

Ionization of heliumlike ions with excitation of nl states by high-energy photon scattering

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We consider the inelastic high-energy photon scattering on heliumlike ions in the ground state, which results in ionization accompanied by simultaneous excitation of the residual ion. Nonrelativistic perturbation theory is employed as a method. The cross sections of the process for transitions into the ns and np states are deduced in the analytical form. A comparison of our results with those of approximated calculations is given.

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The ionization with excitation caused by impact of a single photon is one of the fundamental processes, which occurs exclusively due to the interelectron correlations and, therefore, serves as a tool for quality test of different theoretical models. Two-electron targets are the simplest atomic systems, where this process can take place. Analytical results for cross sections are of particular importance.

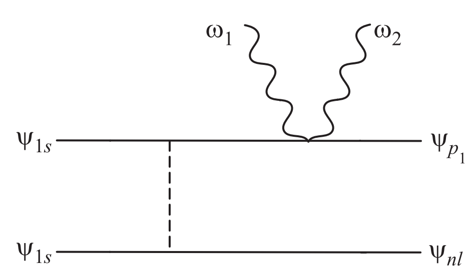
Up to now, the experimental investigations have been mainly focused on helium atom [1–3]. However, due to recent developments of novel sources of synchrotron radiation, the study of correlated processes become actual for other atomic targets, in particular, for heliumlike ions. Multicharged ions allow of consistent description within the framework of QED perturbation theory. The bound K-shell electron is characterized by the averaged momentum $\eta = m\alpha Z$ and the binding energy $I = \eta^2/(2m)$, where Z is the nuclear charge, α is the fine-structure constant, and m is the electron mass ($\hbar = 1$, $c = 1$). Photoionization of heliumlike ions accompanied by excitation of the nl states is studied within entire nonrelativistic range of the incident photon energies $\omega_1 \ll m$, including the threshold range [4, 5]. However, at asymptotically high energies $\omega_1 \gg \eta$, the process of ionization with excitation occurs predominantly due to the photon scattering, but not due to the photoabsorption [4, 6, 7].

In the following, we shall consider the photon energy range characterized by $\eta \ll \omega_1 \ll m$. In works [4, 8], the inelastic Compton scattering on heliumlike ions was studied within the framework of nonrelativistic perturbation theory. The quantity of experimental interest is the following cross-section ratio:

$$R_{nl} = \frac{\sigma_{nl}^{+*}}{\sigma^+} = \frac{Q_{nl}}{Z^2}. \qquad (1)$$

Here $\sigma^+ = 2\sigma_T$ is the cross section of the ordinary Compton scattering on heliumlike ions, where $\sigma_T = (8/3)\pi r_e^2$ is the Thomson limit and $r_e = \alpha/m$ is the classical radius of the electron. The cross section σ_{nl}^{+*} describes the inelastic photon scattering on two-electron atomic target, which causes ionization of one K-shell electron and excitation of another one into the nl state. The second equality in Eq. (1) is the universal scaling, which is obtained within the framework of perturbation theory, taking into account the leading orders with respect to small parameters $1/Z$ and αZ. The dimensionless function Q_{nl} does not depend on Z explicitly.

At high energies $\omega_1 \gg \eta$, the dominant contribution to the total cross section σ_{nl}^{+*} appears from the contact (seagull) diagram, which describes the interelectron interaction in the initial state (see Fig. 1). In this case,



Dominant diagram for ionization of two-electron atom with excitation of the nl state by high-energy photon scattering

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ratio (1) can be cast into the following form [4]:

$$R_{nl} = (4\pi\alpha)^2 \left(-\frac{\partial}{\partial E}\right) \sum_{m'=-l}^{l} \langle \phi_{nl}^{m'} | G(E) | \phi_{nl}^{m'} \rangle, \quad (2)$$

$$\langle \phi_{nl}^{m'} | = N_{1s}^2 \frac{\partial^2}{\partial \nu_1 \partial \nu_2} \int \frac{d\mathbf{f}}{(2\pi)^3} \langle \psi_{nl}^{m'} | V_{i\nu_1} | \mathbf{f} \rangle \frac{1}{f^2} \langle -\mathbf{f} | V_{i\nu_2}, \quad (3)$$

where $N_{1s}^2 = \eta^3/\pi$. The energy of the nonrelativistic Coulomb Green's function $G(E)$ is given by $E = 2E_{1s} - E_{nl} = -I(2-n^{-2})$. In Eq. (3), the derivatives over ν_1 and ν_2 are evaluated at the point $\nu_1 = \nu_2 = \eta$. The atomic electrons exchange with each other by the momentum $\mathbf{f}$, which has the characteristic scale of the order $f \sim \eta$. The matrix element

$$\langle \mathbf{f}' | V_{i\lambda} | \mathbf{f} \rangle = \frac{4\pi}{(\mathbf{f}' - \mathbf{f})^2 + \lambda^2} \quad (4)$$

is the Fourier transform from the Yukawa potential $e^{-\lambda r}/r$.

In work [4], in order to calculate the cross-section ratio R_{nl}, the Coulomb Green's function was approximated by three terms of the Sturm expansion. We shall evaluate Eqs. (2) and (3) exactly.

Let us consider first the excitations into the ns states ($l = 0$). In the momentum representation, the electron Coulomb wave function ψ_{ns} reads

$$\langle \psi_{ns} | \mathbf{f} \rangle = N_{ns} D_\nu \left(-\frac{\partial}{\partial \nu}\right) \langle 0 | V_{i\nu} | \mathbf{f} \rangle, \quad (5)$$

$$D_\nu = \sum_{k=0}^{n-1} \frac{(n-1)!(2\eta_n)^k}{(n-k-1)!k!(k+1)!} \frac{\partial^k}{\partial \nu^k}, \quad (6)$$

where $N_{ns}^2 = \eta_n^3/\pi$ and $\eta_n = \eta/n$. After taking derivatives over ν, one should set $\nu = \eta_n$.

By virtue of Eq. (5) and the operator identity

$$-\frac{\partial}{\partial \nu} V_{i\nu} V_{i\lambda} = -\frac{\partial}{\partial \nu} V_{i\lambda} V_{i\nu} = V_{i(\nu+\lambda)}, \quad (7)$$

one can write

$$\langle \psi_{ns} | V_{i\nu_1} | \mathbf{f} \rangle = N_{ns} D_\nu \langle 0 | V_{i(\nu+\nu_1)} | \mathbf{f} \rangle. \quad (8)$$

Substituting Eq. (8) into Eq. (3) and using the identity

$$f^{-2} \langle \mathbf{f} | V_{i\mu} | 0 \rangle = \mu^{-2} \langle \mathbf{f} | (V_0 - V_{i\mu}) | 0 \rangle, \quad (9)$$

we obtain

$$\langle \phi_{ns} | = N_{1s}^2 N_{ns} \Gamma_\mu \langle 0 | V_{i\zeta}, \quad (10)$$

$$\Gamma_\mu = D_\mu \frac{\partial}{\partial \mu} \frac{1}{\mu^2}, \quad (11)$$

where $\zeta = \eta + \mu$. In Eq. (10), the derivatives over μ are evaluated at the point $\mu = \eta + \eta_n$. The differential operator Γ_μ possesses by the following property: acting on the function, which does not depend on μ, it results in zero after setting $\mu = \eta + \eta_n$. This property has been used in derivation of Eq. (10).

Due to relation (10), formula (2) reads

$$R_{ns} = (4\pi\alpha)^2 N_{1s}^4 N_{ns}^2 \frac{m}{p} \frac{\partial}{\partial p} \Gamma_{\mu_1} \Gamma_{\mu_2} \langle 0 | V_{i\zeta_2} G(p') V_{i\zeta_1} | 0 \rangle, \quad (12)$$

where $p' = \sqrt{2mE + i0} = ip$, $\zeta_k = \eta + \mu_k$ ($k = 1, 2$). After taking derivative over the momentum p, one should set $p = \eta\sqrt{2 - n^{-2}}$.

In Eq. (12), the matrix element with the Coulomb Green's function can be evaluated analytically [9, 10]

$$\langle 0 | V_{i\zeta_2} G(p') V_{i\zeta_1} | 0 \rangle = 16\pi m \frac{ip'}{a_+^2} \int_1^\infty \frac{t^{i\xi} dt}{(t-a)^2} = -\frac{2^4 \pi m p}{a_+^2 (1-\gamma)} \, {}_2F_1(2, 1-\gamma; 2-\gamma; a), \quad (13)$$

where $a = a_-/a_+$, $a_\pm = (p \pm \zeta_1)(p \pm \zeta_2)$, $\gamma = i\xi = \eta/p$, and ${}_2F_1$ is the hypergeometric function.

In order to get the universal scaling, it is convenient to introduce the dimensionless quantities, calibrating all momenta involved into the problem in the units of η. Then the ratio R_{ns} takes the form (1) with the function

$$Q_{ns} = \frac{2^8}{n^3} \frac{1}{\sqrt{2 - n^{-2}}} \left(-\frac{\partial}{\partial p}\right) p \Gamma_{\mu_1} \Gamma_{\mu_2} \times \frac{{}_2F_1(2, 1-\gamma; 2-\gamma; a)}{(1-\gamma) a_+^2}. \quad (14)$$

Here after evaluation of derivatives, one should set $\mu_1 = \mu_2 = 1 + n^{-1}$ and $p = \sqrt{2 - n^{-2}}$. The variable γ becomes to be equal to $\gamma = 1/p$, while $\zeta_k = 1 + \mu_k$ ($k = 1, 2$). The differential operators Γ_{μ_1} and Γ_{μ_2} are defined by formulas (6) and (11), where $\eta_n = 1/n$.

Now we shall evaluate the contribution due to the excitations of the np states ($l = 1$). In this case, the electron Coulomb wave function can be represented in the form

$$\langle \psi_{np}^{m'} | \mathbf{f} \rangle = N_{np} \left(\mathbf{e}_{m'} \cdot \nabla_k \right) D_\lambda \left(-\frac{\partial}{\partial \lambda}\right) \langle \mathbf{k} | V_{i\lambda} | \mathbf{f} \rangle, \quad (15)$$

$$D_\lambda = \frac{\eta^{-2}}{(n-2)!} \frac{\partial^{n-2}}{\partial \lambda^{n-2}} (\lambda + \eta_n)^{n+1}, \quad (16)$$

$$N_{np}^2 = \frac{3}{2^4 \pi} \frac{\eta_n^3}{(1 - n^{-2})}, \quad (17)$$

where $\nabla_k = \partial/\partial\mathbf{k}$ and $\mathbf{e}_{m'}$ ($m' = \pm 1, 0$) are the polarization vectors, which satisfy to the normalization condition $(\mathbf{e}_{m'} \cdot \mathbf{e}_{m'}^*) = 1$. After taking the derivatives with respect to λ and the gradient ∇_k, one should set $\lambda = \eta_n$ and tend the variable k to zero.

The integration over the momentum $\mathbf{f}$ in (3) is performed by using the following relation [11]

$$\int \frac{d\mathbf{f}}{(2\pi)^3} \langle \mathbf{k}|V_{i(\lambda+\nu)}|\mathbf{f}\rangle \frac{1}{f^2} \langle -\mathbf{f}|V_{i\mu} = \\ = \frac{1}{2}\int_0^1 \frac{dz}{\Omega}\langle -\mathbf{k}z|V_{iL}, \quad (18)$$

where $\Omega = \sqrt{(\lambda+\nu)^2 z + k^2 z(1-z)}$ and $L = \Omega + \mu$.

Inserting (15) into (3) and taking into account formula (18) yield

$$\langle \phi_{np}^{m'}| = N_{1s}^2 N_{np} \frac{\partial^2}{\partial\nu\partial\mu} D_\lambda \left(\mathbf{e}_{m'} \cdot \nabla_k\right) \times \\ \times \int_0^1 dx \frac{x}{\Omega}\langle -\mathbf{k}x^2|V_{iL}. \quad (19)$$

In the integral, we have changed the variable by $z = x^2$. The derivatives over ν and μ are evaluated at the point $\nu = \mu = \eta$.

By virtue of Eqs. (2) and (19), one arrives at the following expression:

$$\left(\mathbf{e}_{m'} \cdot \nabla_k\right)\left(\mathbf{e}^*_{m'} \cdot \nabla_{k'}\right)\langle \mathbf{k}'y^2|V_{iL_2} G(p') V_{iL_1}|\mathbf{k}x^2\rangle = \\ = -\frac{2^7 \pi m (xy)^2 p^3}{b_+^4 (2-\gamma)} \, {}_2F_1(4, 2-\gamma; 3-\gamma; b), \quad (20)$$

where $p' = ip$, $p = \sqrt{2m|E|}$, $\gamma = \eta/p$, $b = b_-/b_+$, $b_\pm = (p \pm \Lambda_1)(p \pm \Lambda_2)$. Here, we used the integral representation for the matrix element involving the Coulomb Green's function obtained in works [9, 10]. Formula (20) is written taking into account the terms nonvanishing in the limit $k \to 0$ and $k' \to 0$ only, so that $L_1 = \Omega_1 + \mu_1 \to \Lambda_1 = (\lambda_1 + \nu_1)x + \mu_1$ and $L_2 = \Omega_2 + \mu_2 \to \Lambda_2 = (\lambda_2 + \nu_2)y + \mu_2$.

Now we again express all momenta of the problem in units of $\eta = m\alpha Z$. Then the cross-section ratio R_{np} is reduced to the universal scaling (1), where the dimensionless function Q_{np} is given by

$$Q_{np} = \frac{2^8}{n(n^2-1)} \frac{1}{\sqrt{2-n^{-2}}} \left(-\frac{\partial}{\partial p}\right) p^3 \Gamma^{\lambda_1}_{\nu_1\mu_1} \Gamma^{\lambda_2}_{\nu_2\mu_2} \times \\ \times \int_0^1 dx x^2 \int_0^x dy y^2 \frac{{}_2F_1(4, 2-\gamma; 3-\gamma; b)}{(2-\gamma) b_+^4}. \quad (21)$$

Here after evaluation of derivatives, one should set $\nu_1 = \nu_2 = \mu_1 = \mu_2 = 1$, $\lambda_1 = \lambda_2 = 1/n$, and $p = \sqrt{2-n^{-2}}$. The variable γ is just $\gamma = 1/p$. The differential operators $\Gamma^{\lambda_1}_{\nu_1\mu_1}$ and $\Gamma^{\lambda_2}_{\nu_2\mu_2}$ are defined by the formula:

$$\Gamma^\lambda_{\nu\mu} = 3D_\lambda \frac{\partial^2}{\partial\nu\partial\mu} \frac{1}{(\lambda+\nu)}, \quad (22)$$

where the operator D_λ is given by Eq. (16) with $\eta = 1$ and $\eta_n = 1/n$.

In Table, the results of our numerical calculations of the functions Q_{nl} are compared with those obtained in work [4]. For transitions into the ns states, the agreement between the exact and approximated values becomes significantly better with increase of the principal quantum number n. In the case of the np excitations, the disagreement amounts to about 12% and does not diminish with increase of n.

To summarize, we have deduced the analytical formulas for total cross sections of nonrelativistic high-energy photon scattering, which causes ionization accompanied by simultaneous excitation of the nl states. Expressions (14) and (21) are our main result. The heliumlike ions characterized by the small parameters $1/Z \ll 1$ and $\alpha Z \ll 1$ are considered as a target. Due to the universal scaling behavior, the results obtained can be also employed for more complicated atomic systems, in particular, for stable multicharged ions with more than two electrons [12].

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Numerical values of the function Q_{nl} for the ns and np states (top rows, from Ref. [4]; bottom rows, present work)

n	Q_{ns}	Q_{np}
2	$0.5884 \cdot 10^{-1}$	$0.479 \cdot 10^{-2}$
	$0.5921 \cdot 10^{-1}$	$0.4271 \cdot 10^{-2}$
3	$0.1023 \cdot 10^{-1}$	$0.115 \cdot 10^{-2}$
	$0.1035 \cdot 10^{-1}$	$0.1019 \cdot 10^{-2}$
4	$0.3656 \cdot 10^{-2}$	$0.451 \cdot 10^{-3}$
	$0.3689 \cdot 10^{-2}$	$0.3988 \cdot 10^{-3}$
5	$0.1739 \cdot 10^{-2}$	$0.224 \cdot 10^{-3}$
	$0.1751 \cdot 10^{-2}$	$0.1974 \cdot 10^{-3}$

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