

High-frequency two-electron photoionization cross section of triplet statesR. Krivec,¹ M. Ya. Amusia,^{2,3} and V. B. Mandelzweig²¹*Department of Theoretical Physics, J. Stefan Institute, P.O. Box 3000, 1001 Ljubljana, Slovenia*²*Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel*³*Ioffe Physico-Technical Institute, St. Petersburg, 194021, Russia*

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Using high precision wave functions describing the triplet ground and excited 3S states of the He atom and heliumlike ions, the cross sections of single- and double-electron photoionization are calculated. The dependence of the ratio R of the double and single ionization cross sections on the nuclear charge Z and the principal quantum number of excitation n is studied. The results obtained are compared to those for previously studied singlet states.

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I. INTRODUCTION

This paper presents the results of calculations of the photoionization cross sections with elimination of one or both electrons from two-electron atomic systems in their triplet excited 3S states: the He* atom and the corresponding excited heliumlike two-electron ions. We study excited states that can be roughly considered monopole, i.e., s excitations of one of the electrons. In the one-electron approach all these 3S states can be described as $1s, ns$ configurations with $n > 2$. We concentrate on high photon frequencies $\omega \gg I^{++}$, where I^{++} is the two-electron ionization potential. The problem of the photoionization cross section of helium and heliumlike ion triplet states was recently discussed in Ref. [1]. A highly precise variational wave function was used to calculate the cross sections and their ratios. This wave function was calculated with the Correlation Function Hyperspherical Harmonic Method (CFHHM) and contains all the necessary logarithmic terms of the Fock expansion, which are computed directly from the three-body Schrödinger equation. The aim of this paper is to study the photoionization cross sections and their ratios, and their dependence on the nuclear charge Z and the principal quantum number n of the target object initial state. Our first priority is to see to which extent the results obtained in Ref. [1] are sensitive to the wave function. Therefore, in this paper a completely different, non-variational, and locally correct, wave function calculated in Refs. [2–4] was used.

We shall also consider some ratios that were not directly addressed in Ref. [1]. We chose those that emphasize the peculiarities of the double-electron photoionization of the triplet states more clearly than the usually considered double-to-single ionization cross sections.

The interest for the problem of elimination of two electrons by a single photon goes back to the late 60s and early 70s of the last century [5–8]. It has remained being motivated by the fact that without interaction between atomic electrons, the ejection of two electrons by a single photon is impossible. So studying this process reveals valuable information on the effects of electron interaction inside an atom. Eight to nine years ago the revived interest in this problem sparked an explosion of activity (see Refs. [9–15] and references therein). The research is summarized and a number of

new results presented in a recent book [16]. Such intensive development has been stimulated by the progress in experimental possibilities for measuring the yield of double-charged ions and thus the two-electron ionization cross section, particularly at high energies. The ratio of the yields of He⁺⁺ and He⁺ was measured in a broad photon frequency region, up to 20 keV [17].

However, most research concentrated on singlet states (1S), in which the electron spins are antiparallel and the Pauli principle does not prevent the electrons from coming close to each other. In the 3S states the electron spins are parallel, so the Pauli principle prevents them from approaching each other. Therefore, the effects of electron interaction are expected to be considerably, if not qualitatively, different. These effects are additionally suppressed in the lowest-energy 3S states, because the two electrons in such states have different principal quantum numbers: $1s$ and $2s$ instead of $1s^2$ in the 1S state of He. Despite the theoretical and experimental interest for the 3S states, until now there has been only one paper [1] dedicated to their double-electron photoionization [29].

For two-electron systems in the high but nonrelativistic frequency [30] limit, the cross section of the two-electron ionization $\sigma^{++}(\omega)$, the ionization with excitation $\sigma^{+*}(\omega)$, and the one-electron ionization $\sigma^+(\omega)$ are entirely determined by the initial state wave function with one electron at the nucleus (see, e.g., Ref. [18]). So the profound difference between the wave functions of the 3S and 1S states will be reflected in the above-mentioned cross sections. Using very accurate and locally correct [2–4] initial state wave functions, one expects to get precise values for the cross sections. Studying the cross section dependence on Z and n reveals how the variation of the mean interelectron distance (measured in units of the $1s$ orbit radius) affects the probability of the two-electron ionization or ionization with excitation. By comparing the results of this paper with the results for the 1S states (see, e.g., Refs. [19,20]), it will be possible to observe the changing role of the electron interaction when going from the 1S to the 3S ground state.

There is a qualitative difference between the 3S and the 1S states: the asymptotic ratios for triplet states, valid at any photon energy ω including $\omega \gg c^2$, are expressed via the initial state wave function with one electron at the nucleus. In

contrast, the high frequency ($\omega \gg c^2$) ratios for the singlet states are determined mainly by the initial state wave function with both electrons at the same point anywhere inside the atom, not only at the nucleus (see Ref. [21] and references therein). The nonrelativistic asymptotics for 1S states, expressed via the wave function with one electron at the nucleus (see, e.g., Refs. [19,20] and [1]), have corrections of the order of ω/c^2 that become noticeable, for helium, starting already from $\omega = 10$ keV [22].

At a first glance, the system of two electrons in the field of a nucleus seems to be quite simple. However, despite the progress in computational power, it is still an unsolved problem to find accurate enough continuous spectrum wave functions for this system. Accurate wave functions can be obtained only for its ground and low-lying excited states. Therefore, it is of particular interest to study the high-energy cross sections, which are expressible solely via bound-state wave functions that are reliably established. It is also essential to note [18] that the ω dependence of the cross sections at high ω is known and depends not on the initial state wave function but on the angular momentum of the eliminated electrons. Therefore, a given initial state wave function is able to describe the single and double ionization and ionization with excitation cross sections in a broad photon frequency region $\omega \gg I^{++}$.

The Z dependence of the high-energy double-electron photoionization cross section was considered in Ref. [23] and then discussed in a number of papers, e.g., in Ref. [9].

The interest for the double-ionization process is not purely theoretical: it was shown that it is possible to separate experimentally the contributions to two-electron ionization and ionization with excitation caused by either photon absorption or by scattering (Compton effect) [24]. This is of great importance for investigations at high ω since the cross sections of the latter processes, $\sigma_C^{++}(\omega)$, $\sigma_C^{+*}(\omega)$, and $\sigma_C^+(\omega)$, are almost independent of ω while the cross sections of photoionization are rapidly decreasing with ω . The cross sections of 1S and 3S states have the same asymptotic dependence on ω : $\sim \omega^{-7/2}$, but the coefficients in front of $\omega^{-7/2}$ are considerably different even for $\sigma^+(\omega)$. For the helium 1S state, these cross sections become equal at approximately 6 keV [25] and we have checked that the same is valid for 3S . For the same state, the two-electron ionization Compton scattering starts to dominate over photoionization even at considerably smaller energies.

One should keep in mind that the 3S state in helium has a long lifetime of about 11 minutes. Although with increasing Z this time decreases rapidly in the heliumlike ions, the experimentation with these objects seems to be possible in principle. Considering the fact that several sources of high-intensity, high-frequency, continuous spectrum electromagnetic radiation have been or are being constructed, a growing interest for more detailed studies of two-electron processes can be anticipated. It is quite probable that not only the lowest energy metastable state 3S of two-electron systems but also excitations of the $1s, ns$ 3S type, of neutral atoms and positive ions, will attract attention. This is why we concentrate here on 3S states of the helium atom and the heliumlike

ions, in their lowest energy and $1s, ns$ ($n > 2$) states.

In view of the differences between the 3S and 1S states explained above, qualitative differences of $\sigma^{++}(\omega)$, $\sigma^{+*}(\omega)$, and $\sigma^+(\omega)$ between these states are quite natural. In particular, one expects much larger $\sigma^{+*}(\omega)$ since the outer electron in 3S has (for the same n) a weaker binding than in the 1S state. Of special interest is the comparison of these cross sections for the excited configuration $1s, 2s$, belonging to states 3S and 1S . Another object of our study will be the deexcitation process: the transition of the excited electron without spin and angular momentum change to states with lower principal quantum number $n \rightarrow n'$ ($n' < n$).

Note that along with the 3S states there exists another group of triplet metastable states, namely, 3P , which, however, will not be considered in this paper. The method to obtain the 3P wave function is different from that for 3S and we plan to discuss this issue on another occasion.

Since the ω dependencies of $\sigma^{++}(\omega)$, $\sigma^{+*}(\omega)$, and $\sigma^+(\omega)$ at high ω are the same, it is convenient to study, just as it was done for the 1S states, the ω -independent ratios

$$R^{(3)} = \frac{\sigma^{(3)++}(\omega)}{\sigma^{(3)+}(\omega) + \sigma^{(3)+*}(\omega)} \Bigg|_{\omega \rightarrow \infty}, \quad (1)$$

$$R^{(3)*} = \frac{\sigma^{(3)+*}(\omega)}{\sigma^{(3)+}(\omega)} \Bigg|_{\omega \rightarrow \infty}, \quad (2)$$

$$R_0^{(3)} = \frac{\sigma^{(3)++}(\omega)}{\sigma^{(3)+}(\omega)} \Bigg|_{\omega \rightarrow \infty} = R^{(3)}(1 + R^{(3)*}), \quad (3)$$

and

$$R_1^{(3)} = \frac{\sigma^{(3)+}(\omega) + \sigma^{(3)++}(\omega) + \sigma^{(3)+*}(\omega)}{\sigma^{(3)+}(\omega)} \Bigg|_{\omega \rightarrow \infty} = (1 + R^{(3)})(1 + R^{(3)*}). \quad (4)$$

The notation of our previous papers [19,20] where 1S states were treated is used; the triplet nature of the states is noted by the superscript 3 in parentheses.

One can expect that the ratio $R_n^{(3)}$ decreases with Z , since the mean interelectron radius measured in units of the $1s$ electron orbit increases, causing the relative role of the interelectron interaction that causes double ionization to decrease. Qualitatively one can expect also that $R^{(3)*}$ will increase with n since the main mechanism of ionization with excitation is shake off [18].

The leading order of the Z dependence of $R^{(3)}$ for $Z \gg 1$ is very simple: $R^{(3)} \sim Z^{-2}$ [23], just as that of R in singlet states. The estimate $\sim Z^{-2}$ can be easily obtained in the first order of the interelectron interaction. However, as we saw for the 1S state with $n \geq 2$, this Z^{-2} dependence starts only at $Z \geq 8-10$. In this paper, we shall obtain numerical coefficients in front of Z^{-2} for all considered states and objects, using extrapolation in Z .

We shall calculate here $R^{(3)}$ and $R^{(3)*}$ employing specially calculated accurate and locally correct [2–4] initial state wave functions, using the CFHHM. This same method has recently been applied by us [19,20] to calculate the corresponding ratios for 1S states. In this method, the initial 3S state wave function $\Psi_i^{(3)}$ is decomposed as

$$\Psi_i^{(3)} = e^f \phi, \quad (5)$$

where f is the *correlation function* describing the singularities of $\Psi^{(3)}$ and ϕ is a smooth remainder, which can be expanded in a fast converging hyperspherical harmonic (HH) expansion. The function f depends on the interparticle distances, which 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 [26] exactly. $\Psi^{(3)}$ is obtained by a direct solution of the three-body Schrödinger equation guaranteeing local correctness [2–4] of $\Psi_i^{(3)}$ because the convergence of $\Psi_i^{(3)}$ across the configurations space is uniform.

II. DETAILS OF CALCULATIONS

To obtain the expressions for the ratios $R_i^{(3)}$ and $R_i^{(3)*}$, we use the rather general approach presented in Ref. [18]. Keeping in mind that for high ω the main contribution to $\sigma_i^{(3)++}(\omega)$ comes from the strongly asymmetric energy sharing between the outgoing electrons of which one is fast while the other is slow, simplifies considerably the expression for $\sigma_i^{(3)++}(\omega)$, which is basically the same for the 3S and 1S states:

$$\sigma_i^{(3)++}(\omega) \approx \frac{32\sqrt{2}Z^2\pi^2}{3c\omega^{7/2}} \left\{ \int |\Psi_i^{(3)}(0,\mathbf{s})|^2 d\mathbf{s} - \sum_{\nu lm} \left| \int \Psi_i^{(3)}(0,\mathbf{s}) \psi_{\nu lm}(\mathbf{s}) d\mathbf{s} \right|^2 \right\}, \quad (6)$$

where $\Psi_i^{(3)}$ is the initial 3S state three-body wave function and $\psi_{\nu lm}(\mathbf{s})$ is the unperturbed single-particle wave function of the second electron in the field of the nucleus, after the first electron has left. $\Psi_i^{(3)}$ depends on the Jacobi coordinates \mathbf{r} and \mathbf{s} , where \mathbf{r} connects the nucleus and one electron, and \mathbf{s} connects the center of mass of these two particles with the other electron. In the framework of the present approximation, we set $\mathbf{r}=0$; then \mathbf{s} represents the distance of the second electron from the nucleus. Thus, $\Psi_i^{(3)}(0,\mathbf{s})$ represents the three-body wave function at the coalescence, or cusp, region, in which, as one can see from the discussion in the Introduction and from references cited there, high accuracy of the wave function is especially difficult to obtain. ν is the single-particle principal quantum number, l and m are the angular momentum quantum numbers, and c is the speed of light.

As shown in Ref. [18] we have the following expressions for the total angular momentum $L=0$ and $\omega \rightarrow \infty$, again basically the same for the 3S and 1S states:

$$\sigma_i^{(3)++}(\omega) = \frac{32\sqrt{2}Z^2\pi^2}{3c\omega^{7/2}} \left(\langle \delta(\mathbf{r}) \rangle_i^{(3)} - \sum_{\nu} I_{i\nu 0}^{(3)} \right), \quad (7)$$

where $\langle \delta(\mathbf{r}) \rangle_i^{(3)}$ is the expectation value of the operator $\delta(\mathbf{r})$ in the 3S state and

$$I_{i\nu 0}^{(3)} = 4\pi \left| \int_0^\infty \Psi_i^{(3)}(0,s) R_{\nu 0}(qs) s^2 ds \right|^2, \quad (8)$$

where $q=2Zm_\alpha/(1+m_\alpha)$ and $R_{\nu l}$ are the one-electron bound state Coulomb radial functions.

The total photoabsorption cross section $\sigma_i^{(3)}(\omega)$ can be measured experimentally and is given by

$$\begin{aligned} \sigma_i^{(3)}(\omega) &\equiv \sigma_i^{(3)+}(\omega) + \sigma_i^{(3)++}(\omega) + \sigma_i^{(3)+*}(\omega) \\ &= \frac{32\sqrt{2}Z^2\pi^2}{3c\omega^{7/2}} \langle \delta(\mathbf{r}) \rangle_i^{(3)} = \frac{A_i^{(3)}(Z)}{\omega^{7/2}}. \end{aligned} \quad (9)$$

The asymptotic value of $A_i^{(3)}(Z)$ can be estimated from rather simple considerations, taking into account that the main contribution to $\sigma_i^{(3)}(\omega)$ is determined by the ionization of the inner, nonexcited electron. Indeed, the photoabsorption cross section of an electron in the state ns can be estimated as $\sigma_i(\omega) \sim I_i^{5/2}/\omega^{7/2}$, where I_i is the i th electron ionization potential. Thus, the asymptotic contribution of the outer (o) and inner (i) electrons is estimated as $\sigma_o(\omega)/\sigma_i(\omega) \sim (I_o/I_i)^{5/2}$. The ratio I_o/I_i can be estimated as $I_o/I_i \sim (n_i/n_o)^2$, so that $\sigma_o(\omega)/\sigma_i(\omega) \sim (n_i/n_o)^5 \ll 1$ even for $n_i=1$ and $n_o=2$. So with increasing excitation principal quantum number $n_o \geq 2$ the outer electron's contribution becomes negligible and the coefficient $A_i^{(3)}(Z)$ can be calculated in the hydrogenic approximation (see, for example, Ref. [18]):

$$A_i^{(3)}(Z) = 16\sqrt{2}\pi Z^5/3cn_i^5 \sim 0.17291Z^5/n_i^5. \quad (10)$$

The other quantity that can, in principle, be measured in experiment, which counts the number of produced single-charged ions, is given by the sum [18]

$$\sigma_i^{(3)+}(\omega) + \sigma_i^{(3)+*}(\omega) = \frac{32\sqrt{2}Z^2\pi^2}{3c\omega^{7/2}} \sum_{\nu} I_{i\nu 0}^{(3)}, \quad (11)$$

so that

$$R_i^{(3)} = \frac{\langle \delta(\mathbf{r}) \rangle_i^{(3)} - \sum_{\nu} I_{i\nu 0}^{(3)}}{\sum_{\nu} I_{i\nu 0}^{(3)}} \quad (12)$$

and

$$R_i^{(3)*} = \frac{\sigma_i^{(3)+*}(\omega)}{\sigma_i^{(3)+}(\omega)} = \frac{\sum_{\nu} I_{i\nu 0}^{(3)} - I_{i0}^{(3)}}{I_{i0}^{(3)}} = \frac{\sum_{\nu \geq 2} I_{i\nu 0}^{(3)}}{I_{i0}^{(3)}}. \quad (13)$$

TABLE I. $B_n^{(3)}(Z)$ values for the n^3S states in the helium iso-electronic sequence, in a.u.

Z	n			
	2	3	4	5
2	0.1938	0.0486	0.0190	0.0093
3	2.495	0.6737	0.2720	0.1357
4	13.05	3.626	1.484	0.7459
5	44.82	12.65	5.212	2.631
6	120.2	34.24	14.17	7.175
7	273.6	78.44	32.57	16.52
8	554.0	159.6	66.40	33.72
9	1028.0	297.0	123.8	62.93
10	1781.0	516.0	215.4	109.6

The two other ratios, namely, $R_{0i}^{(3)}$ and $R_{1i}^{(3)}$, are expressed via $R_i^{(3)}$ and $R_i^{(3)*}$, using Eqs. (3) and (4), respectively.

Of special interest is the single-electron photoionization cross section $\sigma_i^{(3)+}(\omega)$, which is determined by the following expression:

$$\sigma_i^{(3)+}(\omega) = \frac{32\sqrt{2}Z^2\pi^2}{3c\omega^{7/2}} I_{ii0}^{(3)} \equiv \frac{B_i^{(3)}(Z)}{\omega^{7/2}}, \quad (14)$$

and it is interesting to compare it with $\sigma_i^+(\omega)$ from Ref. [19]. It is natural to expect that $\sigma_i^{(3)+}(\omega)/\sigma_i^+(\omega) = I_{ii0}^{(3)}/I_{ii0} \gg 1$, since the binding of the outer electron in the triplet states is smaller than that in the singlet states.

As was mentioned above, the two-electron ionization at high energies is determined mainly by the mechanism in which almost all photon energy is accepted by one electron, while the second leaves the atom slowly. On qualitative grounds one can foresee that for high ω the cross section $\sigma_i^{(3)+*}(\omega)$, determined by the expression

$$\sigma_i^{(3)+*}(\omega) = \frac{32\sqrt{2}Z^2\pi^2}{3c\omega^{7/2}} \sum_{\nu \neq i} I_{i\nu 0}^{(3)}, \quad (15)$$

will be larger than $\sigma_i^{(3)+}(\omega)$. Indeed, the photon is absorbed by the electron on the $1s$ level acquiring almost all ω , while

TABLE II. $A_n^{(3)}(Z)$ values for the n^3S states in the helium iso-electronic sequence, in a.u.

Z	n			
	2	3	4	5
2	5.739	5.585	5.554	5.544
3	44.63	42.72	42.31	42.16
4	190.6	180.8	178.6	177.9
5	586.5	553.4	545.7	543.1
6	1468.0	1380.0	1359.0	1352.0
7	3186.0	2986.0	2940.0	2923.0
8	6231.0	5829.0	5734.0	5701.0
9	11256.0	10512.0	10337.0	10275.0
10	19100.0	17815.0	17511.0	17404.0

TABLE III. $I_{n\nu 0}^{(3)}$ values for the lowest n^3S states of He* ($Z=2$).

ν	n			
	2	3	4	5
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

the second electron is “shaked” to one of the nearest upper levels, thus going from ns to $n's$, with $n' > n$.

It has been demonstrated already long ago in Ref. [23] (see also Ref. [27]) that there exists the so-called *quasifree* (QF) mechanism, which leads to emission of both electrons with comparable energies. The QF mechanism leads to R increasing with ω , up to ultrarelativistic energies $\omega \gg c^2$ where R again becomes constant but with a much larger value. For not too high ω the QF mechanism leads to a correction of the first order in $\omega/c^2 \ll 1$ [23,27,28], which can be expressed via $\Psi_i^{(3)}(\mathbf{r}, \mathbf{r})$. The same is valid for ultrarelativistic corrections (see Ref. [21] and references therein). But according to the Pauli principle $\Psi_i^{(3)}(\mathbf{r}, \mathbf{r}) = 0$, so that in the triplet state the term $\sim \omega/c^2$ as well as ultrarelativistic corrections disappear, contrary to the case of the singlet state [22].

III. RESULTS OF CALCULATIONS

The calculated values of $A_i(Z), B_i(Z), \zeta_i(Z) = A_i(Z)/B_i(Z), I_{i\nu 0}^{(3)}$ and of different cross section ratios $R_i^{(3)}, R_i^{(3)*}, R_{0i}^{(3)}$, and $R_{1i}^{(3)}$ for the ground $i \equiv n=2$ and excited states $n^3S, n=3,4,5$ of He* and its isoelectronic sequence $Z=2-10$ are presented in Tables I–VII.

TABLE IV. $R_n^{(3)}(Z) \times 10^3$ and $\eta_n(Z)$ values for the n^3S states in the helium isoelectronic sequence.

Z	n							
	2		3		4		5	
	$R_2^{(3)}$	η_2	$R_3^{(3)}$	η_3	$R_4^{(3)}$	η_4	$R_5^{(3)}$	η_5
2	3.116	0.35	1.965	0.53	1.043	0.62	0.573	0.65
3	3.040	0.25	3.662	0.44	3.076	0.56	2.332	0.65
4	2.222	0.22	3.420	0.40	3.526	0.52	3.198	0.60
5	1.615	0.21	2.811	0.39	3.218	0.50	3.211	0.58
6	1.209	0.20	2.262	0.38	2.755	0.49	2.911	0.57
7	0.933	0.20	1.830	0.37	2.321	0.48	2.546	0.56
8	0.739	0.20	1.500	0.37	1.957	0.48	2.204	0.56
9	0.599	0.19	1.247	0.37	1.660	0.48	1.906	0.55
10	0.495	0.19	1.050	0.37	1.421	0.48	1.655	0.55

TABLE V. Comparison of $R_n^{(3)}(Z) \times 10^3$, $\eta_n(Z)$, $R_n^{ur(1)}(Z) \times 10^3$, and $\eta_n^{ur}(Z)$ values for the helium isoelectronic sequence.

Z	n							
	2		2		3		3	
	$R_2^{(3)}$	η_2	$R_2^{ur(1)}$	η_2^{ur}	$R_3^{(3)}$	η_3	$R_3^{ur(1)}$	η_3^{ur}
2	3.116	0.35	15.69	1.74	1.965	0.53	5.59	1.51
3	3.040	0.25	18.44	1.53	3.662	0.44	10.23	1.23
4	2.222	0.22	14.92	1.50	3.420	0.40	10.01	1.18
5	1.615	0.21	11.48	1.49	2.811	0.39	8.45	1.16
6	1.209	0.20	8.90	1.50	2.262	0.38	6.90	1.15
7	0.933	0.20	7.03	1.50	1.830	0.37	5.64	1.15
8	0.739	0.20	5.67	1.50	1.500	0.37	4.65	1.15
9	0.599	0.19	4.66	1.51	1.247	0.37	3.88	1.14
10	0.495	0.19	3.89	1.51	1.050	0.37	3.28	1.14

We found that most of the results can be obtained with a small HH basis with $K_m=40$, for lower states even with $K_m=32$. Here K_m is the maximum global angular momentum used in the HH expansion. As Z decreases towards 2(He*), the excited states assume a true three-body character, their spectrum becomes dense, and their spatial extents become similar, so their properties can no longer be estimated by scaling in Z from large Z , and K_m up to 100 is necessary to get accurate higher excited states. We also used extrapolation in K_m for all states, relying on checked power-type convergence.

The ratios $R_i^{(3)}$ for $n=2,3,4$ calculated in Ref. [1] disagree with ours at $Z=2$, where the rounded values differ by 2×10^{-6} ($n=2,3$) and 1×10^{-6} ($n=4$); for $Z>2$ Ref. [1] gives values rounded up to one place less and these agree with us.

To calculate the cross section ratios, we have used 200 single-particle states and a stable extrapolation in their number, so that the error of summation over states is negligible and we do not have to resort to estimating the remainder as in Ref. [19].

According to Eq. (15), the cross section $\sigma_i^{(3)+}(\omega)$ is totally characterized by the values of $B_i^{(3)}(Z)$, which are pre-

TABLE VI. $R_n^{(3)*}(Z)$ and $\eta_n^*(Z)$ values for the n^3S states in the helium isoelectronic sequence.

Z	n							
	2		3		4		5	
	$R_2^{(3)*}$	η_2^*	$R_3^{(3)*}$	η_3^*	$R_4^{(3)*}$	η_4^*	$R_5^{(3)*}$	η_5^*
2	28.53	1.5	113.79	1.6	291.18	1.6	595.76	1.6
3	16.83	1.3	62.19	1.3	154.06	1.4	309.04	1.4
4	13.58	1.2	48.70	1.2	118.96	1.3	236.66	1.3
5	12.06	1.2	42.63	1.2	103.37	1.2	204.73	1.2
6	11.20	1.2	39.20	1.2	94.63	1.2	186.89	1.2
7	10.63	1.1	37.00	1.1	89.05	1.1	175.55	1.1
8	10.24	1.1	35.47	1.1	85.19	1.1	167.71	1.1
9	9.95	1.1	34.35	1.1	82.36	1.1	161.97	1.1
10	9.72	1.1	33.49	1.1	80.19	1.1	157.60	1.1

TABLE VII. $R_{1n}^{(3)}$ values for the n^3S states in the helium isoelectronic sequence.

Z	n			
	2	3	4	5
2	29.62	115.0	292.5	597.1
3	17.89	63.42	155.5	310.8
4	14.61	49.87	120.4	238.4
5	13.09	43.75	104.7	206.4
6	12.21	40.29	95.89	188.4
7	11.64	38.07	90.26	177.0
8	11.25	36.53	86.36	169.1
9	10.95	35.39	83.49	163.3
10	10.73	34.52	81.31	158.9

sented in Table I. The values of $A_i^{(3)}(Z)$ are collected in Table II. Table III displays the results of $I_{n\nu_0}^{(3)}$ for the lowest He* 3S state. The values of the ratios $R_i^{(3)}$, $R_i^{(3)*}$, $R_{1i}^{(3)}$, and $R_{0i}^{(3)}$ for the states n^3S , $n=2, \dots, 5$ of the helium isoelectronic sequence from $Z=2$ to $Z=10$ are presented in Tables IV, V, VI, VII, and VIII, respectively.

As is seen from Table I, the parameter $B_n^{(3)}(Z)$ depends strongly on Z and n , rapidly decreasing with n and impressively increasing with Z . Note that the cross section $\sigma_n^{(3)+}(\omega)$ is considerably smaller than $\sigma_n^+(\omega)$ obtained in Ref. [19]. In general, since in the triplet state the average distance between electrons is larger than that in the singlet state, the effects of the interelectron interaction in 3S is weaker, and the corresponding effects are smaller. This can be seen from comparing the results of this paper with those from Ref. [19].

Table II demonstrates the magnitude of $\sigma_n^{(3)}(\omega)$, which is at least by an order of magnitude larger than $\sigma_n^{(3)+}(\omega)$. This emphasizes the relatively low probability of a process in which the state of the outer electron remains unaltered while the inner one is ionized. The value of $A_n^{(3)}(Z)$, starting from $Z=3-4$ follows the $1/Z^5$ relation in Eq. (14). Indeed, for $Z=10$, Eq. (14) gives $A_2^{(3)}(10) \sim 17291$, which is quite close to the corresponding value in Table II, 19100. For $Z=2$, $A_2^{(3)He} \sim 5.533$, which is very close to the tabulated

TABLE VIII. $R_{0n}^{(3)}(Z)$ values for the n^3S states in the helium isoelectronic sequence.

Z	n			
	2	3	4	5
2	0.0920	0.2254	0.3048	0.3421
3	0.0542	0.2314	0.4771	0.7232
4	0.0324	0.1700	0.4230	0.7602
5	0.0211	0.1226	0.3359	0.6606
6	0.0147	0.0909	0.2635	0.5470
7	0.0108	0.0696	0.2090	0.4495
8	0.0083	0.0547	0.1687	0.3718
9	0.0066	0.0441	0.1384	0.3106
10	0.0053	0.0362	0.1153	0.2625

value of 5.74. Note that the corresponding values for a given Z are slowly decreasing with n , which is the consequence of a small contribution of the outer electron to $A_n^{(3)}(Z)$. This is understandable since the outer electron asymptotic photoionization cross section, according to Eq. (14), decreases rapidly, as $\sim n^{-5}$, with n .

Table III demonstrates that after photon absorption, the most probable transition is that of the outer electron to one of the nearest excited levels. Indeed, one can see that for $n=2$ the probability for the second electron to remain on the same level is the largest ($I_{220}^{(3)}=1.033$), while to be excited to the next level it is noticeably smaller ($I_{230}^{(3)}=0.2287$). Note, however, that ionization with deexcitation, i.e., with transition to the level $1s$, is much smaller ($I_{210}^{(3)}=0.04458$). For $n>2$ the probability for the second electron to remain at its initial level decreases rapidly, while the most probable process becomes the excitation to the next level ($n \rightarrow n+1$) and, for higher n , even to $n+2$. The deexcitation (the transition $n \rightarrow n-1$) probability is always much smaller.

According to Table IV the cross section ratio $R_n^{(3)}(Z)$ for $n=2$ decreases with Z monotonically, while for $n \geq 2$ it first increases and then decreases. It is seen that the ratio $\eta_n(Z) \equiv R_n^{(3)}(Z)/R_n(Z)$ [the data for $R_n(Z)$ are from Table II of Ref. [20]] is considerably smaller than 1. This fact demonstrates that for the triplet state the role of ionization with excitation is even greater than for excited singlet states. For $Z>2$ and $n>2$ the variation of $R_n^{(3)}(Z)$ is relatively small. From an experimental point of view, we observe here very good agreement with the results obtained using the variational wave function, since the results of Ref. [1] and of the present paper are currently impossible to distinguish experimentally. However, despite using the same equations we detected a noticeable numerical difference of about 0.1–0.2%, which is far larger than expected from the accuracies of the wave functions used by us and in Ref. [1]. This means that the results are sensitive to the fact that the wave functions are locally somewhat different.

We also calculated the dependence of $R_n^{(3)}(Z)$ on Z , not only for $n=2$ as in Ref. [1], but also for $n=3,4,5$. The latter turned out to be qualitatively different from the $n=2$ case.

As was explained in the Introduction, the relativistic asymptotics of $R_n^{ur(1)}$ for $1S$ states [21] differs considerably from the corresponding nonrelativistic values $R_n^{(1)}$ obtained earlier (see Refs. [20] and [1]). Therefore, Table V presents the results of calculations for $R_n^{(3)}(Z)$, $\eta_n(Z)$, $R_n^{ur(1)}$, and $\eta_n^{ur}(Z) \equiv R_n^{(3)}(Z)/R_n^{ur}(Z)$. An impressive difference due to relativistic effects is clearly seen.

Table VI presents the data for $R_n^{(3)*}(Z)$, which are everywhere much larger than 1, up to two orders of magnitude, demonstrating that excitation with ionization is much more probable than the single-electron ionization. The latter proceeds, for excited states at high ω , via a rather improbable process: ionization of the $1s$ electron with subsequent transition of the excited ns electron into the $1s$ state. Table VI presents also the ratio $\eta_n^*(Z) \equiv R_n^{(3)*}(Z)/R_n^*(Z)$ [the data for $R_n^*(Z)$ are from Table III of Ref. [20]], which is everywhere considerably larger than 1. As it was expected, $R_n^{(3)*}(Z)$ for

all n decreases with Z . For a given Z , the increase is really rapid, by a factor of about 20 when n goes from 2 to 5.

It seems that $R_n^{(3)*}(Z)$ emphasizes explicitly the relative role of ionization with excitation relative to the single ionization. For the first time we demonstrate clearly the dominance of ionization with excitation. According to Eqs. (1) and (2), the ratios $R_n^{(3)*}(Z)$ and $R_n^{(3)}(Z)$ are algebraically independent.

Now we turn to the calculation of the ratios $R_{1n}^{(3)*}$ and $R_0^{(3)}$. Although according to Eqs. (3) and (4) they can be expressed algebraically via $R_n^{(3)*}(Z)$ and $R_n^{(3)}(Z)$, these ratios are instructive since they present the ratios of double and total ionization cross sections to the pure single-electron ones. They emphasize clearly the relative role of double ionization and ionization with excitation.

The values of $R_{1n}^{(3)}$ in Table VII are close to those of $R_{1n}^{(3)*}$ in Table VI, since for the triplet state $\sigma_n^{(3)+*}(\omega)$ is much larger than both of $\sigma_n^{(3)+}(\omega)$ and $\sigma_n^{(3)++}(\omega)$. Interesting is the tendency of “saturation” of the values in Tables VI and VII with increasing Z that obviously approach the asymptotic $Z \rightarrow \infty$ limits. The corresponding values are increasing with n . This is a direct consequence of $\sigma_n^{(3)+}(\omega)$ decreasing with n .

Table VIII presents the results for $R_{0n}^{(3)}(Z)$. From the behavior of $R_0^{(3)}$ it is seen that the excitation of one of the electrons in helium or in the heliumlike ions increases the relative probability of double ionization, but by far not so strongly as that of the ionization with excitation. Note that with growing n , $R_{0n}^{(3)}(Z)$ increases and finally exceeds 0.76. This indicates that the two-electron ionization can become more probable than one-electron ionization. This is, in fact, a manifestation of the competition between two processes: ionization with excitation and ionization with deexcitation to the one-electron state $1s$, the outcome of which depends mainly on n , but also on Z .

In Refs. [1,23] the leading term of the Z dependence of R was estimated and shown to be $1/Z^2$. Our calculations in this paper demonstrate that for $R_n^{(3)}$ with $n=2$, $R_2^{(3)}$, the Z^{-2} dependence already appears only for $Z>4$. For larger n , the Z value at which the Z^{-2} dependence starts is increasingly higher.

To reveal the Z^{-2} dependence and to find the asymptotics at $Z \rightarrow \infty$ one can use three-term fits in inverse powers of Z but it is necessary to go to higher values of Z , $Z>10$, particularly for $n>3$.

IV. CONCLUSION

The cross sections $\sigma_n^{(3)}(\omega)$ and $\sigma_n^{(3)+}(\omega)$, the parameter $I_{i\nu 0}^{(3)}$, and the ratios $R_n^{(3)}$, $R_n^{(3)*}$, $R_{1n}^{(3)}$, and $R_{0n}^{(3)}$ have been calculated for the n^3S states, $n=2, \dots, 5$, of the helium isoelectronic sequence from $Z=2$ to $Z=10$. The peculiarities of these values as functions of Z and n were discussed at length. It was demonstrated that the ratios $R_n^{(3)}$ for the ground state decrease very fast with Z . But already starting from $R_3^{(3)}$, these ratios at first increase with Z and only after reaching a maximum start to decrease. Specifically, $R_n^{(3)*}$ increases dra-

matically with n for any Z . The Z dependence of $R_n^{(3)*}$ proved to be qualitatively the same for all n , exhibiting a not too fast decrease with Z growth.

In the helium ($Z=2$) case, it was necessary to employ a nonlinear correlation function f in Eq. (5) to calculate the cross sections and the corresponding ratios, but for $Z>2$ a simple linear f and a rather small value of $K_m=32$ (81 HH states) were sufficient for most states, except for the higher excited states where it was prudent to use $K_m=40$ (121 HH states) although some value $32<K_m<40$ could be sufficient, and for the higher excited states of helium where K_m up to 100 was needed because of their close spacing and, consequently, different structure than for $Z>2$. In all cases the three cusp conditions were fulfilled exactly.

As it was discussed above our results proved to be numerically quite close to $R_2^{(3)}(Z)$ calculated in Ref. [1]. The difference between the asymptotic values for the ratios of double-to-single ionization cross sections of triplet and singlet states appeared to be much larger, due to strong relativistic effects exclusive to the singlet states.

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- [1] R.C. Forrey, H.R. Sadeghpour, J.D. Baker, J.D. Morgan III, and A. Dalgarno, *Phys. Rev. A* **51**, 2112 (1995).
- [2] M. Haftel and V.B. Mandelzweig, *Phys. Rev. A* **42**, 6342 (1990).
- [3] M. Haftel, R. Krivec, and V.B. Mandelzweig, *J. Comput. Phys.* **123**, 149 (1996).
- [4] R. Krivec, V.B. Mandelzweig, and K. Varga, *Phys. Rev. A* **61**, 062503 (2000).
- [5] T.A. Carlson, *Phys. Rev.* **156**, 142 (1967).
- [6] F.W. Byron and C.J. Joachain, *Phys. Rev.* **164**, 1 (1967).
- [7] T. Aberg, *Phys. Rev. A* **2**, 1736 (1970).
- [8] M.Ya. Amusia and M.P. Kazachkov, *Phys. Lett.* **A28**, 27 (1968).
- [9] A. Dalgarno and H. Sadeghpour, *Phys. Rev. A* **46**, R3591 (1992).
- [10] K. Hino, T. Ishihara, F. Shimizu, N. Toshima, and J.H. McGuire, *Phys. Rev. A* **48**, 1271 (1993).
- [11] T. Surić, K. Pisk, B.A. Logan, and R.H. Pratt, *Phys. Rev. Lett.* **73**, 790 (1994).
- [12] J.H. McGuire, N. Berrah, R.J. Bartlett, J.A.R. Samson, J.A. Tanis, C.L. Cocke, and A.S. Schlachter, *J. Phys. B* **28**, 913 (1995).
- [13] M. Pont, R. Shakeshaft, F. Maulbetsch, and J.S. Briggs, *Phys. Rev. A* **53**, 3671 (1996).
- [14] A.S. Kheifets and I. Bray, *Phys. Rev. A* **54**, R995 (1996).
- [15] Y. Qiu, J.-Z. Tang, and J. Burgdörfer, *Phys. Rev. A* **57**, R1489 (1998).
- [16] J.H. McGuire, *Electron Correlation Dynamics in Atomic Collisions* (Cambridge University Press, Cambridge, 1997).
- [17] J.C. Levin, G.B. Armen, and I.A. Sellin, *Phys. Rev. Lett.* **76**, 1220 (1996).
- [18] M. Ya. Amusia, *Atomic Photoeffect* (Plenum, New York, 1990).
- [19] R. Krivec, M.Ya. Amusia, and V.B. Mandelzweig, *Phys. Rev. A* **62**, 064701 (2000).
- [20] R. Krivec, M.Ya. Amusia, and V.B. Mandelzweig, *Phys. Rev. A* **63**, 052708 (2001).
- [21] M.Ya. Amusia, E.G. Drukarev, R. Krivec, and V.B. Mandelzweig, *Phys. Rev. A* **66**, 052706 (2002).
- [22] R. Krivec, M.Ya. Amusia, and V.B. Mandelzweig, *Phys. Rev. A* **64**, 012713 (2001).
- [23] M.Ya. Amusia, E.G. Drukarev, V.G. Gorshkov, and M.P. Kazachkov, *J. Phys. B* **8**, 1248 (1975).
- [24] J. Ullrich, R. Moshhammer, R. Dörner, O. Jagutzki, V. Mergel, H. Schmidt-Böcking, and L. Spielberger, *J. Phys. B* **30**, 2917 (1997).
- [25] J.A.R. Samson, Z.X. He, R.J. Bartlett, and M. Sagurton, *Phys. Rev. Lett.* **72**, 3329 (1994).
- [26] T. Kato, *Commun. Pure Appl. Math.* **10**, 151 (1957).
- [27] E.G. Drukarev, *Phys. Rev. A* **52**, 3910 (1995).
- [28] M.A. Kornberg and J.E. Miraglia, *Phys. Rev. A* **60**, R1743 (1999).
- [29] Note that $H^- * 3S$ bound states do not exist, contrary to H^- .
- [30] The atomic system of units is used: $m_e = e = \hbar = 1$, with m_e being the electron mass, e its charge and \hbar the Planck constant.