

# High-Energy Two-Electron Photoabsorption as a Three-Body Problem

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**Abstract.** We study the high-energy behaviour of double photoionization and of the ionization accompanied by excitation of the states  $n^1S$  and  $n^3S$  of the  $H^-$  ion, helium atom, and light helium-like ions. We show that the high-energy nonrelativistic limit of the “ionization + excitation” to the single-ionization cross section ratio is still valid for the photon energies, corresponding to the relativistic energies of the outgoing electron. The same applies to the double photoionization of the triplet states. The situation for the double photoionization of singlet states differs due to the quasifree mechanism. All these ionization ratios are calculated by using the high-precision locally correct wave functions for the bound electrons. The importance of using locally correct functions is emphasized.

## 1 Introduction

The analysis of the experimental data on ionization and excitation processes of complicated systems provides the information on their structures. The largest values of the cross sections are achieved in atomic heavy ion collisions. However, in these cases the targets and projectiles are many-body systems. Thus, it is not easy to clarify the mechanisms of the corresponding processes. From this point of view the investigation of photoionization of the two-electron systems, i.e., of the negative hydrogen ion  $H^-$ , the helium atom, and helium-like ions is more instructive, since they are relatively simple three-body systems.

In order to calculate the cross sections one needs the three-body wave functions of both the initial and the final states. It is reasonable to consider the high-energy

limits of the processes since at large values of the photon energy  $\omega$  the interactions of the fast outgoing electrons with the nucleus and between themselves can be treated perturbatively. This does not mean that one can always use the plane waves for the description of the fast electrons. However, several lowest-order terms determine the lowest-order term of the  $\omega^{-1}$  expansion of the cross sections. Thus, the investigation of the high-energy ionization provides information about the initial-state wave function  $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ .

At photon energies exceeding 6 keV, ionization accompanied by radiation of the photon, i.e., the Compton scattering is known to provide the largest contribution as compared to the other processes, in which one or both electrons are eliminated from the helium atom. However, it is possible to separate experimentally the contributions to the two-electron ionization and ionization with excitation caused by either photon absorption (photoionization) or by photon scattering. In these processes the wave function  $\Psi(\mathbf{r}_1, \mathbf{r}_2)$  is probed in different regions of the distances  $r_1$  and  $r_2$ . The cross section of the Compton scattering is determined by the kinematical region, in which the process on the free electrons is allowed. Thus, the distances  $r_{1,2} \sim r_b$ , with  $r_b$  being the size of the bound state dominating in the process. Photoionization with excitation is not allowed for free electrons. Thus, one of the electrons should transfer the large momentum to the nucleus. This requires one of the distances  $r_1$  or  $r_2$  to be small and therefore the function  $\Psi(0, r)$  at  $r \sim r_b$  is probed [1]. The same refers to the double photoionization at nonrelativistic energies of the outgoing electrons. In the relativistic case there is an additional contribution due to the quasifree mechanism (QFM) [2–4], in which the electrons exchange the large momentum, transferring only the small momentum  $q \sim r_b^{-1}$  to the nucleus. This probes the wave function at  $r_{1,2} \sim r_b$ ,  $|\mathbf{r}_1 - \mathbf{r}_2| \rightarrow 0$ .

The motion of the initial-state electrons at distances of the order  $r_b$  can be treated in the nonrelativistic approximation if the averaged velocities are small enough,

$$\frac{(\alpha Z)^2}{n^2} \ll 1, \quad (1)$$

with  $Z$  denoting the charge of the nucleus,  $\alpha = \frac{1}{137}$  being the fine-structure constant, and  $n$  being the principal quantum number. If the energies  $\omega$  of the photons are as large as the rest energy of the electron, i.e.,  $\omega \sim m$  (we use the system of units  $\hbar = c = 1$ , and the electron mass is kept as  $m$ ), momentum  $q$  transferred to the nucleus in the photoionization process becomes of the order of the electron mass  $m$ . Thus, the wave function  $\Psi(r_1 \sim q^{-1}, r_2 \sim r_b)$  requires relativistic treatment. The main relativistic effects can be accounted for by the Furry-Sommerfeld-Maue (FSM) wave functions [5], which have the form of a differential operator acting on the nonrelativistic wave function. The higher-order relativistic corrections are of the order  $(\alpha Z/n)^2$ . In a similar way the FSM function describes the configuration  $r_{1,2} \sim r_b$ ,  $|\mathbf{r}_1 - \mathbf{r}_2| \lesssim 1/m$  with the accuracy  $\alpha^2$ . Thus, for the adequate description of the photoionization processes, it is sufficient to have a good nonrelativistic initial-state wave function.

The final-state wave function can be presented as the power series in the Sommerfeld parameter

$$\xi_Z = \frac{E_1 \alpha Z}{p_1} \quad (2)$$

of the interaction of the fast outgoing electron with energy  $E_1 = (p_1^2 + m^2)^{1/2}$  and the three-dimensional momentum  $p_1$  with the nucleus.

This parameter is of the order  $\alpha Z$  at  $\omega \sim m$ . At these values of the photon energies the first-order interaction between the fast electron and the nucleus contributes to the lowest-order expansion of the amplitude [5]. The higher-order corrections are of order  $\xi_Z \approx \alpha Z$ . In contrast to the nonrelativistic case, one cannot carry out the expansion in powers of the ratio  $k/p$  ( $k$  stands for the photon momentum). Thus, there is no dipole approximation in the relativistic case.

In the amplitudes of the ‘‘ionization with excitation’’ processes one can separate the amplitude of the single ionization as a factor. The accuracy of such a presentation is  $(\alpha Z)^2$ . This is because the ionization with excitation can be viewed as a kind of a two-step process, in which single ionization is followed by the shake-off of the second electron, in the whole region  $\omega \gg I$  with  $I$  denoting the binding energy. Thus, the ratios of the cross sections of these processes to the cross section of single photoionization are determined by the properties of the initial state only. The corrections of the order  $\xi_Z$  cancel out in the shake-off ratios. In this way these ratios can be obtained with the accuracy  $(\alpha Z)^2$ .

The same applies to the double ionization of the singlet states, when we consider the photon energies  $\omega \ll m$ , corresponding to the nonrelativistic outgoing electrons. At  $\omega \sim m$  an alternative quasifree mechanism (QFM) provides the contribution of the same order as the shake-off. In the QFM large momentum  $q_e \sim m$  is exchanged between the outgoing electrons if  $\omega \sim m$ . Relativistic effects in the initial state are described by the FSM wave function  $\Psi(\mathbf{r}_1, \mathbf{r}_2)$  at  $|\mathbf{r}_1 - \mathbf{r}_2| \sim 1/q_e$ , thus being expressed through the nonrelativistic wave function. In this case the structures of the amplitudes of the single and double ionization processes are different. Therefore the double-to-single ionization ratio of singlet states depends on the ratio  $\omega/m$  in the region  $\omega \sim m$ . It reaches a new asymptotic value in the limit  $\omega \gg m$  [6]. The corrections of the order  $\xi_Z$  do not cancel out in the QFM part of the double-to-single ionization ratio. Thus, we obtain the double-to-single ionization ratios of the singlet states with the accuracy  $\alpha Z$ .

In this paper we present the analysis and the calculations of the high-energy limits of the double photoionization and of the ionization with excitation cross sections for the ground and excited  $n^1S$  and  $n^3S$  states of two-electron systems. We consider the  $H^-$  ion, the helium atom, and the helium-like ions. In the latter case we investigate the cross-sections dependence upon the nuclear charge. We use the approach, traditional for the double photoionization studies, of presenting the double-to-single cross section ratios

$$R_n^{(k)}(\omega) = \frac{\sigma_n^{(k)++}(\omega)}{\sigma_n^{(k)+}(\omega)}, \quad R_n^{(k)*}(\omega) = \frac{\sigma_n^{(k)+*}(\omega)}{\sigma_n^{(k)+}(\omega)}. \quad (3)$$

Here the notations  $+$ ,  $++$ ,  $+*$  correspond to single ionization, double ionization, and ionization with excitation, respectively. The cross sections are summed over all the final states belonging to the discrete spectrum. The upper index  $(k)$  denotes the excited  $n^kS$  initial states with  $n = k = 1$  for the ground state. Note that in the existing experiments somewhat different parameters are detected, with the cross sections  $\sigma_n^{(k)++}$  and  $\sigma_n^{(k)+*}$  related to the total cross section of the formation of the

singly charged ion  $\sigma_n^{(k)+} + \sigma_n^{(k)+*}$ . The expression ‘‘high-energy limit’’ means that the photon energy exceeds strongly the energy of the electron at rest, i.e.,

$$\omega \gg m. \quad (4)$$

In this limit we calculate the leading term of the expansion of the ratios  $R_n^{(k)}$  and  $R_n^{(k)*}$  in powers of  $\omega^{-1}$ . In some cases the ‘‘high-energy nonrelativistic limit’’ can be just expanded to the relativistic region of energies of the outgoing electrons.

As shown above, all what we need is a nonrelativistic wave function of the initial state, which would describe the two-electron system in the configurations where one of the electron-nucleus distances  $r_{1,2}$  or the electron-electron distance  $|\mathbf{r}_1 - \mathbf{r}_2|$  is small. In these cases the behaviour of the solution of the Schrödinger equation is described by the Kato cusp conditions [7]. It was shown in ref. [8] that even the energy of the ground state of helium, i.e., the characteristic, which is determined mainly by the distances  $r_{1,2} \sim r_b$ ,  $|\mathbf{r}_1 - \mathbf{r}_2| \sim r_b$  can be obtained with much better accuracy if the wave function satisfies the Kato conditions. It was shown in refs. [9–11] that the violation of these conditions may cause erroneous results in the high-energy photoionization problem.

We use the initial-state wave functions, obtained by the correlation function hyperspherical harmonic method (CFHHM) in refs. [12–14]. The functions describe the ground states of the two-electron systems, as well as the excited  $n^k S$  states.

In Sect. 2 we analyze the shake off and quasifree mechanisms in detail. We discuss the choice of the initial-state wave function in Sect. 3. We present our numerical results for the singlet and triplet states in Sects. 4 and 5, providing the summary in Sect. 6.

## 2 Shake-Off and Quasifree Mechanisms

The single-photoionization and the shake-off-mechanism contributions to the ionization with excitation and to double ionization can be considered in a similar way. The general expression for the amplitudes is  $F_\mu(\omega) = F^0(\omega)J_\mu$  with  $F^0$  being the amplitude of the single ionization process and  $\mu$  denoting the state of the secondary electron, while [1]

$$J_\mu = \int \Psi(0, r) \varphi_\mu(r) d^3 r, \quad (5)$$

with  $\varphi_\mu$  being the electron wave function in the Coulomb field of the residual nucleus. The ground state is labeled by  $\mu = 1$ . Thus, we obtain

$$R_n^* = \sum_b \frac{|J_b|^2}{|J_1|^2}, \quad R_n^+ = \sum_c \frac{|J_c|^2}{|J_1|^2}, \quad (6)$$

with  $b$  and  $c$  standing for the final bound and continuum states.

Actually, the wave function  $\Psi(r_1 \sim q^{-1}, r_2 \sim r_b)$  enters the integrand on the right-hand side of Eq. (5). The momentum  $q$  transferred to the nucleus is of the order  $m$  in the relativistic case. The relativistic wave function  $\Psi(r_1 \sim q^{-1}, r_2 \sim r_b)$  can be expressed in terms of the nonrelativistic one by using the lowest-order

iteration of the Bethe-Salpeter equation

$$\Psi = \Psi_0 + GV\Psi \quad (7)$$

with  $V$  standing for the interactions inside the system, while  $G$  is the relativistic Green function of two free electrons. The higher-order iterations provide the terms of higher orders of the expansion in powers of  $p_1^{-2}$ . This equation connects the wave function  $\Psi(r_1 \sim p_1^{-1}, r_2 \sim r_b)$  with the wave function  $\Psi(r_1 \sim r_b, r_2 \sim r_b)$ . This becomes quite explicit in the momentum space, where

$$\Psi_F(\mathbf{p}_1, \mathbf{p}_2) = \frac{8\pi\alpha Z}{p_1^4} \left( 1 + \frac{(\boldsymbol{\alpha}\mathbf{p}_1)}{2m} \right) \int \frac{d^3f}{(2\pi)^3} \Psi_F(\mathbf{f}, \mathbf{p}_2) \quad (8)$$

with  $\Psi_F(\mathbf{p}_1, \mathbf{p}_2)$  being the Fourier transform of the function  $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ , while  $\boldsymbol{\alpha}$  are the standard Dirac matrices. The integral on the right-hand side of Eq. (8) is saturated by momenta  $f$  of the order of the binding momentum of the atom. The latter is of the order  $m\alpha Z$ . Thus, the nonrelativistic function  $\Psi_F(\mathbf{f}, \mathbf{p}_2)$  can be employed on the right-hand side of Eq. (8) with the accuracy  $(\alpha Z)^2$ . Hence, Eq. (8) presents the relativistic wave function in terms of the nonrelativistic one. All the relativistic effects are contained in the factor  $GV$  on the right-hand sides of Eqs. (7) and (8). Note that Eq. (8) is just the representation of the FSM function of the relative motion of the electrons.

Thus the ratios  $R_n^{(k)}$  and  $R_n^{(k)*}$  determined by Eq. (3) are expressed by Eq. (6) in the whole region  $\omega \gg I$  and do not depend on  $\omega$ , although the cross sections in the numerators and denominators depend on the parameter  $\omega/m$ . This becomes important in the region  $\omega \gtrsim m$ . The situation differs for the double photoionization of the singlet states due to the QFM contribution.

The main point of QFM is that two free electrons at rest can be moved to continuum by interaction with a photon. This contrasts with the single photoionization which is not allowed for free electrons. The cross section of the QFM contribution is thus proportional to the probability for the two electrons composing a bound state with the principal quantum number  $n$  to come to the same point,

$$C_n = \int |\Psi_n(\mathbf{r}, \mathbf{r})|^2 d^3r = \int |\tilde{\Psi}_n(R, 0)|^2 d^3R, \quad (9)$$

expressed in terms of the nonrelativistic function  $\tilde{\Psi}_n(\mathbf{R}, \rho) = \Psi_n(\mathbf{r}_1, \mathbf{r}_2)$  with  $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ ,  $\rho = \mathbf{r}_1 - \mathbf{r}_2$ . The FSM terms presented by Eq. (8) are included into the cross section of the free process  $\sigma_0^{++}(\omega)$  and QFM contributes

$$\sigma_{\text{QFM}}^{(1)++}(\omega) = C_n \sigma_0^{++}(\omega), \quad (10)$$

with  $C_n$  defined by Eq. (9).

Thus, the double-to-single ionization ratio  $R_n^{(1)}$  is the sum of the shake-off contribution given by Eq. (6) and the QFM one,

$$(R_n^{(1)})_{\text{QFM}} = \frac{C_n \sigma_0^{++}(\omega)}{\sigma_n^{(1)+}(\omega)}. \quad (11)$$

In contrast to the shake-off term (6), the QFM ratio (11) depends on the parameter  $\omega/m$ . The contribution (11) is  $\omega/m$  times smaller than that of the shake-off. The two terms are of the same order at  $\omega \sim m$ . Their sum reaches a new asymptotic

value at  $\omega \gg m$  [6]. The QFM for the triplet states is quenched by a factor of the order  $(m\alpha Z/\omega)^2$ , reflecting a small probability for the two bound electrons to be separated by a small distance  $1/\omega$  in a space-asymmetric state.

All the ratios considered above drop as  $Z^{-2}$  at large  $Z$ . Note that the values of  $Z$  are limited by the condition (1) which ensures that the relativistic effects at the distances  $r \sim r_b$  are small.

### 3 The Wave Function of the Initial State

The parameters of the double-ionization processes are very sensitive to the choice of the approximate initial-state wave function  $\psi_{\text{appr}}$ . Even for the best studied case of the helium atom the discrepancy of the characteristics of the double photoionization provided by different types of functions exceeds strongly the discrepancy of the values of the ground-state binding energy. For example, the Hartree-Fock value of  $R_1^{(1)}$  underestimates the experimental one by a factor of 3 [15]. One needs a variational wave function with a large number of parameters to reproduce the experimental data. The value also differs by several times for different functions [16]. The uncertainties are even larger for the excited states. As we have seen, the values of the ratios are determined by the wave function at  $r_1 \rightarrow 0$  and  $|\mathbf{r}_1 - \mathbf{r}_2| \rightarrow 0$ . The dependence of the wave functions of the initial state (which can be either the ground or the excited state) on the components of the vectors  $\mathbf{r}_1$  and  $\boldsymbol{\rho}$  is non-analytic at these points due to the singularities of the Coulomb interactions

$$V_{eN} = \frac{-\alpha Z}{r_1} \quad \text{and} \quad V_{ee} = \frac{\alpha}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (12)$$

The behaviour of the wave functions near these points is determined by the Kato conditions [7]. For the ground state

$$r_0 \frac{\partial \Psi(\mathbf{r}_1, \mathbf{r}_2)}{\partial r_1} = -Z\Psi(\mathbf{r}_1, \mathbf{r}_2) \quad (13)$$

at  $r_1 \rightarrow 0$  and

$$r_0 \frac{\partial \tilde{\Psi}(\mathbf{R}, \rho)}{\partial \rho} = \frac{1}{2} \tilde{\Psi}(\mathbf{R}, \rho) \quad (14)$$

at  $\rho = |\mathbf{r}_1 - \mathbf{r}_2| \rightarrow 0$ . Here  $r_0$  is the Bohr radius. Eqs. (13) and (14) can be viewed as the conditions of the cancellation of the singularities in the Schrödinger equation for the helium atom at  $r_1 \rightarrow 0$  and at  $\rho \rightarrow 0$ .

The calculation of the amplitude of the double ionization with the ‘‘accurate’’ approximate wave functions which, however, do not satisfy the Kato cusp conditions, may lead to controversial results. For example, it was noted recently in ref. [11] that the coefficient  $C_1 = C$ , being expressed by Eq. (9) if the amplitude is evaluated by using the Bethe-Salpeter equation (7), becomes rather

$$C = \int \left| 2r_0 \frac{\partial \tilde{\Psi}(\mathbf{R}, \rho = 0)}{\partial \rho} \right|^2 d^3 R$$

in the original formalism of quantum mechanics. The two values coincide for the exact wave function  $\Psi$  due to Eq. (14). However, they may differ for the

approximate functions. Somewhat more dramatical examples of the erroneous results, which can originate from the violation of the Kato conditions, are analyzed in refs. [9] and [10].

However, even if the short-distance behaviour is treated properly, the various approximate wave functions still provide numbers which differ rather strongly [10]. This increases the necessity to have a proper wave function of the initial state.

We use the functions obtained in refs. [12–14] for the description of the initial state, which can be either the ground or an excited state of the system. They were found by using the correlation function hyperspherical harmonic method. The initial wave function is decomposed as

$$\Psi = e^f \Phi, \quad (15)$$

where  $f$  is the correlation function describing the singularities of  $\Psi$ , and  $\Phi$  is a smooth part which can be expanded in a fast converging hyperspherical harmonic (HH) expansion. The function  $f$  depends on the interparticle distances, what is necessary and sufficient to take into account analytically the two- and three-body Coulomb singularities (cusps) in the wave function, i.e., it satisfies the Kato cusp conditions [7] exactly. Here  $\Psi$  is obtained by direct solution of the three-body Schrödinger equation, which guarantees local correctness [12–14] of  $\Psi$  because the convergence of  $\Psi$  across the configurations space is uniform.

The accuracy of the CFHHM wave function has previously been studied in ref. [12] for the ground and the  $2^1S$  excited state of the helium atom and for the ground state of the positronium ion ( $\text{Ps}^-$ ). In ref. [12], the correlation function  $f$  linear in interparticle coordinates was used. However, a linear  $f$  satisfying all cusp conditions, including the repulsive one, has a wrong asymptotic behaviour which becomes critical for spatially extended systems [8]. Indeed, for the ground state of the helium atom, the inclusion of all cusp conditions in  $f$  yielded better  $D = H\Psi/E\Psi - 1$  than if the repulsive cusp condition was omitted, while for the  $2^1S$  excited state of helium and for the ground state of  $\text{Ps}^-$ , the  $D$  values were much better at distances of a few a.u. if the repulsive cusp condition was omitted. As expected, the behaviour of  $\Psi$  near the coalescence points was always improved [12] by the inclusion of the cusp conditions, by up to 6 orders of magnitude for the  $2^1S$  state of the helium atom, compared with omitting the repulsive cusp condition.

The necessity of a proper description of local properties of the wave function also in variational calculations was stressed in ref. [17] where a variational principle for the minimization of the local energy  $\epsilon = H\Psi/\Psi - E$  instead of  $E$  was developed and realized within the quantum Monte Carlo method. The two best calculations of the helium atom ground state gave  $E$  with errors of 0.004 a.u. and  $2 \times 10^{-6}$  a.u., respectively. The corresponding standard deviations of the local energy,  $\sigma$ , were 0.14 a.u. and 0.001 a.u., respectively. This shows that the error in energy was still decreasing faster than  $\sigma$ . An example of a CFHHM calculation with the same precision  $2 \times 10^{-6}$  a.u. in energy is the CFHHM calculation of the  $2^1S$  state with  $K_m = 32$  [8]. Here  $K_m$  is the maximum value of the global angular momentum used in the hyperspherical expansion of the smooth factor  $\phi$ . The measure of the local accuracy analogous and comparable to  $\sigma$ , the expectation

value  $\langle |\epsilon| \rangle = E \langle |D| \rangle$  was 0.0023 a.u., which is of the same order of magnitude as 0.001 a.u. [17], indicating that the proposed variational principle in this reference, while giving better accuracy of the wave function than the ordinary Ritz variational approach, is roughly equivalent in precision to the CFHHM approach using relatively small  $K_m$ . Namely, the CFHHM calculation in ref. [8] was done for  $K_m$  up to 56, where  $\langle |\epsilon| \rangle$  fell to 0.0003 a.u. and  $E$  improved by two digits. For the helium atom, the particles  $\{1, 2, 3\}$  correspond to  $\{e, e, \alpha\}$ , where  $\alpha$  denotes the  ${}^4\text{He}^{++}$ . For  $\text{Ps}^-$ , the particles  $\{1, 2, 3\}$  correspond to  $\{e, e, e^+\}$ , where  $e^+$  denotes the positron. The Jacobi vectors, the first connecting the  $k$ -th, or  $ij$ -th, pair, and the second connecting the center of mass of the  $k$ -th pair with the third particle, are denoted by  $\mathbf{r}_k$  and  $\mathbf{s}_k$ , respectively. The angle between  $\mathbf{r}_k$  and  $\mathbf{s}_k$  is denoted by  $\phi_k$ . The odd-man out notation and the explicit pair notation for relative coordinates are used interchangeably. Thus,  $\mathbf{r}_1 = \mathbf{r}_{e\alpha}$  in the case of the helium atom.

The general nonlinear form of  $f$  is [18]

$$f = \sum_{k=1}^3 [a_k + (b_k - a_k) \exp[-r_k / (n_k \bar{r}_k)]] r_k, \quad (16)$$

where  $\bar{r}_k$  are approximate values of the expectation values of interparticle distances, and  $n_k$  are free parameters which are optimized for a faster convergence of the method. Putting  $b_k = Z_i Z_j m_i m_j / (m_i + m_j)$ , where  $m_i$  and  $Z_i$  are particle masses and charges, respectively, assures that the Kato cusp conditions are satisfied exactly.

Only a nonlinear dependence of  $f$  on interparticle distances assures that  $f$  can have a proper asymptotic behaviour and can incorporate all cusp conditions. In the  $\text{Ps}^-$  calculation [19] employing nonlinear  $f$  the convergence of the method was improved by orders of magnitude compared to the calculation employing a linear  $f$ . For the helium atom states [8] it is, however, enough to employ the linear correlation function obtained from Eq. (16) with  $a_k = b_k$ ,  $k = 1, 2, 3$ , and the helium ion mass of 7294.2996 a.u.

The highly accurate wave function of the He atom in its ground and several lowest excited  $n^1S$  states with  $n = 2, \dots, 5$  can be used not only in calculations of some ground-state observable characteristics, but also to determine cross sections of atomic processes. Such are the high-energy photoionization cross sections, which can be expressed solely via the initial-state wave functions. For example, recently the cross sections for the two-electron photoionization and photoionization with excitation of the He atom and helium-like ions in the limit of very high photon energy  $\omega$  were calculated [20, 21]. It was demonstrated there that the two-electron photoionization cross section and photoionization with excitation and their ratio to the one-electron photoionization cross section depend strongly upon the quality of the initial-state wave function. Another interesting process occurs if the initial state is excited, in which case photoionization with de-excitation can take place.

#### 4 Results for the Singlet States

We start with the results for the total values of the double-to-single ionization ratios  $R_n^{(1)}$ . The largest value is obtained for  $n = 1$  with  $R_1^{(1)} = 0.0837$  for the ionization



**Table 1.** Ratio  $R_n^{(1)}$  as function of  $Z$  and  $n$ 

$n$	1	2	3	4	5
$Z$	$R_1^{(1)}$	$R_2^{(1)}$	$R_3^{(1)}$	$R_4^{(1)}$	$R_5^{(1)}$
1	0.08366				
2	0.07615	0.01569	0.00559	0.00247	0.00127
3	0.04347	0.01844	0.01023	0.00627	0.00402
4	0.02733	0.01492	0.01001	0.00741	0.00563
5	0.01864	0.01148	0.00845	0.00692	0.00579
6	0.01349	0.00890	0.00690	0.00600	0.00532
7	0.01020	0.00703	0.00564	0.00510	0.00469
8	0.00798	0.00567	0.00465	0.00431	0.00408
9	0.00641	0.00466	0.00388	0.00367	0.00354
10	0.00526	0.00389	0.00328	0.00315	0.00308

of the negative ion of hydrogen  $H^-$ . For the ground state of helium we find  $R_1^{(1)} = 0.0762$ . For large  $Z$  the ratio is expected to drop as  $Z^{-2}$ . However, for the ground states of the light helium-like ions the ratio drops slower with  $Z$ . The numerical results are presented in Table 1.

Now we follow the relative role of the QF mechanism in the ionization of  $n^1S$  states as a function of the nuclear charge  $Z$ . Since the contributions of both the shake-off and QF mechanisms drop as  $Z^{-2}$  at large  $Z$ , their relative contribution does not depend on  $Z$  in the limit  $Z \gg 1$ . The role of the QF mechanism is determined by the function  $\zeta(n, Z)$  defined in such a way that

$$R_n^{(1)} = R_{n,s.o.}^{(1)} \cdot \zeta(n, Z), \quad (17)$$

where  $R_{n,s.o.}^{(1)}$  is the shake-off contribution, for the limiting values of  $R_n^{(1)}$ . We expect, thus, the function  $\zeta$  to depend smoothly on  $Z$  with  $Z$ -dependence ceasing at large  $Z$ . For the ground states of  $H^-$  and He the values of  $\zeta$  are  $\zeta(1, 1) = 5.22$  and  $\zeta(1, 2) = 4.63$ . For the helium-like ions  $\zeta(1, 2)$  increases slowly with the

**Table 2.** Factors  $\zeta(n, Z)$  as functions of  $Z$  and  $n$ 

$n$	1	2	3	4	5
$Z$	$\zeta(n, Z)$				
1	5.222				
2	4.632	1.737	1.515	1.462	1.444
3	5.081	1.531	1.232	1.148	1.115
4	5.380	1.500	1.180	1.095	1.062
5	5.583	1.495	1.161	1.077	1.046
6	5.727	1.497	1.153	1.069	1.039
7	5.835	1.500	1.148	1.064	1.035
8	5.919	1.503	1.145	1.062	1.032

high  $Z$  limit being  $\zeta \approx 6.3$ . However, for  $Z > 8$  the neglected corrections of the order  $\alpha Z$  may appear to be more important than the change of the function  $\zeta(1, Z)$  with  $Z$ .

The results for the function  $\zeta(n, Z)$  are presented in Table 2.

In Table 5 we show the results for “ionization with excitation” for several lowest values of  $n$  and  $Z$ .

## 5 Results for the Triplet States

In the case of the singlet states the single photoionization was the main channel of the process. In contrast, the excited ions are created with the largest probability in the ionization of the triplet states. This is because the photon interacts mostly with the inner electron and thus it is most probable to find the  $ns$ -excited ion in the final state. For example, in the ionization of the  $2^3S$  state of the atom of helium, the probabilities to find the final-state electron in the states  $1s$  and  $3s$  are, correspondingly, 23 and 4.5 times smaller than to obtain it in the state  $2s$ . The double ionization provides a still smaller fraction  $3.3 \cdot 10^{-3}$  of the main channel.

In Table 3 we present the results for the limiting value of the cross-section ratio

$$\tilde{R}_n^{(3)} = \frac{\sigma_n^{(3)++}}{\sigma_n^{(3)+} + \sigma_n^{(3)+*}}, \quad (18)$$

where  $\sigma_n^{(3)+*}$  is the sum of the “ionization with excitation” cross section over the final states of the discrete spectrum. The ratio  $\tilde{R}_n^{(3)}$  describes the fraction of the double ionization in the inclusive ionization processes. The data placed in Table 3 show the dependence of this ratio on the value of  $n$  and on the charge of the helium-like ions. The values for the ratios  $R_n^{(3)*}$ , defined by Eq. (3), are given in Table 4. The distributions  $a_{n\mu}^{(3)} = |J_\mu|^2$  over the final excited states, where  $J_\mu$  is defined by Eq. (5), are shown in Table 5.

**Table 3.**  $\tilde{R}_n^{(3)}(Z) \times 10^3$  values for the  $n^3S$  states in the helium isoelectronic sequence

$n$	2	3	4	5
$Z$	$\tilde{R}_2^{(3)}$	$\tilde{R}_3^{(3)}$	$\tilde{R}_4^{(3)}$	$\tilde{R}_5^{(3)}$
2	3.116	1.965	1.043	0.573
3	3.040	3.662	3.076	2.332
4	2.222	3.420	3.526	3.198
5	1.615	2.811	3.218	3.211
6	1.209	2.262	2.755	2.911
7	0.933	1.830	2.321	2.546
8	0.739	1.500	1.957	2.204
9	0.599	1.247	1.660	1.906
10	0.495	1.050	1.421	1.655

**Table 4.**  $R_n^{(3)*}(Z)$  values for the  $n^3S$  states in the helium isoelectronic sequence

$n$	2	3	4	5
$Z$	$R_2^{(3)*}$	$R_3^{(3)*}$	$R_4^{(3)*}$	$R_5^{(3)*}$
2	28.53	113.79	291.18	595.76
3	16.83	62.19	154.06	309.04
4	13.58	48.70	118.96	236.66
5	12.06	42.63	103.37	204.73
6	11.20	39.20	94.63	186.89
7	10.63	37.00	89.05	175.55
8	10.24	35.47	85.19	167.71
9	9.95	34.35	82.36	161.97
10	9.72	33.49	80.19	157.60

**Table 5.**  $a_{n\mu}$  values for the lowest  $n^3S$  states of  $\text{He}^*$  ( $Z = 2$ )

$n$	2	3	4	5
$\mu$				
1	0.04458	0.01118	0.00436	0.00214
2	1.033	0.07593	0.02170	0.00934
3	0.2287	0.5211	0.1154	0.04498
4	0.00583	0.6719	0.09669	0.05350
5	0.00179	0.00073	0.9702	0.00758
6	0.00080	0.00046	0.06774	0.8569
7	0.00044	0.00033	0.00011	0.2967
8	0.00027	0.00021	0.00005	0.00353
9	0.00018	0.00014	0.00005	0.00001

## 6 Summary

We calculated the relativistic high-energy limit of the “ionization + excitation” to single ionization and of double-to-single ionization ratios. We obtained also the results for the distribution between the final states in “ionization of excitation” processes. The calculations are carried out for the atoms of helium, for helium-like ions, and for the  $\text{H}^-$  negative ion. The ground states as well as the excited  $n^1S$  and  $n^3S$  states are considered as the initial states.

We showed that, although the corresponding cross sections depend on the photon energy  $\omega$  strongly in the region  $\omega \sim m$ , the “ionization with excitation” to the single-ionization cross section ratios do not. The same refers to the double-to-single cross section ratios of the triplet states. Thus the results of our earlier calculations of these ratios in the high-energy non-relativistic limit [20–22] can be expanded to the whole region  $\omega \gg I$ .

These calculations as well as the calculations of the double-to-single ratio of the singlet states, where the specific quasifree mechanism is very important, were carried out by using very precise locally correct initial-state wave functions [12–14]. The proper description of the quasifree mechanism relies strongly on these

properties of the wave functions. For example, if the function  $\Psi(r, r)$  involved in the calculation of the QF mechanism is approximated by a product of the Coulomb functions, the contribution appears to be overestimated by a factor of 2.

The expansion of the approach to the heavier helium-like ions requires account of the relativistic corrections of higher order to the wave function of the initial state and more precise treatment of the wave function of the final state.

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