be characterized by moderate values of the nuclear charge number Z.

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I. INTRODUCTION

The double ionization of inner-shell electrons by a single photon has been intensively investigated during recent decades. Since the incident photon interacts with each electron separately, the simultaneous ejection of two bound electrons is caused exclusively by the interelectron interaction. The helium atom and heliumlike ions are the simplest atomic systems, where the double ionization can occur. Consideration of such targets allows one to test the quality of theoretical description of the electron-electron correlations within the framework of different approaches.

In this work, we employ nonrelativistic perturbation theory with respect to the electron-electron interaction. Two small parameters are assumed to be available, namely, $1/Z \ll 1$ and $\alpha Z \ll 1$, where Z is the nuclear charge number and α is the fine-structure constant. As the zeroth approximation, the complete set of the Coulomb wave functions is used. The characteristic momentum of K-shell electron and its binding energy in the Coulomb field of nucleus are given by $\eta = m\alpha Z$ and $I = \eta^2/(2m)$, respectively, where m is the electron mass $(\hbar = 1, c = 1)$.

The atomic ionization can proceed due to both the absorption and the scattering of photons. As long as the photon energy ω is not too high ($\omega \leq \eta$), the photoabsorption dominates over the Compton scattering. However, if $\omega \gtrsim \eta$, the Compton effect becomes the dominant process. It is well known that, at high nonrelativistic energies, the ratio of cross sections for double-to-single photoabsorption $R_p = \sigma_p^{++} / \sigma_p^{+}$ does not depend on the photon energy ω [1,2]. At present, the most accurate calculations give $R_p = 1.67\%$ for the helium atom at $\omega \gg I$. The theoretical result is in agreement with experimental measurements [3]. However, at $\omega \gtrsim 7$ keV, the ejection of electrons from the helium atom proceeds mainly due to the scattering, but not due to the absorption of photons. If any ions are registered experimentally, without regard to the particular way they are prepared, all possible ionization channels should be taken into account in the theoretical calculations.

In the high-energy limit, the double-to-single cross section ratio $R_C = \sigma_C^{++}/\sigma_C^+$ for the Compton scattering was

calculated with the use of multiparametrical variational wave functions for the initial atomic state [4,5]. In the case of He, it was found that $R_C \simeq 0.8\%$. At the asymptotic energy range characterized by $I \ll \omega \ll m$, analytical evaluation of the Compton contribution to the double ionization was performed to the first order of nonrelativistic perturbation theory with respect to the interelectron interaction [6]. For two-electron targets being in the ground state, the ionization cross section ratio was shown to have the simple scaling form

$$R_C \simeq 0.048 Z^{-2}.$$
 (1)

Since 1/Z is the formal expansion parameter of the perturbation theory used in derivation, the higher is Z, the more accurate is formula (1).

Substituting Z = 2 into Eq. (1) yields $R_C \simeq 1.2\%$, which is about 1.5 times larger than the value calculated in Refs. [4,5] by using the highly correlated ground state wave functions. It should be noted that, for He, the authors of work [6] used in Eq. (1) the effective nuclear charge number $Z_{\rm eff} = 27/16$ instead of its true value Z. This assumption significantly increased the ratio R_C , but was not justified (see discussion in Ref. [7]). For heliumlike ions with Z > 2, the numerical calculations were made in work [7] with the use of the variational wave function of Hart and Herzberg [8]. The results obtained for R_C tend also to the asymptotic limit $R_C \simeq 0.05 Z^{-2}$ with increasing Z. The experimental measurements of R_C are available for helium only [9–13]. These studies indicate that, with increasing photon energy, the Compton double-to-single ionization ratio, after attaining a maximum value of about 1.6% near $\omega \simeq 13$ keV, declines slowly approaching the constant limit. At $\omega \simeq 100$ keV, the experimental data still exceed the asymptotic value of 0.8% predicted in Refs. [4,5]. Such slow convergence towards the asymptotic limit seems to be partly explained by the necessity to account for the interaction between ejected electrons [14]. One needs also to analyze the additional approximations made in derivation of Eq. (1).

In work [6], the wave function of the initial state is constructed with the use of the Coulomb Green's function, which is presented by three first terms of the expansion over the Sturm functions of the nonrelativistic Kepler problem. Account for the following terms in the Sturm's expansion faces the problem. Namely, the corresponding contributions to the energy distribution of slow ejected electrons exhibit

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nonphysical rise at the electron energies much larger than the ionization potential I. Therefore, exact estimate of the contributions neglected in work [6] is absent. In this work, we employ the closed expression for the Coulomb Green's function [15], which allows one to perform accurate calculations.

II. AMPLITUDE FOR DOUBLE COMPTON EFFECT IN THE ASYMPTOTIC HIGH-ENERGY RANGE

We shall assume that the incident photon energy ω_1 is restricted by the condition $\eta \ll \omega_1 \ll m$, which is called by the asymptotic nonrelativistic range. In this case, the dominant contribution to the cross section arises from the A^2 term of the operator of photon-electron interaction, where A is the vector potential of the electromagnetic field. Taking into account the symmetry of two-electron wave function and the possibility of photon scattering on each atomic electron, one can show that the amplitude \mathcal{M} for the double Compton effect is represented by the Feynman diagram depicted in Fig. 1 (see details in Refs. [6,16]). The corresponding analytical expression is given by the following matrix element:

$$\mathcal{M} = \sqrt{2} \langle \psi_{p_1} \psi_{p_2} | UG(E) V | \psi_{1s} \psi_{1s} \rangle.$$
 (2)

Here p_1 and p_2 are the asymptotic momenta of ejected electrons, U is the operator of the A^2 interaction, and G(E) is the single-particle Coulomb Green's function with the energy E. The operator $V = \alpha/|r_1 - r_2|$ describes the Coulomb interaction between atomic electrons with the coordinates r_1 and r_2 . Due to the energy-conservation law, the intermediate energy is given by

$$E = 2E_{1s} - E_{p_2} = -I(2 + \varepsilon_2), \tag{3}$$

where $E_{1s} = -I$, $E_{p_2} = p_2^2/(2m)$, and $\varepsilon_2 = p_2^2/\eta^2$ is the dimensionless energy of the emitted electron.

The main contribution to the cross section arises from the edge range characterized by the inequality $E_{p_1} \gg E_{p_2}$. In this case, it turns out that $p_1 \sim \omega_1$, while the relative contribution of the Feynman diagram with the interchanged final single-electron wave functions $(\psi_{p_1} \rightleftharpoons \psi_{p_2})$ is estimated as $\eta/\omega_1 \ll 1$ [16]. The diagram depicted in Fig. 1 accounts for the interelectron interaction in the initial state only. The diagrams describing the interelectron interaction in the final state contain the additional smallness of the order η/ω_1 and, therefore, can be neglected [16].



FIG. 1. Feynman diagram describing the double Compton ionization of the K shell. Solid lines denote electrons in the Coulomb field of the nucleus, the dashed line denotes the interelectron interaction, and wavy lines denote incident and scattered photons. The electron propagator with dot corresponds to the Coulomb Green's function. In the following, we shall employ the momentum representation. Then the operator V corresponds to the photon propagator $D(f) = 4\pi\alpha/f^2$, where f is the exchange momentum of electrons. Let the incident photon be characterized by the momentum k_1 , the energy $\omega_1 = |k_1|$, and the polarization vector \mathbf{e}_1 , while the scattered photon has the momentum k_2 , the energy $\omega_2 = |k_2|$, and the polarization \mathbf{e}_2 . The kernel of the operator U takes the form

$$\langle \mathbf{f}'|U|\mathbf{f}\rangle = N_{\gamma}\langle \mathbf{f}'|\mathbf{f}+\mathbf{k}\rangle, \quad N_{\gamma} = 2\pi \frac{\alpha}{m} \frac{(\mathbf{e}_{2}^{*} \cdot \mathbf{e}_{1})}{\sqrt{\omega_{1}\omega_{2}}},$$
 (4)

where $\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2$ is the momentum transferred to the atom. The plane-wave states are normalized to δ function in the momenta,

$$\langle f'|f\rangle = (2\pi)^3 \delta(f' - f).$$
⁽⁵⁾

Now we redefine the amplitude as follows: $\mathcal{M} = \sqrt{2}N_{\gamma}F(\boldsymbol{p}_1, \boldsymbol{p}_2)$. Then one has

$$F(p_{1}, p_{2}) = \int \frac{df}{(2\pi)^{3}} \frac{df'}{(2\pi)^{3}} \frac{df_{1}}{(2\pi)^{3}} \frac{df_{2}}{(2\pi)^{3}} \langle \psi_{p_{1}} | f' + k \rangle$$

$$\times \langle f' | G(E) | f_{1} \rangle \langle f_{1} + f | \psi_{1s} \rangle D(f)$$

$$\times \langle \psi_{p_{2}} | f_{2} \rangle \langle f_{2} - f | \psi_{1s} \rangle.$$
(6)

Since $p_1 \sim \omega_1 \gg \eta$, the wave function ψ_{p_1} can be approximated by the plane wave. The Coulomb wave function of the *K*-shell electron is represented as follows [17]:

$$\langle \boldsymbol{f} | \psi_{1s} \rangle = N_{1s} \left(-\frac{\partial}{\partial \eta} \right) \langle \boldsymbol{f} | V_{i\eta} | 0 \rangle,$$
 (7)

$$\langle f'|V_{i\eta}|f\rangle = \frac{4\pi}{(f'-f)^2 + \eta^2},$$
 (8)

where $N_{1s}^2 = \eta^3 / \pi$ and $\eta = m\alpha Z$. Substituting Eq. (7) into amplitude (6), one can perform integrations over the intermediate momenta. It yields

$$F(\boldsymbol{p}_1, \boldsymbol{p}_2) = N_{1s}^2 \frac{\partial^2}{\partial \nu \partial \mu} \int \frac{d\boldsymbol{f}}{(2\pi)^3} \langle \psi_{\boldsymbol{p}_2} | V_{i\nu} | \boldsymbol{f} \rangle D(\boldsymbol{f}) \\ \times \langle -\boldsymbol{f} | V_{i\mu} G(E) | \boldsymbol{q} \rangle, \tag{9}$$

where $q = p_1 - k$. In Eq. (9), after taking derivatives over ν and μ one should set $\nu = \mu = \eta$. Using the expression for the Coulomb Green's function from work [15] and the operator identity

$$-\frac{\partial}{\partial\epsilon}V_{i\epsilon|\epsilon\to0} = 1, \qquad (10)$$

one has

$$\langle -\boldsymbol{f}|V_{i\mu}G(E)|\boldsymbol{q}\rangle = -\frac{\partial}{\partial\epsilon} \langle -\boldsymbol{f}|V_{i\mu}G(E)V_{i\epsilon}|\boldsymbol{q}\rangle_{|\epsilon\to0}$$

$$= -\frac{2m}{q^2+p^2} \bigg\{ \langle \boldsymbol{f}|V_{i\mu}|-\boldsymbol{q}\rangle$$

$$+ \eta \int_0^1 \frac{dx}{\lambda} e(x) \langle \boldsymbol{f}|V_{i(\lambda+\mu)}|-\boldsymbol{q}x\rangle \bigg\}.$$
(11)

Here we used the following notation:

$$e(x) = \left(\frac{(qx)^2 + (p+\lambda)^2}{x(q^2 + p^2)}\right)^{\zeta},$$
 (12)

where $\lambda = \sqrt{(p^2 + q^2 x)(1 - x)}$, $p = \sqrt{2m|E|} = \eta\sqrt{2 + \varepsilon_2}$, and $\zeta = \eta/p = 1/\sqrt{2 + \varepsilon_2}$. Substituting Eq. (11) into Eq. (9) and using the results of work [18], the integration over the momentum f can be reduced to the single integral:

$$\int \frac{df}{(2\pi)^3} \langle \psi_{p_2} | V_{i\nu} | f \rangle \frac{1}{f^2} \langle f | V_{i(\lambda+\mu)} | - qx \rangle$$

= $2\pi N_{p_2} \int_0^1 \frac{dy}{\lambda_1} \frac{a^{i\xi_2 - 1}}{b^{i\xi_2}},$ (13)

$$a = (\mathbf{p}_2 + \mathbf{q} x y)^2 + (\lambda_1 + \nu)^2,$$

$$b = (q x y)^2 + (\lambda_1 + \nu - i p_2)^2,$$
(14)

$$\lambda_1 = \sqrt{(qx)^2 y(1-y) + (\lambda + \mu)^2 y},$$
(15)

$$N_{p_2}^2 = rac{2\pi\xi_2}{1 - e^{-2\pi\xi_2}} \simeq 2\pi\xi_2,$$

where $\xi_2 = \eta/p_2 = 1/\sqrt{\varepsilon_2}$. Using Eqs. (13)–(15) and taking derivatives with respect to μ and ν , amplitude (9) can be cast in the following compact form:

$$F(\boldsymbol{p}_1, \boldsymbol{p}_2) = -N\left\{Q(1) + \int_0^1 dx \left(1 + \frac{\eta}{\lambda}\right) e(x)Q(x)\right\},$$
(16)

$$Q(x) = \int_0^1 dy \frac{y}{\lambda_1^2} \left(-\frac{1}{\lambda_1} + \frac{\partial}{\partial \lambda_1} \right) \frac{\partial}{\partial \lambda_1} \frac{a^{i\xi_2 - 1}}{b^{i\xi_2}}, \quad (17)$$

where $N = N_{p_2} N_{1s}^2 (4\pi)^2 m \alpha \eta / (q^2 + p^2)$.

III. ENERGY DISTRIBUTION AND TOTAL CROSS SECTION

The differential cross section for the double Compton ionization of the *K*-shell electrons is related to amplitude (16) as follows:

$$d\sigma_{C}^{++} = \frac{(4\pi\alpha)^{2}}{2m^{2}} \frac{|\mathbf{e}_{2}^{*} \cdot \mathbf{e}_{1}|^{2}}{\omega_{1}\omega_{2}} |F(\boldsymbol{p}_{1}, \boldsymbol{p}_{2})|^{2} d\Gamma, \qquad (18)$$

$$d\Gamma = 2\pi \frac{d\mathbf{p}_1}{(2\pi)^3} \frac{d\mathbf{p}_2}{(2\pi)^3} \frac{d\mathbf{k}_2}{(2\pi)^3} \delta(E_{p_1} + E_{p_2} + \omega_2 - \omega_1 - 2E_{1s}).$$
(19)

Averaging over polarizations of the incident photons and taking summation over polarizations of the scattered photons are equivalent to the substitution

$$|\mathbf{e}_{2}^{*} \cdot \mathbf{e}_{1}|^{2} \rightarrow \overline{|\mathbf{e}_{2}^{*} \cdot \mathbf{e}_{1}|^{2}} = \frac{1}{2} \sum_{\text{pol.}} |\mathbf{e}_{2}^{*} \cdot \mathbf{e}_{1}|^{2} = \frac{1}{2} (1+t^{2}), \quad (20)$$

where $t = (\mathbf{k}_1 \cdot \mathbf{k}_2)/(\omega_1 \omega_2)$ is the cosine of the photon scattering angle.

Since function (16) depends on the scattering angles via the momentum $q = p_1 - k_1 + k_2$ only, it is convenient to express the phase volume $d\Gamma$ via dq instead of dp_1 . In addition, the amplitude $F(p_1, p_2) \equiv F(q, p_2)$ decreases very rapidly with increasing q. Accordingly, the main contribution to the cross section is exhausted at $q \leq \eta$. The energy δ function is

eliminated by integrating over ω_2 due to the relation

$$\delta[\chi(\omega_2)] = \left|\chi'(\omega_2^0)\right|^{-1} \delta(\omega_2 - \omega_2^0).$$
(21)

Here ω_2^0 is the root of the equation: $\chi(\omega_2) = 0$, where

$$\chi(\omega_2) = \omega_2 + E_{p_1} + E_{p_2} + 2I - \omega_1.$$
(22)

Keeping only the leading terms in the expansion over q/m yields

$$E_{p_1} = \frac{p_1^2}{2m} \simeq \frac{k^2}{2m} = \frac{\omega_1^2}{2m} + \frac{\omega_2^2}{2m} - \frac{\omega_1}{m}\omega_2 t, \qquad (23)$$

$$\omega_2^0 \simeq \omega_1 - \frac{\omega_1^2}{m}(1-t), \quad \chi'(\omega_2^0) \simeq 1 + \frac{\omega_1}{m}(1-t).$$
 (24)

Then integration over ω_2 is reduced to the substitution

$$\frac{d\Gamma}{\omega_1\omega_2} \to \left(1 - \frac{2\omega_1}{m}(1-t)\right) \frac{d\boldsymbol{q}}{(2\pi)^3} \frac{d\boldsymbol{p}_2}{(2\pi)^3} \frac{dt}{2\pi}.$$
 (25)

Here it is also taken into account that the phase volume of the scattered photons is given by $d\mathbf{k}_2 = 2\pi\omega_2^2 d\omega_2 dt$.

Let us denote the integral over q as follows:

$$S = \int \frac{d\boldsymbol{q}}{(2\pi)^3} |F(\boldsymbol{q}, \boldsymbol{p}_2)|^2$$
(26a)

$$= \int_{0}^{q_{\text{max}}} \frac{dqq^2}{(2\pi)^2} \int_{-1}^{+1} dt_2 |F(q,t_2,p_2)|^2, \qquad (26b)$$

where $t_2 = (\mathbf{q} \cdot \mathbf{p}_2)/(qp_2)$. Since the integral over q is saturated at $q \leq \eta$, the upper integration limit $q_{\text{max}} \sim \omega_1$ can be replaced by infinity. Then, after integrations over \mathbf{q} and t, Eq. (18) reads

$$d\sigma_C^{++} = \sigma_C^+ S \frac{d \boldsymbol{p}_2}{(2\pi)^3},\tag{27}$$

$$\sigma_C^+ = 2\sigma_T \left(1 - 2\frac{\omega_1}{m} \right), \quad \sigma_T = \frac{8}{3}\pi r_e^2.$$
(28)

Here $r_e = \alpha/m$ is the classical electron radius, σ_T is the Thomson cross section of photon scattering by a free electron, and σ_C^+ is the single ionization cross section of photon scattering by two-electron target. As seen from Eq. (27), in the high-energy range, the double-to-single cross section ratio for the Compton scattering does not depend on the incident photon energy ω_1 . The angular distribution of slow electrons is isotropic, since *S* does not depend on the direction of their ejection. Accordingly, one can write that $d\mathbf{p}_2 = 4\pi m p_2 dE_{p_2} = 2\pi \eta^3 \xi_2^{-1} d\varepsilon_2$. It is also convenient to express all momenta and energies involved into the problem in units of η and *I*, respectively. Then one has

$$\frac{d\sigma_C^{++}}{\sigma_C^{+}} = Z^{-2} J(\varepsilon_2) d\varepsilon_2, \qquad (29)$$

$$J(\varepsilon_2) = \frac{2^5}{\pi} \int_0^\infty \frac{d\varkappa \varkappa^2}{(\varkappa^2 + \zeta^{-2})^2} \int_{-1}^{+1} dt_2 |\mathcal{F}(\varkappa, t_2, \varepsilon_2)|^2.$$
(30)



FIG. 2. Universal function $J(\varepsilon_2)$ vs the dimensionless energy ε_2 .

Here

$$F(\varkappa, t_2, \varepsilon_2) = Q(1) + \int_0^1 dx \left(1 + \frac{1}{\lambda}\right)$$
$$\times \left(\frac{(\varkappa x)^2 + (\lambda + \zeta^{-1})^2}{x(\varkappa^2 + \zeta^{-2})}\right)^{\zeta} Q(x), \quad (31)$$

$$a = \varepsilon_2 + 2\varkappa xyt_2\sqrt{\varepsilon_2} + (\varkappa xy)^2 + (\lambda_1 + 1)^2, \qquad (32)$$

$$b = (\varkappa xy)^2 + (\lambda_1 + 1 - i\sqrt{\varepsilon_2})^2, \qquad (33)$$

$$\lambda_1 = \sqrt{(\varkappa x)^2 y (1 - y) + (\lambda + 1)^2 y},$$
(34)

$$\lambda = \sqrt{(\varkappa^2 x + \zeta^{-2})(1 - x)},$$
(35)

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where $\varkappa = q/\eta$, $\varepsilon_2 = p_2^2/\eta^2$, $\zeta = 1/\sqrt{2+\varepsilon_2}$, and $\xi_2 = 1/\sqrt{\varepsilon_2}$. Functions (31) and (16) are related to each other as follows: $F(q, p_2) = -N\eta^{-6}\mathcal{F}(\varkappa, t_2, \varepsilon_2)$. The function Q(x) is given by Eq. (17). Energy distribution of slow electrons (30) does not depend on Z explicitly. As seen from Fig. 2, it decreases rapidly with increasing ε_2 .

Finally, the double-to-single ionization cross section ratio for the Compton effect reads

$$R_C = \frac{\sigma_C^{++}}{\sigma_C^+} = Z^{-2} \int_0^{\varepsilon_{2\max}} J(\varepsilon_2) d\varepsilon_2.$$
(36)

In Eq. (36), integrating with the upper limit $\varepsilon_{2\text{max}} \gg 1$ yields

$$R_C = 0.050 Z^{-2}.$$
 (37)

This is our main result. Formula (37) is in very good agreement with previous calculations made in works [6,7]. A comparison of Eqs. (1) and (37) shows that approximation of the Coulomb Green's function by three terms of the Sturm's expansion is justified with an accuracy of about 4%.

Concluding, we have evaluated analytically the doubleto-single ionization cross section ratio for the Compton scattering in the asymptotic high-energy range. The derivation is performed to leading order of the nonrelativistic perturbation theory with the use of the Coulomb Green's function in the closed form. The heliumlike ions characterized by the small parameters $\alpha Z \ll 1$ and $1/Z \ll 1$ are considered as a target. The universal scalings (30) and (37) can be also used for more complicated atomic systems, in particular, for stable multicharged ions with more than two electrons [19].

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