Photoionization accompanied by excitation at intermediate photon energies

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(Received 27 September 2007; published 18 January 2008)

We calculate the photoionization-with-excitation to photoionization ratios R_{nl} and $R_n=\Sigma_l R_{nl}$ for atomic helium and positive heliumlike ions at intermediate values of the photon energies. The final-state interactions between the electrons are included in the lowest order of their Sommerfeld parameter. This enables us, in contrast to purely numerical calculations, to investigate the roles of various mechanisms contributing beyond the high-energy limit. The system of two bound electrons is described by the functions obtained by the correlation function hyperspherical harmonic method. For the case of heliumlike ions we present the high-energy limits as a power expansion in the inverse charge of the nucleus. We analyze the contribution of excitation of states with nonzero orbital momenta to the ratios R_n. In the case of helium our results for R_n are in good agreement with those of experiments and of previous calculations.

DOI: 10.1103/PhysRevA.77.012715 PACS number(s): 32.80.Fb, 32.80.Hd, 32.80.Zb

I. INTRODUCTION

Atomic photoionization accompanied by excitation and double photoionization have been thoroughly documented in experimental and theoretical works in connection with the many-electron problem. In the present paper the three-body Coulomb problem in the case of two-electron systems is the subject of investigation.

Most of the attention in experimental studies was focused on the process of double photoionization. Photoionization with additional excitation has not been investigated in detail. The energy dependence of the cross section ratios in a broad interval of the photon energies ω, the dependence of these ratios on the value of nuclear charge Z, and the branching ratios for excitations of nl subshells of a shell with the principal quantum number n remain subjects for future experiments. As it stands now, there are experimental data only for atomic helium. The intensity of excitation of the nth shell relative to the main photoline $n=1$ was measured in Ref. [1] for photon energies up to several hundred eV for the values of $n\leq 6$. A few measurements of $2s$ and $2p$ excitations at smaller values of the photon energies were carried out earlier—see Ref. [1] for examples.

Theoretical investigation of the process requires the knowledge of the wave functions describing two electrons in the field of the nucleus. In the initial state both electrons are bound by the nucleus. In the final state one of the electrons belongs to the continuum, while the second one is in the excited bound state. Certain approximations (models) for the wave functions are required. Somewhat different approximations are reasonable in different regions of the photon energy ω.

We use terminology which is similar to that employed for the much studied double photoionization [2]. It is known that the ratios

$$R_n(\omega)=\frac{\sigma_n^{+*}(\omega)}{\sigma_1^{+}(\omega)} \tag{1}$$

of the cross sections $\sigma_n^{+*}(\omega)$ for ionization with excitation of the second electron to the nth level, to those without excitation $\sigma_1(\omega)$ do not depend on the photon energy in the high-energy limit [3,4]

$$R_n(\omega)=\text{const} \tag{2}$$

for $\omega\to\infty$. This requires that ω greatly exceeds the values of single-particle ionization potentials I

$$\omega\gg I. \tag{3}$$

The analyses of Refs. [3,4] have been carried out by employing the nonrelativistic functions for description of the outgoing electrons. It was shown in Ref. [5] that asymptotics of the ratio $R(\omega)$ remain the same in the whole region (3) including the photon energies corresponding to relativistic outgoing electrons. Recall that this is not true for the double-to-single photoionization ratios [6].

By "high energies" we mean that part of the region (3) where the ratios exhibit behavior described by Eq. (2). At low energies the ratio I/ω cannot be treated as a small parameter. By "intermediate energies" we mean the values of the photon energies where inequality (3) is true, while deviations of the cross section ratios from the high-energy limit are noticeable (with the relative deviations exceeding 10%). For atomic helium this is the region from 300–400 eV to 2 keV. In the systems bound by the nucleus with the charge Z the limits of the interval are proportional to Z^2.

Since the ionization with excitation is a three-body problem, certain approximated wave functions for both initial and final states are required. It was shown in Refs. [3] and [4] that in the high-energy limit the final-state interactions (FSI) between the electrons can be neglected. This simplifies the problem of the description of the final state (under a proper choice of gauge interactions of the outgoing electron with the nucleus can be neglected as well). In Ref. [3] the high-energy limit of the process was expressed in terms of the initial-state wave function $\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)$. The high-energy limits of the ratios R_n for atomic helium were calculated in Refs. [7,8] and dependence on the choice of the approximate function Ψ_i was traced. The calculations of Ref. [6] also include the Z depen-

dence of the high-energy limits of R_n. Results of the high-energy calculations for Li^+ are presented in Refs. [9] and [10].

At low energies there is no small parameter. All the interactions involved should be treated as accurately as possible. In this energy region one must make a choice of both initial and final-state wave functions. The low-energy calculations of the cross sections $\sigma_n^{+*}(\omega)$ have been carried out in Refs. [14,15] for He and in Refs. [14,16] for Li^+. The paper [16] also contains results for partial cross sections $\sigma_{nl}^{+*}(\omega)$ of ionization accompanied by excitation of the remaining bound electron to the subshells with quantum numbers n and l. Low-energy calculations for the two-electron ions with larger values of Z were carried out in Ref. [14].

In the papers [11–14] the intermediate-energy region was approached by extension of the low-energy calculations to this energy interval. In the present paper we move from the high-energy region by including next to leading order of expansion in powers of ω^{-1}. This is achieved by inclusion of the interaction between the final-state electrons in the lowest order of perturbation theory

We find several attractive points in such an approach. It provides the possibility to clarify the role of various mechanisms (in a fixed form of electron-photon interactions) representing their contributions in terms of certain characteristics of the initial wave function. Within the framework of the approach one can estimate the magnitude of the neglected terms, thus controlling the accuracy. At the lower limit of the intermediate-energy region numerical calculations with certain models for the final-state wave functions are more precise. The discrepancy between the results obtained in numerical and perturbative approaches should diminish as ω increases. Hence these two approaches should supplement each other. A similar analysis of the intermediate-energy double photoionization have been carried out earlier [17].

We expect the approach developed in the present paper to be useful also because of certain discrepancies between experimental data for helium [1] and theoretical results. The high-energy limit of the ratio R_n extrapolated from the data obtained in Ref. [1] is in perfect agreement with the calculated one only for $n=2$. The disagreement increases with n reaching a factor of about 2 for $n=5$. There is also visible disagreement between theoretical and experimental results for $R_n(\omega)$ at $\omega \sim 200-400$ eV for $n=2,4,5$ [13,14]. Note also that in the case of helium there is a discrepancy between the calculations employing various approaches (see, e.g., Refs. [13] and [14]). Moving from the high-energy region can be instructive also since (as noted in Ref. [14]) the R matrix approach, widely used in low-energy calculations, becomes unstable at high energies. Finally, studies of the Z dependence of the ratios R_n may be of interest in connection with the increasing attention devoted to the physics of the multicharged ions.

We calculate ratios (1) of photoionization accompanied by excitation of the residual ion for helium atom and light heliumlike positive ions. We also obtain more detailed characteristics

$$R_{nl}(\omega) = \frac{\sigma_{nl}^{+*}(\omega)}{\sigma_{10}^{+}(\omega)}. \tag{4}$$

Such ratios are also detected in the low-energy experiments [18]. The ratios defined by Eq. (1) can be represented as

$$R_n(\omega) = \sum_l R_{nl}(\omega).$$

In this paper the calculations are carried out with inclusion of next-to-leading order terms of expansion of the ratios (1) in powers of ω^{-1}. This means that for ns states we calculate the high-energy limits of the ratios (1) and the correction of the order $1/\omega$. For nl states with $l \geq 1$ we obtain the leading order of expansion in $1/\omega$.

In the limit (3) all the interactions of the outgoing electron can be treated perturbatively [3]. In the high-energy limit of σ_n^{+*} final-state interactions (FSIs) of the outgoing electron with the electron bound in the residual ion can be neglected. The excitation following photoionization is due to the specific correlation in initial state known as shake-up (SU). Only s states can be excited by this mechanism. Excitations of the states with nonzero values of angular momentum l are quenched by a small factor of the order I/ω.

We can present the ratios (4) as

$$R_{ns}(\omega) = A_n + \frac{I_0}{\omega} B_{n0} \tag{5}$$

(where I_0 is the electron binding energy in hydrogen) for $l=0$, while for $l \geq 1$

$$R_{nl}(\omega) = \frac{I_0}{\omega} B_{nl}. \tag{6}$$

In the atomic system of units used throughout the paper ($e=m=\hbar=1$, $c=137$) $I_0=1/2$.

The coefficients A_n and B_{ln} with $l \geq 1$ do not depend on the photon energy, while we show that B_{n0} contains a smooth dependence on ω. Now we can present the ratios R_n defined by Eq. (1) as

$$R_n(\omega) = A_n + \frac{1}{2\omega} B_n, \quad B_n = \sum_l B_{nl}. \tag{7}$$

In the SU mechanism the interactions of the outgoing electron with nucleus can be treated perturbatively [3]. Excited electrons can be described by the Coulomb field wave functions. Thus, all the specifics of this three-body problem is contained in the wave function of the initial state. The ionized electron approaches the nucleus at distances which are much smaller than the size of the atom. The SU cross section is thus determined by initial-state wave function $\Psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)$ at electron-nucleus coalescence point, i.e., by $\Psi_i(\boldsymbol{r}_1=0, \boldsymbol{r}_2)$.

The SU probabilities depend on n in terms of the wave function and of momentum p_n of the outgoing electron

$$p_n^2 = 2\varepsilon_n$$

with ε_n being the energy of the outgoing electron. In the lowest order of expansion in powers of I/ω we can put

$$p_n^2 = p_1^2 = p^2 = 2\omega. \tag{8}$$

The SU terms with this value of p determine the high-energy limit of the ratios

$$\lim_{\omega\to\infty} R_{nl}(\omega) = \lim_{\omega\to\infty} R_{ns}(\omega)\delta_{l0} = A_n. \tag{9}$$

Now we consider three types of contribution beyond the high-energy limit, in the same way as it was done in Ref. [17] for the double photoionization. The kinematical corrections to SU ratios are caused by taking into account n dependence of momentum p_n in the SU amplitudes. This provides the contributions to the terms B_n on the right-hand side (RHS) of Eq. (5). Note that these corrections are proportional to the small parameter I/ω, containing also dependence on specific parameter $\pi\xi_Z$ with

$$\xi_Z = \frac{Z}{p}. \tag{10}$$

One has to have in mind that corrections of the order $\pi\xi_Z/\omega$ drop as $\omega^{-3/2}$ but contain a numerically large coefficient. We shall not treat $\pi\xi_Z$ as a small parameter, but include it exactly. The dependence of the cross sections on $\pi\xi_Z$ is known to be presented by the Stobbe factor $S(\pi\xi)=\exp(-\pi\xi)$ which is common for the photoionization processes [19,20]. These corrections are expressed in terms of SU contributions A_n to the ratios (5), which appear only in the ratios R_{ns}.

In the next to leading order the excitation energy can be transferred to the second electron also by the initial-state interactions (ISIs) beyond the SU. In this case the terms of the order $1/\omega$ and Z^2/ω come from the higher terms r_1^2/r_2^2 and $(\boldsymbol{r}_1\cdot\boldsymbol{r}_2)/r_2^2$ of the expansion of initial-state function $\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)$ at $r_1\to 0$. Thus the contribution will be presented in terms of the derivatives of the initial-state wave function, integrated with the Coulomb field function of the bound state.

The excitation energy can be transferred also by the final-state interactions (FSIs) between the final-state electrons. We include the FSIs by the perturbative method developed in Ref. [21]. The FSI amplitude is presented as a power series of the Sommerfeld parameter of the interaction between the fast outgoing electron and that of the residual ion

$$\xi = \frac{1}{v}, \tag{11}$$

while v is their relative velocity. Thus, the square of the amplitude is presented as a power series in $\xi^2=1/2\varepsilon$ with ε being the energy of the outgoing electron. Looking for terms of the relative order ω^{-1} in the cross sections, we must include the lowest correction of the order ξ^2, putting

$$\xi^2 = \frac{1}{2\omega}. \tag{12}$$

The FSI contributions are presented in terms of matrix elements of relatively simple operators sandwiched by the function $\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)$ and the Coulomb function of the electron in residual ion. The states with any angular momenta l can be excited by the FSI in the next to leading order of ω^{-1} expansion.

Thus, all the contributions up to the order ω^{-1} will be presented in terms of certain characteristics of the initial-state wave functions. We employ the functions obtained by the correlation function hyperspherical harmonic method (CFHHM), obtained in Ref. [22]. The CFHHM functions have been employed successfully for investigation of the parameters of the bound two-electron systems [23] and some characteristics of the double photoionization. Also, the method of inclusion of the FSIs [21] enabled us earlier to remove the discrepancy between experimental and theoretical results in creation of vacancies in electronic shells during nuclear transitions and in single photoionization of the p states [24]. In Ref. [17] it was used for investigation of the double photoionization at intermediate energies. In the present paper we use the CFHHM functions and the perturbative treatment of FSIs for investigation of photoionization with excitation.

Note that for the system containing a larger number of electrons the picture is more complicated. Considering ionization with excitation of the subshell with $l=1$ we find for ionization without excitations $\sigma^{+}\sim\omega^{-9/2}$, while for ionization accompanied by excitation to an s state $\sigma^{+*}\sim\omega^{-7/2}$ (the ISI provides admixture of two s state electrons to the system containing two p state ones). Hence the corresponding ratio increases proportionally to ω.

Our analysis is completely nonrelativistic. We neglect the terms of the order ω/m in the wave function of the final state, and in the operator of the photon-electron interaction. The latter means that we are using the dipole approximation. We also assume $(Z/137)^2 \ll 1$, to neglect relativistic effects in the initial bound system.

II. GENERAL EQUATIONS

The cross section of photoionization accompanied by excitation of the residual ion into a state with the quantum numbers n,l,m can be written as

$$d\sigma_{nl}^{+*} = \frac{2\pi}{\omega c}\sum_m \overline{|F_{nlm}|^2}\,\delta(\omega-\varepsilon_n-I_i)\frac{d^3p_n}{(2\pi)^3}. \tag{13}$$

Here I_i denotes the ionization potential of the K electron in the initial-state atom. The factor 2 is due to two electrons in the K shell. The overbar shows that the averaging over the photon polarizations have been carried out. The angular dependence of the amplitudes can be written explicitly because of the dipole approximation employed. The amplitude

$$F_{nlm} = \langle\Phi_{nlm}|\gamma|\Psi\rangle, \tag{14}$$

with γ being the operator of interaction between the photon and an electron, while Ψ and Φ_{nlm} describe the initial and final two-electron states, can be represented as

$$F_{nlm} = (4\pi)^{1/2}\frac{(\boldsymbol{e}\cdot\boldsymbol{p}_n)}{c}T_{nlm}. \tag{15}$$

After averaging over the photon polarizations one obtains

$$\sigma_{nl}^{+*} = \frac{4}{3}\frac{p_n^3}{c^3\omega}\sum_m |T_{nlm}|^2. \tag{16}$$

If the FSIs are neglected, the final-state function is

$$\Phi_{nlm}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \psi_f(\boldsymbol{p}_n;\boldsymbol{r}_1)\psi_{nlm}(\boldsymbol{r}_2) \tag{17}$$

with the functions ψ_f and $\psi_{n,l,m}$ being just the continuum and bound state single-particle wave functions in the Coulomb field. If condition (3) is valid, the interactions of the outgoing electron with the nucleus can be included perturbatively. Using the velocity gauge for the operator γ, i.e.,

$$\gamma(r) = -i(\boldsymbol{e}\cdot\boldsymbol{\nabla})$$

with $\boldsymbol{e}$ standing for the photon polarization, we obtain the leading contribution of expansion in powers of p^{-2} as coming from the plane waves. Following Ref. [17] we can separate two scales in the interactions between the fast outgoing electron and the nucleus. Those taking place at small distances of the order $p^{-1} \ll r_c$ with $r_c = 1/Z$ being the characteristic size of the atom are expressed in terms of the parameter $\pi\xi_Z^{(n)}$ ($\xi_Z^{(n)} = Z/p^{(n)}$). Such contributions can be calculated explicitly, producing the factor

$$N(\xi_Z^{(n)}) = N_r(\xi_Z^{(n)})e^{-\pi\xi_Z^{(n)}} \tag{18}$$

with $N_r(\xi_Z^{(n)}) = \{2\pi\xi_Z^{(n)}/[1-\exp(-2\pi\xi_Z^{(n)})]\}^{1/2}$ being the normalization factor of the nonrelativistic Coulomb continuum wave function. The interactions which take place at the distances of the order $r \sim r_c$ can be presented as p^{-2} series thus cancelling in the ratios (1) and (2). Thus we can put

$$\Phi_{nlm}^{(0)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = N(\xi_Z^{(n)})e^{i(\boldsymbol{p}_n\cdot\boldsymbol{r})}\psi_{nlm}(\boldsymbol{r}_2). \tag{19}$$

Following Ref. [20] we present the factors $N^2(\xi_Z^{(n)})$ in the cross sections as

$$N^2(\xi_Z^{(n)}) = h(\pi\xi_Z^{(n)})e^{-\pi\xi_Z^{(n)}} \tag{20}$$

with the function $h(\xi_Z^{(n)}) = 2\pi\xi_Z^{(n)}/[\exp(\pi\xi_Z^{(n)}) + \exp(-\pi\xi_Z^{(n)})]$ containing only weak dependence on parameter $\pi\xi_Z^{(n)}$. Thus we can put $h(\pi\xi_Z^{(n)}) = h(\pi\xi_Z)$, with ξ_Z defined by Eq. (10). Hence,

$$N^2(\xi_Z^{(n)}) = h(\pi\xi_Z)e^{-\pi\xi_Z^{(n)}}. \tag{21}$$

The second factor on the RHS of Eq. (21) is the Stobbe factor mentioned above.

We shall also present the perturbative FSI contributions in terms of the function (17). Thus the ratios (1) will be presented in terms of the matrix elements of initial-state two-electron function and the Coulomb function of the excited electron.

III. AMPLITUDES BEYOND THE SHAKE-UP

Following the analysis given above, we present the amplitudes for ionization with excitation beyond the SU as

$$F_{nlm} = F_{nlm}^{(s)} + F_{nlm}^{(i)} + F_{nlm}^{(f)} \tag{22}$$

with $F_{nlm}^{(s)}$ standing for SU amplitude, which includes kinematical corrections to the high-energy limit, while $F_{nlm}^{(i)}$ and $F_{nlm}^{(f)}$ are the contributions caused by correlations in ISIs and FSIs, correspondingly.

A. Amplitudes without inclusion of final-state interactions

Since in this subsection we neglect the interactions between the outgoing electrons, we can use Eq. (14) for the amplitude with the final-state wave function presented by Eq. (17). Recall that we use the operator γ in the velocity form. This provides

$$F_{nlm} = (4\pi)^{1/2}(\boldsymbol{e}\cdot\boldsymbol{p}_n)N(\xi_Z^{(n)})\int d^3r_2\psi_{nlm}^*(\boldsymbol{r}_2)\tilde{\Psi}_i(\boldsymbol{p}_n;\boldsymbol{r}_2). \tag{23}$$

Here

$$\tilde{\Psi}_i(\boldsymbol{p}_n;\boldsymbol{r}_2) = \int d^3r_1\Psi_i(\boldsymbol{r}_1,\boldsymbol{r}_2)e^{-i(\boldsymbol{p}_n\cdot\boldsymbol{r}_1)} \tag{24}$$

is the partial Fourier transform of the initial-state wave function in variable $\boldsymbol{r}_1$.

Since the integral over r_2 on the RHS of Eq. (23) is saturated at $r_2 \sim r_c$, while $p_n \gg r_c^{-1}$, we need expansion of the function $\tilde{\Psi}(\boldsymbol{p}_n;\boldsymbol{r}_2)$ in inverse powers of p_n^2. It is convenient to employ the Lippman-Schwinger equation

$$\tilde{\Psi}_i(\boldsymbol{p}_n;\boldsymbol{r}_2) = \frac{2Z}{p_n^2}J(\boldsymbol{p}_n,\boldsymbol{r}_2), \quad J(\boldsymbol{p}_n,\boldsymbol{r}_2) = \int\frac{d^3r}{r}e^{-i(\boldsymbol{p}_n\cdot\boldsymbol{r})}\Psi_i(\boldsymbol{r},\boldsymbol{r}_2). \tag{25}$$

The integral on the RHS is dominated by $r \sim p_n^{-1} \ll r_2$. Thus the expansion in p_n^{-2} can be carried out by expanding the function $\Psi(\boldsymbol{r},\boldsymbol{r}_2)$ in powers of r in the integrand on the RHS of Eq. (25).

1. Shake-up with kinematical corrections

Presenting

$$J(\boldsymbol{p}_n,\boldsymbol{r}_2) = \lim_{\delta\to 0}\int\frac{d^3r}{r}e^{-i(\boldsymbol{p}_n\cdot\boldsymbol{r})-\delta r}\Psi_i(\boldsymbol{r},\boldsymbol{r}_2), \tag{26}$$

we obtain for the leading order contribution

$$J(\boldsymbol{p}_n,\boldsymbol{r}_2) = \frac{4\pi}{p_n^2}\Psi(0,r_2), \tag{27}$$

which enables us to write for the SU amplitudes

$$F_{nlm}^{(s)} = a(p_n)S_n\delta_{l0}\delta_{m0}, \quad S_n = (4\pi)^{1/2}\int dr_2r_2^2\psi_{n0}^{(r)}(r_2)\Psi(0,r_2) \tag{28}$$

with

$$a(p_n) = (4\pi)^{1/2}(\boldsymbol{e}\cdot\boldsymbol{p}_n)N(\pi\xi_Z^{(n)})\frac{8\pi Z}{p^2p_n^2}, \tag{29}$$

while the upper index (r) in Eq. (28) labels the radial part of the Coulomb function ψ_{n0}. In the leading order we should neglect the dependence of p_n on n, putting $p_n = p$, just as in

Eq. (8). The high-energy limit of the amplitude (28) is thus

$$F^{(0)}_{n00} = a(p) S_n. \tag{30}$$

In the next to leading term we must include the n dependence of p_n. Since the residual ion contains only one electron, the latter is described by the Coulomb wave function, and thus

$$p_n^2 = p^2 - 2\delta_n, \tag{31}$$

where

$$\delta_n = \frac{Z^2}{2}\left(1 - \frac{1}{n^2}\right) \tag{32}$$

is the excitation energy of the electron in the final-state ion.

2. Contributions of correlations in the initial state

Now we return to Eqs. (24) and (25), looking for higher order terms of expansion of the function $\Psi_i(\boldsymbol{r},\boldsymbol{r}_2)$ at $r \to 0$. Since the CFHHN functions are expressed in terms of variables $r=|\boldsymbol{r}|$, $r_2=|\boldsymbol{r}_2|$, $\rho=|\boldsymbol{r}-\boldsymbol{r}_2|$, we present the expansion in terms of the function $\Psi(r,r_2,\rho)=\Psi_i(\boldsymbol{r},\boldsymbol{r}_2)$

$$\Psi(r,r_2,\rho) = \left(1 + r_i \boldsymbol{\nabla}_i + \frac{1}{2} r_i r_j \boldsymbol{\nabla}_i \cdot \boldsymbol{\nabla}_j\right) \Psi(r,r_2,|\boldsymbol{r}-\boldsymbol{r}_2|). \tag{33}$$

Here we put $\Psi(r,r_2,|\boldsymbol{r}-\boldsymbol{r}_2|)=\Psi(0,r_2,r_2)$ after the derivatives are calculated. Using Eq. (33) we find that at small r

$$\begin{aligned}\Psi(r,r_2,\rho) = {} & \Psi(0,r_2,r_2) + r\Psi'_r(r,r_2,r_2) - r\tau\Psi'_\rho(0,r_2,\rho) \\ & + \frac{r^2}{2}\Psi''_r(r,r_2,r_2) + \frac{r^2(1-\tau^2)}{r_2}\Psi'_\rho(0,r_2,\rho) \\ & + \frac{r^2\tau^2}{2}\Psi''_\rho(0,r_2,\rho) - r^2\tau\Psi'_{r\rho}(r,r_2,\rho).\end{aligned} \tag{34}$$

Here $\tau=(\boldsymbol{r}\cdot\boldsymbol{r}_2)/rr_2$. The derivatives Ψ'_r and Ψ'_ρ (and those of the second order) are taken at the points $r=0$ and $\rho=r_2$. The higher terms of expansion in r contribute to the higher order corrections in $1/p$ to the amplitudes. Thus, they are neglected. While evaluating the next to leading order terms we must put $p_n=p$.

Using Eqs. (26) and (34) we find nonzero contributions to the amplitudes with the angular momenta $l=0$ and 1. For excitation to s states we obtain

$$\begin{aligned}F^{(2)}_{n00} = {} & a(p) Q_n \frac{1}{p^2}, \quad Q_n = -(4\pi)^{1/2} \int dr_2 r_2^2 \psi^{(r)}_{n0}(r_2) \\ & \times \left[\Psi''_r(r,r_2,r_2) + \frac{1}{3}\Psi''_\rho(0,r_2,\rho) + \frac{2}{3r_2}\Psi'_\rho(0,r_2,\rho)\right] r_0^2\end{aligned} \tag{35}$$

with the upper index (r) labeling the radial part of the single-particle Coulomb field function as in Eq. (28). The function $a(p)$ is determined by Eq. (29). Other notations are explained in the text below Eq. (26). For excitation into p states, choosing the direction of the outgoing electron momentum as the axis of quantization of the angular momentum, we obtain

$$F^{(2)}_{n1m} = ia(p) P_n \frac{\delta_{m0}}{p},$$

$$P_n = (4\pi)^{1/2} \frac{2\sqrt{3}}{3} \int dr_2 r_2^2 \psi^{(r)}_{n1}(r_2) \Psi'_\rho(0,r_2,\rho) r_0.$$

Thus interactions in the initial state provide corrections of the order p^{-2} to the cross sections of excitations into s states. The dependence of the wave function on the interelectron distances $\rho=|\boldsymbol{r}_1-\boldsymbol{r}_2|$, which describes the electron correlations also enables excitations into p states. Excitation to the states with higher orbital momenta due to the ground-state correlations only are still impossible.

B. Contribution of the final-state interactions

Now we include the final-state interactions. Following Refs. [21,24] we present the final-state wave function as

$$\Phi^{(f)} = (1 + GV_{ee} + GV_{ee}GV_{ee})\Phi^{(0)} \tag{37}$$

with $\Phi^{(0)}$ being the wave function (17), where the FSIs have been neglected (here we omit lower indices), V_{ee} is the electron-electron interactions, and G is the propagator of the system of two noninteracting electrons in the Coulomb field of the nucleus. The second and third terms on the RHS of Eq. (37) correspond to one and two interactions between the final-state electrons, thus being proportional to the powers of the parameter ξ defined by Eq. (11).

The last two terms on the RHS contain infrared divergent contributions caused by the Coulomb interactions V_{ee}. It was shown in Ref. [21] that the infrared divergent terms cancel in each order of the expansion of the square of the amplitude $|F|^2$. The situation is similar to that with the infrared singularities in the e-N scattering analyzed in Ref. [25]. The cancellation can be illustrated by assuming the electron interactions to be defined as $V_{ee}(r)=\lim_{\nu\to 0} e^{-\nu r}/r$. The contributions $\ln \nu$ emerge in intermediate steps but vanish in the final expression for $|F|^2$.

Explicit expressions which include FSIs in the process with the fast outgoing electron up to terms of the order ξ^2 have been obtained in Refs. [21,24]. The first order amplitude $F^{(f1)}$, corresponding to the second term on the RHS of Eq. (37) is mostly imaginary. The real part of $F^{(f1)}$ is suppressed by additional power of p^{-1} and thus can be written as being proportional to ξ^{-1}. The second order amplitude is mostly real. Thus $\mathrm{Im}\, F^{(f1)} \sim \xi$, $\mathrm{Re}\, F^{(f1)} \sim \xi^2$, $\mathrm{Re}\, F^{(f2)} \sim \xi^2$, and $\mathrm{Im}\, F^{(f2)} \sim \xi^3$ (we do not trace the dependence on Z here). The FSI amplitudes can be presented as [21]

$$F^{(f1)}_{nlm} = a(p)\left(i\xi\langle\psi_{nlm}|\ln(r_2 - r_{2z})\nu|\Psi_i\rangle + \frac{\xi^2}{2}\langle\psi_{nlm}|r_0\frac{d}{dr_2}|\Psi_i\rangle\right), \tag{38}$$

$$F^{(f2)}_{nlm} = -\frac{a(p)\xi^2}{2}\langle\psi_{nlm}|\ln^2(r_2 - r_{2z})\nu|\Psi_i\rangle. \tag{39}$$

Here $\Psi_i \equiv \Psi_i(r_1=0,r_2)$ is a function of $r_2=|\boldsymbol{r}_2|$ and z is the direction of the momentum of the outgoing electron. Recall

that the z axis is chosen for the quantization of angular momentum and r_0 is the Bohr radius. Thus all the contributions to $F^{(f)}_{nlm}$ have nonzero values only for $m=0$.

For s states both amplitudes F^{f1} and F^{f2} are important, since the terms containing the factor ξ^2 interfere with the SU amplitude. For s states

$$F^{(f1)}_{ns} = a(p)(i\xi U_n + \xi^2 V_n), \quad F^{(f2)}_{ns} = -a(p)\xi^2 W_n, \quad (40)$$

with

$$U_n = (4\pi)^{1/2}\int dr_2 r_2^2 \psi^{(r)}_{n0}(r_2)\ln r_2 \nu \Psi_i(0,r_2),$$

$$V_n = \frac{(4\pi)^{1/2}}{2}\int dr_2 r_2^2 \psi^{(r)}_{n0}(r_2)\frac{d\Psi_i(0,r_2)}{dr_2} r_0,$$

$$W_n = -\frac{(4\pi)^{1/2}}{2}\int dr_2 r_2^2 \psi^{(r)}_{n0}(r_2)\ln^2(r_2\nu)\Psi_i(0,r_2). \quad (41)$$

For the states with $l \neq 0$ there is no interference with the SU amplitude. Thus only the first term of the amplitude $F^{(f1)}$ is important. We can present

$$F^{(f1)}_{nl} = ia\xi S_{nl} c_l + O(\xi^2) \quad (42)$$

with

$$S_{n\ell} = (4\pi)^{1/2}\int dr_2 r_2^2 \psi^{(r)}_{n\ell}(r_2)\Psi(0,r_2), \quad (43)$$

while

$$c_\ell = \frac{\sqrt{2l+1}}{2}\int_{-1}^{1} dt\, \ln(1-t)\mathrm{P}_l(t) = -\frac{\sqrt{2l+1}}{l(l+1)}, \quad (44)$$

and P_l is the Legendre polynomial.

IV. THE RATIOS

Now we can calculate the cross sections and the ratios (1) and (4). The cross sections are related to the squares of the amplitudes $|F|^2$ by Eqs. (13) and (16). We start with calculation of the values of $|F|^2$.

A. Excitation of s states

Expressions for excitation of s states have the most complicated structure

$$|F_{ns}|^2 = a^2(p_n)S_n^2 + \frac{a^2(p)}{2\omega}[2S_n Q_n + 2S_n(V_n + W_n) + U_n^2]. \quad (45)$$

Here the first term on the RHS stands for the SU contribution taking account of kinematical corrections (28) and (29). The first term in the square brackets comes from interference between SU and ISI amplitudes (30) and (35). The second term in brackets is caused by interference of the SU amplitude presented by Eq. (30) with the first and second order FSI amplitudes presented by Eqs. (40) and (41). The last term in brackets is purely a FSI contribution.

In order to obtain contribution of the first term on the RHS of Eq. (45) to the ratio (1) we must include the n dependence of the phase volume in Eq. (13) for the cross section. As a result, for the purely SU ratio we find

$$R^{\mathrm{SU}}_{ns} = \frac{S_n^2}{S_1^2}\frac{p}{p_n}e^{-\pi(\xi^{(n)}_Z - \xi)}, \quad (46)$$

with p_n defined by Eq. (31). In the lowest order of expansion in powers of I/ω the dependence of R^{SU}_n on parameter $\pi\xi_Z$ is just the same as it would result in expansion of the RHS of Eq. (46) in powers of $\pi\xi_Z$. However, this is not true for the higher order terms of the I/ω expansion.

The contribution of the other terms to the ratios R_n can be found as their ratios to squared amplitude of photoionization without excitation $|F_{1s}|^2$, where the corrections of the order I/ω should also be included. This gives

$$R_{ns}(\omega) = \frac{S_n^2}{S_1^2} + \frac{1}{2\omega}\left[\frac{S_n^2}{S_1^2}\frac{Z^2}{2}\left(1-\frac{1}{n^2}\right)(1-\pi\xi_Z) + \frac{2S_n}{S_1^2}\left(Q_n + V_n + W_n - \frac{S_n}{S_1}(Q_1 + V_1 + W_1)\right) + U_n^2 - \frac{S_n^2}{S_1^2}U_1^2\right]. \quad (47)$$

The first term on the RHS is the high-energy limit of the ratio. Note that Eq. (47) provides exact dependence on parameter $\pi\xi_Z$ in next to leading order of the I/ω expansion. The expression in square brackets on the RHS of Eq. (47) should be identified with parameter B_{n0} introduced by Eq. (5). Separating energy independent contributions and the terms, which depend on the photon energy through parameter $\pi\xi_Z$ we write

$$B_{n0} = d_n + \pi\xi_Z f_n, \quad (48)$$

with

$$d_n = \frac{S_n^2}{S_1^2}\frac{Z^2}{2}\left(1-\frac{1}{n^2}\right) + \frac{2S_n}{S_1^2}\left(Q_n + V_n + W_n - \frac{S_n}{S_1}(Q_1 + V_1 + W_1)\right) + U_n^2 - \frac{S_n^2}{S_1^2}U_1^2, \quad f_n = -\frac{S_n^2}{S_1^2}\frac{Z^2}{2}\left(1-\frac{1}{n^2}\right). \quad (49)$$

B. Excitation of p states

Excitations of the states with $l \neq 0$ can take place only beyond the SU approximation. The contributions of ISIs and FSIs are expressed by Eq. (36) and by the first term in brackets on the RHS of Eq. (38), correspondingly:

$$F_{n1} = i\frac{1}{p}(P_n + S_{n1}), \quad (50)$$

leading to

$$R_{n1}(\omega) = \frac{1}{2\omega}\frac{(P_n + S_{n1})^2}{S_1^2}. \quad (51)$$

C. Excitation of the states with $l \geq 2$

In this case only the FSIs contribute. The amplitude is expressed by Eq. (43) giving

TABLE I. The high-energy limits of the ratios R_{ns} in percent for a helium atom. The column "theory-I" [7] stands for early high-energy calculations with a variational initial-state function and "theory-II" [9] are results obtained using many-body perturbation theory. Theory-III [13] and theory-IV [14] are the extensions of the low-energy results with multiconfiguration Hartree-Fock and variational ground-state wave functions, correspondingly. The last column shows the result obtained in Ref. [1] by extrapolation of the experimental data of Ref. [1] with statistical errors given in parentheses.

n	Theory-I	Theory-II	Theory-III	Theory-IV	This work	Experiment
2	5.34	4.79	4.78	4.79	4.80	4.80 (13)
3	0.66	0.592	0.605	0.596	0.590	0.543(33)
4	0.21	0.19	0.200	0.197	0.195	0.118(37)
5	0.100	0.09	0.092	0.091	0.0900	0.048(30)
6	0.055	0.05	0.050	0.0515	0.0493	

$$R_{nl}(\omega) = \frac{1}{2\omega}\frac{c_l^2 S_{nl}^2}{S_1^2} \tag{52}$$

with c_l defined by Eq. (44). Now we turn to analysis of particular cases.

V. THE CASE OF HELIUM

A. High-energy limit

In Table I we compare our results for the high-energy limits with those extrapolated from the experimental data [1] and with the results of previous calculations [7,9,13,14]. There were also several publications of the high-energy limit for R_{2s} only. The pioneering calculation [26] provided $R_{2s}=4.61\times10^{-2}$, while the latest available result is $R_{2s}=4.79\times10^{-2}$ [27].

One can see that various theoretical approaches provide very close values for high-energy limits at $n\leq 6$. However, the values of these limits extrapolated in Ref. [1] from the experimental data are in perfect agreement with the theoretical results only for $n=2$. Discrepancy between theoretical and experimental results increases with n rapidly.

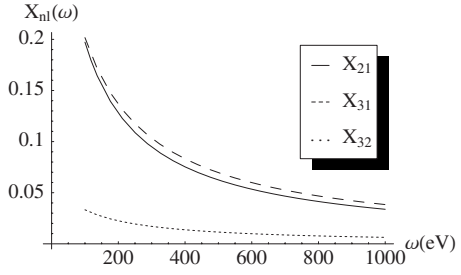

FIG. 1. Energy dependence of the relative role of excitations to the states with $l>0$, expressed by the ratio $X_{nl}=\sigma_{nl}^{+*}/\sigma_n^{+*}=R_{nl}/R_n$ for the case of helium ($Z=2$).

B. Beyond the high-energy limit

Now we consider the contributions beyond the limit (9). Let us start with excitation of ns states. As we showed above, the contributions beyond the high-energy limits come from kinematical corrections to the SU term and from the initial and final-states electron-electron interactions. One can see from Table II that the FSI and ISI contributions are positive, with the FSI term being about three times larger than the ISI one for all values of n. The kinematical corrections are negative at $\mu>1$, corresponding to $\omega<540$ eV. At larger ω values they become positive. Their contribution to the parameter B_{n0} defined by Eq. (5) does not exceed 10% for $\omega\lesssim 1$ keV. They increase with ω, becoming as large as 25 -30 % in the limit $\mu\ll 1$ ($\omega\gg 500$ eV). In this limit the FSI contribution determines about one half of the parameter B_{n0}. Note that the relative role of the three contributions does not vary much with n.

Contributions to excitation of p states come from FSIs and ISIs. Actually the former one dominates, providing more than 4/5 of the total contribution to B_{n1}. The result of calculations are presented in Table III. One can see that B_{n0} and B_{n1} provide contributions of the same order of magnitude to the energy dependent part of the ratio $R_n(\omega)$ defined by Eqs. (1) and (7).

TABLE II. Contributions of various mechanisms to the value B_{n0} defined by Eq. (5) for the case of helium. Here $\mu=\pi\xi_Z$, $\mu=1.04$ or $\omega=500$ eV, $\mu=0.73$ for $\omega=1$ keV.

n	Kinematical corrections	ISI	FSI	B_{n0}
2	$0.072(1-\mu)$	0.027	0.094	$0.193-0.072\mu$
3	$0.105(1-\mu)(-1)$	0.50(−2)	1.46(−2)	$(3.01-1.05\mu)(-2)$
4	$0.036(1-\mu)(-1)$	1.76(−3)	5.00(−3)	$(1.04-0.36\mu)(-2)$
5	$0.174(1-\mu)(-2)$	0.85(−3)	2.40(−3)	$(4.99-1.74\mu)(-3)$
6	$0.095(1-\mu)(-2)$	0.47(−3)	1.35(−3)	$(2.77-0.95\mu)(-3)$

TABLE III. Parameters B_{nl} and B_n of the energy-dependent contributions to the ratios R_{nl} and R_n defined by Eqs. (5)–(7).

States	B_{nl}	B_n
$2s$	$0.193-0.072\mu$	
$2p$	0.130	$0.323-0.072\mu$
$3s$	$(3.01-1.05\mu)(-2)$	
$3p$	$1.86(-2)$	$(5.13-1.05\mu)(-2)$
$3d$	$3.07(-3)$	
$4s$	$(1.04-0.36\mu)(-2)$	
$4p$	$0.62(-2)$	$(1.80-0.36\mu)(-2)$
$4d$	$1.35(-3)$	
$4f$	$3.9(-5)$	
$5s$	$(4.99-1.74\mu)(-3)$	
$5p$	$2.93(-3)$	$(0.86-0.17\mu)(-2)$
$5d$	$0.70(-3)$	
$6s$	$(2.77-0.95\mu)(-3)$	
$6p$	$1.63(-3)$	$(4.80-0.95\mu)(-3)$
$6d$	$0.40(-4)$	

Thus the energy-dependent parts of the ratios $R_n(\omega)$ determined by parameters B_n, are dominated by contributions of s and p states. The d states provide corrections of about 10%, while contributions of states with larger values of orbital momenta are negligibly small. The coefficients B_n are dominated by FSI which provide more than 70% of the values.

Excitation of the states with $l \geq 2$ are due to FSIs only. The cross sections of d states excitations are several times smaller than those of p states still providing noticeable contributions to parameter B_n [Eq. (71)] for $n \geq 3$. The relative role of excitation of d states slowly increases with increasing n—see Table III. Excitation of states with higher values of l drops rapidly with increasing of l. For example, the cross section for excitation of $4f$ state is about twenty times smaller than that of $4d$ state. The values of B_{nl} and B_n are presented in Table III. The energy dependence of the relative role of excitations to the states with $l>0$, expressed by the ratio $\sigma_{nl}^{+*}/\sigma^{+*}=R_{nl}/R_n$ is shown in Fig. 1.

The ratios B_n/A_n converge to certain limiting values while n increases. This is due to similar n^{-3} behavior of both characteristics at large n.

C. Comparison with earlier results

Now we compare our result with experimental and theoretical data obtained by the others. In Fig. 2 we present the ratios R_n for $2 \leq n \leq 6$, calculated in the present work and measured in Ref. [1]. We also show the results of calculations carried out in Ref. [14], where the intermediate-energy region was reached by moving from the low energies.

We see that for $n=2$ our results are in good agreement with those of Refs. [1,14] for $\omega \geq 400$ eV. As expected, there are noticeable deviations from results of Refs. [1,14] at smaller values of ω. We do not show the results of calculations for $\omega \sim 900$ eV obtained in Refs. [11,27], which are also in good agreement with those of the present paper. For $n=3$ we find a good agreement with experimental and theoretical results at all values of ω. For the cases $n=4$ and $n=5$ our results are close to those of Ref. [14], with both sets of the calculated values exceeding the experimental data at $\omega \sim 300-400$ eV. For $n=6$ the experimental results are available only for $\omega \leq 160$ eV, where the accuracy of our approach is poor since $\xi_Z^2 \geq 0.34$. However, the deviations between our results and experimental data are not large for $n=6$, as well as for the other values of n in this energy region.

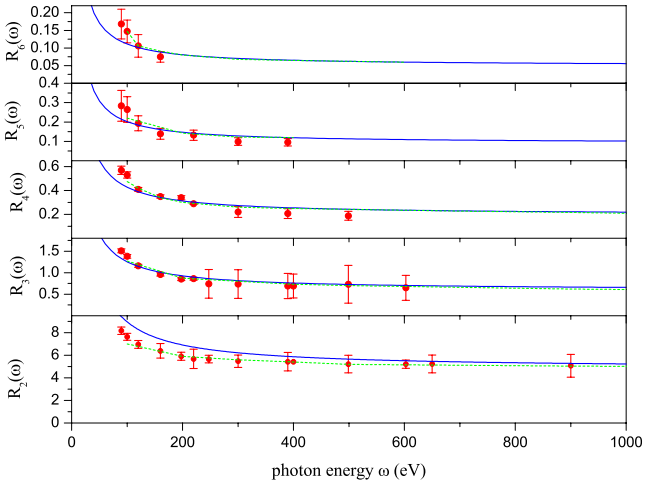

FIG. 2. (Color online) Energy dependence of the ratios R_n in 10^{-2} units for the case of helium. The dots stand for the experimental data of Ref. [1]. The solid lines show the results of the present work. The dashed lines show the results of the calculations carried out in Ref. [14].

VI. Z DEPENDENCE

A. High-energy limit

It was shown in Ref. [6] that the SU ratios A_n drop as Z^{-2} at $Z \gg 1$. The tendency is illustrated by the results of calculations for $Z \leq 10$ presented in Table IV. One can see that the convergence to Z^{-2} law becomes better for larger values of n. In Ref. [28] the Z dependence of high-energy limits for double-to-single photoionization ratio was traced and presented as a Z^{-1} series. We can write a similar presentation for the ionization followed by excitation. Assuming that A_n can be approximated by two terms of the series one has

TABLE IV. The values $A_n Z^2 \times 10^2$, with A_n defined by Eq. (9).

n	$Z=2$	$Z=3$	$Z=4$	$Z=6$	$Z=10$
2	19.1	14.9	12.8	11.4	10.4
3	2.36	2.18	2.06	1.93	1.84
4	0.781	0.749	0.722	0.692	0.660
5	0.360	0.351	0.340	0.327	0.316
6	0.197	0.193	0.188	0.182	0.176

TABLE V. The values of coefficients a_n and b_n in Eq. (53) and of coefficients c_n in Eq. (54).

n	$a_n(-2)$	$b_n(-2)$	$c_n(-2)$
2	8.9	15.0	9.2
3	1.7	1.4	1.7
4	0.61	0.48	0.64
5	0.30	0.16	0.30
6	0.17	0.08	0.17

$$A_n = \frac{a_n}{Z^2} + \frac{b_n}{Z^3}. \tag{53}$$

The values of a_n and b_n are given in Table V. The convergence of the Z^{-1} series is faster than in the case of double photoionization [28]. Also, in contrast to the double photoionization case, the leading Z^{-2} terms underestimate the values of the ratios. Note that in approach of Ref. [6], where all the interactions between the electrons where treated perturbatively,

$$A_n = \frac{c_n}{Z^2} \tag{54}$$

with c_n also presented in Table V (a numerical error was corrected in Ref. [10]). As expected, our values of a_n are close to c_n.

The results presented in Table V also illustrate the tendency to n^{-3} behavior. The values of the product $n^3 R_{ns}^{(0)}$ for $n=5$ and 6 differ by 5% for $Z=2$ and by 4% for $Z=10$.

B. Beyond the high-energy limits

In this case Eq. (3) can be written as

$$\omega \gg \frac{Z^2}{2}.$$

In order to trace Z dependence of the characteristics, we consider the limit $Z \gg 1$. Let us start with excitations of s states. One can see that in Eqs. (48) and (49) the ratio $s_1/S_n \sim 1/Z$, while $Q_n/S_1 \sim Z$, $V_n/Z \sim Z$, $W_n/S_1 \sim 1$, $U_n/S_1 \sim 1$. Thus in Eq. (5) $A_n \sim 1/Z^2$, $B_{ns} \sim 1$. Hence, we can present

$$R_{n0} = \left(1 + \frac{Z^2}{2\omega} r_{n0}\right) A_n, \tag{55}$$

with $r_{n0} = B_{n0}/Z^2 A_n$. Using Eqs. (48) and (49) we can write

$$r_{n0} = r_{n0}^d + \pi \xi_Z r_{n0}^f \tag{56}$$

with $r_{n0}^d = d_n/Z^2 A_n$ and

$$r_{n0}^f = \frac{f_n}{Z^2 A_n} = -\frac{n^2 - 1}{2n^2}. \tag{57}$$

In a similar way we can present for $l \geq 1$

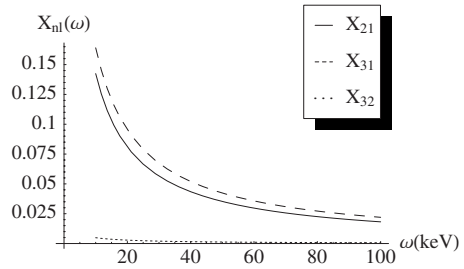

FIG. 3. Energy dependence of the relative role of excitations to the states with $l>0$, expressed by the ratio $X_{nl}=\sigma_{nl}^{+*}/\sigma_n^{+*}=R_{nl}/R_n$ for the case $Z=10$.

$$R_{nl} = \frac{Z^2}{2\omega} r_{nl} A_n, \tag{58}$$

with $r_{nl}=B_{nl}/Z^2 A_n$, while parameters B_{nl} are introduced by Eq. (6).

For the cross section ratios R_n defined by Eq. (1) we present

$$R_n = \left(1 + \frac{Z^2}{2\omega} r_n\right) A_n, \quad r_n = r_n^d + \pi \xi_Z r_n^f, \quad r_n^d = r_0^d + \sum_{\ell>0} r_{nl}, \quad r_n^f = r_{n0}^f. \tag{59}$$

For illustration we present characteristics of the process for $Z=10$. Interplay of the three types of contributions to the parameter B_{n0} describing excitation of s states is shown in Table VI. As in the case $Z=2$ the FSIs provide the main contribution. However, the domination is less pronounced than in the case of helium.

As one can see from Eq. (57), the ratios r_{n0}^f do not depend on Z. Dependence of parameters r_{nl} and r_n on Z is illustrated by the results presented in Table VII. The values of r_n^d for $Z=10$ are somewhat larger than for $Z=2$. This is mainly due to the larger contribution for excitation of p states in the case $Z=10$. On the other hand the role of excitation of d states becomes smaller—see Fig. 3. The ratio of r_n^d for $Z=2$ and $Z=10$ exhibits very weak dependence on n. The values of r_{nl} and r_n converge to certain limiting values while n increases. This is due to similar n^{-3} behavior of the parameters B_{nl} and A_n at large n.

To estimate the limiting behavior of the ratios R_n for $Z \gg 1$, note that the first term on the RHS of Eq. (7) for R_n depends on the nuclear charge as Z^{-2}. Since the values of r_n^f are several times smaller than r_n^d they can be neglected for $\pi \xi_Z \lesssim 1$. At these energies the second term contains only weak dependence on Z.

VII. SUMMARY

We have considered photoionization accompanied by excitation for helium atoms and positive two-electron ions. We focused on the case of intermediate photon energies, for which expansion of the amplitudes in powers of ω^{-1} is possible, while account of the lowest term only is not sufficient. We included the final-state interactions between the electrons

TABLE VI. Contributions of various mechanisms to the value B_n defined by Eq. (5) for the case $Z=10$, $\mu=\pi\xi_Z$.

n	Kinematical corrections	ISI	FSI	B_{n0}
2	$0.390(1-\mu)(-1)$	$1.91(-2)$	$4.96(-2)$	$0.104-0.039\mu$
3	$0.820(1-\mu)(-2)$	$0.41(-3)$	$1.00(-2)$	$(2.23-0.82\mu)(-2)$
4	$0.326(1-\mu)(-2)$	$1.56(-3)$	$3.85(-3)$	$(8.67-3.26\mu)(-3)$
5	$0.152(1-\mu)(-2)$	$0.76(-3)$	$1.91(-3)$	$(4.19-1.52\mu)(-3)$
6	$0.856(1-\mu)(-2)$	$0.43(-3)$	$1.07(-3)$	$(2.36-0.86\mu)(-3)$

in the lowest order of their Sommerfeld parameter. This enabled us to analyze the role of various mechanisms of transferring the excitation energy. We calculated the ratios R_{nl} of the cross sections σ_{nl}^{+*} for ionization, accompanied by transition of the second electron to the bound state with quantum numbers n,l to the cross section for ionization without excitations σ_{10}^{+}, and also found the sums $R_n=\Sigma_l R_{nl}$—Eq. (47), (51), and (52).

Following Ref. [17], we separated three types of contributions beyond the high-energy limit. These are the kinematical correction to the shake-up (SU) terms, and the contributions describing the transfer of excitation energy by initial-state and final-state interactions. The FSIs were included by the perturbative approach developed in Ref. [21] and employed in Ref. [24]. This enabled us to extract the energy-dependent factors, presenting the amplitudes in terms of the matrix elements containing the initial-state wave functions. The latter were obtained in Ref. [22] using the correlation function hyperspherical harmonic method. These functions were employed in atomic physics calculations earlier [23].

We carried out the calculations taking into account the next-to-leading terms of expansion in powers of ξ_Z^2. The kinematical corrections to the SU terms also depend on the parameter $\pi\xi_Z$. Dependence on this parameter was included exactly.

The cross sections for excitation of ns states have the most complicated structure. In this case we had to include kinematical corrections to SU terms. The ISI amplitudes are proportional to ξ_Z^2, and we included their interference with the SU amplitudes. The first and second order FSI amplitudes contain the factors $i\xi$ and ξ^2. Thus we had to include the interference between SU and FSI amplitudes and a purely FSI term. All the corrections should be included in the expressions for ionization cross sections without excitation σ_{10}^{+} as well. The cross section for excitation of p states was determined by ISI and FSI mechanisms, with both amplitudes being proportional to $i\xi$. Ionization accompanied by excitations to the state with $l\geq 2$ took place only due to the FSIs.

For the case of helium we found the values of the high-energy limits for $n\leq 6$ to be in agreement with those calculated by others—Table I. For excitations of ns states we found that FSIs provide the largest contributions. Excitations of np and ns states provide contributions of the same order of magnitude as the energy-dependent parts of the ratios R_n.

TABLE VII. The values of characteristics r_{n0}^d for $l=0$ and r_{nl} for $l>0$ and r_n^d defined by Eqs. (58), (55), and (56) for $Z=2$ and $Z=10$.

	$Z=2$		$Z=10$	
State	$r_{n0}^d, r_{n\ell}$	r_n^d	$r_{n0}^d, r_{n\ell}$	r_n^d
$2s$	1.01		1.00	
$2p$	0.68	1.69	1.38	2.38
$3s$	1.28		1.21	
$3p$	0.77	2.18	1.68	2.94
$3d$	0.13		0.05	
$4s$	1.33		1.31	
$4p$	0.80	2.33	1.80	3.18
$4d$	0.17		0.07	
$4f$	5.0(−3)		2.0(−3)	
$5s$	1.39		1.33	
$5p$	0.82	2.40	1.86	3.27
$5d$	0.19		0.08	
$6s$	1.40		1.34	
$6p$	0.83	2.43	1.89	3.31
$6d$	0.20		0.08	

Excitations of nd states determine a corrections of about 10% to R_n. Excitation of states with $l\geq 3$ are negligibly small—Tables II and III. For atomic helium we carried out detailed comparison with earlier experimental and theoretical results. We found good agreement at $\omega\geq 400$ eV for $n=2$ and even at smaller values of ω for the larger values of n—Fig. 2.

For larger Z we found an approximate formula (53), which presents the high-energy limits in the form of the Z^{-1} series, with the leading terms of expansion being consistent with the earlier results [6,10]. Excitation of ns states beyond the high-energy limit is still dominated by the FSIs. The role of excitation of the states with $l=1$ increases, e.g., for $Z=10$ transitions to np states provide the largest contribution to the energy-dependent part of R_n. The role of excitation of nd states drops with Z. These results are illustrated by Table VII and Fig. 3. In the limit $Z\gg 1$ the ratios R_n can be presented as the sums of two terms. The high-energy limit term does not depend on ω, dropping with Z as Z^{-2}. The second term drops as ω^{-1}, varying with Z slowly.

For the case of helium, as well as for the ions with larger values of Z, the contribution of ISIs to the ratios R_n is about 10%. Hence, the ratios R_n are determined by the kinematical corrections to SU and by the FSIs.

ACKNOWLEDGMENTS

One of us (E.G.D.) is thankful for the hospitality during the visit to Hebrew University. M.Ya.A. is grateful for support by the ISF Grant No. 134.03 and by the Hebrew University Intramural Funds.

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