CALCULATION OF THE PHOTOIONIZATION
WITH DE-EXCITATION CROSS SECTIONS OF He
AND HELIUM-LIKE IONS

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We discuss the results of the calculation of the photoionization with de-excitation of excited He and helium-like ions Li^+ and B^{3+} at high but nonrelativistic photon energies ω. Several lower ^1S and ^3S states are considered. We present and analyze the ratios R_d^{+*} of the cross sections of photoionization with de-excitation, $\sigma_{(d)}^{+*}(\omega)$, and of the photoionization with excitation, $\sigma^{+*}(\omega)$. The dependence of R_d^{+*} on the excitation of the target object and the charge of its nucleus is presented. In addition to theoretical interest, the results obtained can be verified using long-lived excited states such as 2^3S of He.

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1. INTRODUCTION

The processes of two-electron photoionization and ionization with excitation have been attracting the attention of theorists and experimentalists for a long time. A steady increase of activity occurred during the last decade [1–8]. The interest in these processes is motivated to a large extent by the desire to test our ability to reliably calculate the two-electron wave function and to understand the mechanisms of the processes that take place solely due to the interelectron interaction.

The simplest objects where the interelectron interaction can manifest itself are the two-electron systems such as the He atom and helium-like ions. There-

fore, they represent the main targets of investigation. Recently, a number of studies have been carried out of the two-electron photoionization cross sections of these systems, including the corresponding ratios of the two-electron and single-electron cross sections, at high but nonrelativistic photon energies ω (see [9–12] and the references therein).

In the high photon energy region, the cross sections of two-electron processes can be expressed via the initial-state wave functions. The initial states considered were the ground and excited states of He and the helium-like ions.

For high but nonrelativistic ω, the dominating mechanisms of the two-electron ionization and ionization with excitation are twofold: shake-off and initial state correlations. Both exhibit the same dependence on ω at high ω. The contribution of the final-state in-

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teraction, where the second electron is excited or ionized due to a collision with the primary eliminated electron that absorbs the incoming photon, decreases with ω faster than the shake-off contribution. The quasi-free mechanism [13] operates in the situation where both electrons are ionized and acquire almost equal energies. Therefore, the quasi-free mechanism is not taken into consideration in the framework of the ionization with excitation or de-excitation.

If the initial state is excited, the elimination of one of the electrons can be accompanied not only by the excitation of the second one but also by de-excitation. As far as we are aware, the de-excitation process almost completely escaped theoretical investigation. However, it is expressed by integrals similar but not identical to those entering the expressions for the cross sections of the two-electron ionization and ionization with excitation [9–11, 14]. The aim of this paper is to study the photoionization accompanied by de-excitation. In principle, this process can be separated experimentally from the other two-electron processes, i.e., the double ionization and ionization with excitation, if the photoelectron energy for the given incoming photon frequency ω is detected.

We obtain the initial-state wave function using the correlation function hyperspherical harmonic method (CFHHM). The local accuracy of this wave function was previously studied for the ground and the 2^1S state of the He atom in Ref. [15], where it was shown that the local deviation of the CFHHM wave function from the exact value is extremely small. Very accurate nonvariational CFHHM wave functions of the He atom and helium-like ions in their ground and several lowest excited ^1S and ^3S states [16, 17] were therefore used to calculate the cross sections of the processes of interest. We calculated the high-energy photoionization cross sections that can be expressed solely through the initial-state two-electron wave functions $\Psi_i(\mathbf{r}_1, \mathbf{r}_2)$.

In this work, we use these nonvariational wave functions for the He atom and the helium-like ions in several lowest excited ^1S and ^3S states to calculate the high-energy limits of the cross sections of photoionization with de-excitation. The results of these limits are compared with the cross sections of the photoionization with excitation and with the single-electron photoionization cross sections. To study the theoretically interesting nuclear charge dependences of the considered values, we also investigate the Li$^+$ and B^{3+} ions.

Unfortunately, until now, only the double- and single-charge ions have been counted in the absolute majority of experiments. Therefore, the excitation and de-excitation processes remained undetected but included into the yield of single-charge ions.

2. MAIN FORMULAS

We start from the formula for the two-electron photoionization cross section at asymptotically high ω obtained in [9] and recently rederived in [10, 11]. In this ω region, the cross section $\sigma^{+*}(\omega)$ of the ionization with excitation for the He atom and the helium-like ions in their excited states is expressed as

$$\sigma_i^{+*}(\omega) = \frac{32Z^2\sqrt{2}\pi^2}{3c\omega^{7/2}} \sum_{n_f} I_{n_f n_i}, \tag{1}$$

where

$$I_{n_f n_i} = 4\pi \left| \int\limits_0^\infty \Psi_i(0, r) R_{n_f 0}(r) r^2 dr \right|^2 \tag{2}$$

is square modulus of the overlap integral. Here, Z is the nuclear charge, $i(n_i)$ denotes the initial state, $R_{n_f 0}(r)$ are the hydrogen single-electron radial wave functions with the principal quantum number n_f and angular momentum zero. We use the atomic units. We note that the excitations of states with nonzero angular momenta l decrease faster than $\omega^{-7/2}$, namely, as $\omega^{-(7/2+l)}$.

The photoionization cross section $\sigma^+(\omega)$ of the inner electron, without alteration of the state of the outer one, is given by

$$\sigma_i^+(\omega) = \frac{128Z^2\sqrt{2}\pi^3}{3c\omega^{7/2}} \left| \int\limits_0^\infty \Psi_i(0, r) R_{n_i 0}(r) r^2 dr \right|^2. \tag{3}$$

The cross section $\sigma_{(d)}^{+*}$ of the photoionization with de-excitation is calculated using expressions (1) and (2) where the summations over n_f include values that are different from those for ionization with excitation. As was mentioned above, we classify the initial state by its principal quantum number n_i. The ground state can be considered approximately as a state with $n_i = 1$. The next state is $n_i = 2$, and so on: the higher the excitation, the more precise becomes the assignment of a given state to an integer principal quantum number. With increasing the excitation principal quantum number n_i, the wave function approaches a symmetrized product of two pure Coulomb wave functions. One of these is the $1s$ electron function in the nuclear field with charge Z, and the other is a function in the $(Z-1)$ field. Thus, $\sigma^{+*}(\omega)$ includes the summation over $n_f > n_i$, while $\sigma_{i(d)}^{+*}(\omega)$ includes the summation over $n_f < n_i$.

Table 1. Values of the ratios $I_{n_f n_i}$ and R_{id}^{+*} for the singlet states of the helium atom

n_f	n_i						
	1	2	3	4	5	6	7
1	0.9295	0.0493	0.0136	0.0055	0.0028	0.0016	0.0010
2	0.0446	0.5346	0.0702	0.0231	0.0106	0.0059	0.0036
3	0.0055	0.3993	0.1668	0.0533	0.0237	0.0131	0.0079
4	0.0018	0.0035	0.7319	0.0019	0.0063	0.0051	0.0037
5	0.0008	0.0017	0.0131	0.7761	0.0594	0.0107	0.0029
6	0.0005	0.0009	0.0001	0.1380	0.4997	0.1430	0.0541
7	0.0003	0.0005	0.0001	0.0003	0.3865	0.1606	0.1129
8	0.0002	0.0003	0.0001		0.0103	0.5996	0.0025
9	0.0001	0.0002	0.0001			0.0597	0.6106
10	0.0001	0.0002	0.0001			0.0001	0.1969
11	0.0001	0.0001					0.0035
12		0.0001					0.0000
R_{id}^{+*}		0.0523	0.0917	0.0893	0.0452	0.0378	0.0790

Table 2. The same as in Table 1, but for the triplet states of the helium atom

n_f	n_i					
	2	3	4	5	6	7
1	0.0338	0.0087	0.0034	0.0017	0.0009	0.0006
2	0.7823	0.0591	0.0170	0.0073	0.0039	0.0023
3	0.1733	0.4053	0.0902	0.0352	0.0177	0.0103
4	0.0044	0.5231	0.0760	0.0419	0.0228	0.0137
5	0.0014	0.0006	0.7595	0.0059	0.0005	0.0016
6	0.0006	0.0004	0.0526	0.6723	0.0995	0.0247
7	0.0003	0.0003	0.0001	0.2324	0.3434	0.1470
8	0.0002	0.0002		0.0027	0.4812	0.0615
9	0.0001	0.0001			0.0299	0.6144
10	0.0001	0.0001				0.1225
11	0.0001	0.0001				0.0012
12						0.0000
R_{id}^{+*}	0.0350	0.0728	0.124	0.0942	0.0479	0.0562

The ratio R_{id}^{+*} of the cross section $\sigma_{i(d)}^{+*}(\omega)$ to the sum of $\sigma_i^+(\omega)$ and $\sigma_i^{+*}(\omega)$ is given by

$$R_{id}^{+*} \equiv \frac{\sigma_{i(d)}^{+*}(\omega)}{\sigma_i^+(\omega) + \sigma_i^{+*}(\omega)} = \frac{\sum\limits_{n_f < n_i} I_{n_f n_i}}{\sum\limits_{n_f \geq n_i} I_{n_f n_i}}. \qquad (4)$$

It is seen from Eq. (2) that σ_i^{+*} and $\sigma_{i(d)}^{+*}$ probe different parts of the initial-state wave function $\Psi_i(0, r)$.

3. RESULTS OF CALCULATIONS

The Tables present the results of our calculations for the singlet and triplet states of the He atom (Tables 1 and 2) and helium-like ions Li$^+$ (Tables 3 and 4) and B^{3+} (Tables 5 and 6).

Most results can be obtained using a small hyperspherical harmonic basis with $K_m = 48$, for some ground states even with $K_m = 40$, where K_m is the maximum global angular momentum used in the hyperspherical harmonic expansion. The main problem is the calculation of the overlap integrals (2) between the accurate CFHHM wave function and the hydrogen single-electron ones of higher orders. Very precise calculations of the CFHHM wave function $\Psi_i(0, r)$ at the

Table 3. Values of the ratios $I_{n_f n_i}$ and R_{id}^{+*} for the singlet states of the Li^+ ion

n_f	n_i						
	1	2	3	4	5	6	7
1	0.9716	0.0718	0.0210	0.0087	0.0044	0.0025	0.0016
2	0.0157	0.7456	0.0516	0.0147	0.0064	0.0034	0.0020
3	0.0023	0.1528	0.5476	0.0835	0.0293	0.0141	0.0080
4	0.0008	0.0102	0.3561	0.3000	0.0813	0.0347	0.0183
5	0.0004	0.0032	0.0082	0.5824	0.1053	0.0523	0.0276
6	0.0002	0.0015	0.0029	0.0009	0.7627	0.0100	0.0177
7	0.0001	0.0008	0.0014	0.0013	0.0052	0.8381	0.0107
8	0.0001	0.0005	0.0008	0.0008	0.0003	0.0417	0.7807
9	0.0001	0.0003	0.0005	0.0005	0.0003	0.0000	0.1314
10	0.0000	0.0002	0.0003	0.0003	0.0002	0.0001	0.0000
11	0.0000	0.0002	0.0002	0.0002	0.0002	0.0001	0.0000
12	0.0000	0.0001	0.0002	0.0002	0.0001	0.0001	0.0000
R_{id}^{+*}		0.0784	0.0790	0.120	0.139	0.120	0.0815

Table 4. The same as in Table 3, but for the triplet states of the Li^+ ion

n_f	n_i					
	2	3	4	5	6	7
1	0.0559	0.0158	0.0064	0.0032	0.0018	0.0011
2	0.8762	0.0316	0.0079	0.0032	0.0017	0.0010
3	0.0574	0.7283	0.0771	0.0241	0.0109	0.0060
4	0.0044	0.2085	0.4788	0.0982	0.0375	0.0188
5	0.0013	0.0070	0.4194	0.2340	0.0836	0.0391
6	0.0006	0.0022	0.0031	0.6321	0.0649	0.0467
7	0.0003	0.0010	0.0016	0.0003	0.7789	0.0011
8	0.0002	0.0005	0.0008	0.0006	0.0179	0.8094
9	0.0001	0.0003	0.0005	0.0004	0.0001	0.0747
10	0.0001	0.0002	0.0003	0.0003	0.0001	0.0000
11	0.0001	0.0002	0.0002	0.0002	0.0002	0.0001
12	0.0000	0.0001	0.0001	0.0001	0.0001	0.0000
R_{id}^{+*}	0.0594	0.0499	0.101	0.148	0.157	0.127

first electron–nucleus distance zero and for large values of r are required. The precision of the CFHHM wave function, including its values for large r, then increases slowly with increasing K_m, while the calculation time increases considerably as K_m grows. We here use the hyperspherical harmonic basis with $K_m = 100$ for the excited $2S - 7S$ both singlet and triplet states of He atom and the one with $K_m = 64$ for the other ions in the excited states, which makes the calculation quite difficult. This gives the data with the accuracy well above experimentally obtainable in foreseeable future.

In the Tables, we presented only several first terms ($n_f \leq 12$) of the set of integrals (2). However, we have used 200 single-particle states to calculate the cross section ratios, and hence the error of summation over states is at least the error of the data presented in the Tables.

4. DISCUSSION AND CONCLUSIONS

In all cases, the probability of the initially excited electron to remain on the same level ($n_f = n_i$) decreases with n_i. In principle, this is quite natural because the higher n_i, the easier it is to alter the electron state in the course of the rapid elimination of the $1S$

Table 5.   Values of the ratios $I_{n_f n_i}$ and R_{id}^{+*} for the singlet states of the B^{3+} ion

n_f	n_i						
	1	2	3	4	5	6	7
1	0.9905	0.0892	0.0270	0.0114	0.0058	0.0034	0.0020
2	0.0047	0.8485	0.0235	0.0057	0.0023	0.0012	0.0007
3	0.0008	0.0448	0.8156	0.0495	0.0138	0.0060	0.0031
4	0.0003	0.0054	0.1098	0.7053	0.0725	0.0228	0.0102
5	0.0001	0.0018	0.0094	0.2009	0.5663	0.0877	0.0300
6	0.0001	0.0009	0.0030	0.0116	0.3131	0.4197	0.0900
7	0.0000	0.0005	0.0014	0.0036	0.0112	0.4376	0.2746
8	0.0000	0.0003	0.0008	0.0017	0.0037	0.0080	0.5493
9	0.0000	0.0002	0.0005	0.0010	0.0018	0.0030	0.0036
10	0.0000	0.0001	0.0003	0.0006	0.0009	0.0019	0.0015
11	0.0000	0.0001	0.0002	0.0004	0.0007	0.0006	0.0036
12	0.0000	0.0001	0.0002	0.0003	0.0004	0.0007	0.0000
R_{id}^{+*}		0.0987	0.0536	0.0718	0.105	0.138	0.158

Table 6.   The same as in Table 5, but for the triplet states of the B^{3+} ion

n_f	n_i					
	2	3	4	5	6	7
1	0.0764	0.0228	0.0095	0.0048	0.0028	0.0017
2	0.9025	0.0122	0.0027	0.0010	0.0005	0.0003
3	0.0162	0.8914	0.0359	0.0091	0.0038	0.0020
4	0.0019	0.0613	0.8004	0.0622	0.0179	0.0078
5	0.0006	0.0054	0.1337	0.6722	0.0840	0.0272
6	0.0003	0.0017	0.0084	0.2306	0.5265	0.0964
7	0.0002	0.0008	0.0025	0.0095	0.3460	0.3783
8	0.0001	0.0004	0.0012	0.0030	0.0082	0.4717
9	0.0001	0.0003	0.0006	0.0014	0.0028	0.0045
10	0.0000	0.0002	0.0004	0.0008	0.0014	0.0023
11	0.0000	0.0001	0.0003	0.0005	0.0008	0.0013
12	0.0000	0.0001	0.0002	0.0003	0.0005	0.0005
R_{id}^{+*}	0.0829	0.0364	0.0507	0.0839	0.123	0.157

electron. This decrease is monotonic for pure hydrogenic functions; in the lowest order in the interelectron interaction, this result can be demonstrated analytically [18]. For the He atom, the decrease is nonmonotonic and the overlap integral in Eq. (2) reaches its minimum value at $n_i = n_f = 4$ for the singlet states and at $n_i = n_f = 5$ for the triplet states. This is a consequence of the strong deviation of $\Psi_i(0, r)$ from its simplest approximation. A trace of the helium-like behavior can be found in the minimum of $I_{n_f n_i}$ at $n_i = n_f = 7$ for singlet states in Li^+.

The B^{3+} ion is already purely hydrogen-like, the role of its interelectron interaction being relatively smaller than in He. This brings about the decrease of $I_{n_f n_i}$ for $n_f = n_i$ with increasing n_i. As a result, the probability for the initially excited electron to remain on the same level after the inner $1S$ electron is photoionized increases. Indeed, I_{77} for B^{3+} is about 30 times larger than for Li^+. The corresponding ratio for the triplet I_{77} values is even larger by an additional factor of 15. As can be seen from the Tables, the most probable process is the ionization with excitation to the next one or two levels. The ratio R_{id}^{+*} varies relatively little, from 0.035 to 0.158. It has quite a complex form, with at least two minima for the He atom and at least

one minimum for the singlet and triplet states of B^{3+}.

We must bear in mind that the process of photoionization with excitation can be relatively easily distinguished from other two-electron processes, from the two-electron ionization in particular. This can be achieved simply by detecting photoelectrons with energies larger than the energy of the incoming photon. The ratio R_{id}^{+*} of the cross section of the ionization with de-excitation and the cross section of the ionization with excitation presents a rather complex function of the initial state and is completely determined by its wave function. Observation of this process could serve as an additional (to studies of ionization with excitation) verification of the quality of the wave functions used in describing the initial state of the target atoms or ions.

We note that a target consisting of excited atoms can be produced by the initial illumination of a He gas volume, e.g., by laser light. The p-excited states then radiatively decay into excited s-states.

Targets of triplet excited states can be produced by colliding at small angles an α-particle beam with a magnetized metallic surface, i.e., the surface occupied by electrons with the same spin orientation.

The development of experimental technique and growth of intensity of available high photon beams will lead without a doubt to the experiments in which, for a given photon frequency, the outgoing photoelectron energy will be detected accurately enough. It will allow studying ionization with excitation and de-excitation. A good object for de-excitation studies would be the 2^3S state of He, whose lifetime is about eight minutes. Experimental detection of ionization with de-excitation is, of course, an experimental challenge and we do believe that it will attract experimentalists very soon.

REFERENCES

1. T. A. Carlson, Phys. Rev. **156**, 142 (1967).

2. F. W. Byron and C. J. Joachain, Phys. Rev. **164**, 1 (1967).

3. T. Aberg, Phys. Rev. A **2**, 1736 (1970).

4. A. Dalgarno and H. Sadeghpour, Phys. Rev. A **46**, 3591 (1992).

5. 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).

6. A. S. Kheifets and I. Bray, Phys. Rev. A **54**, R995 (1996).

7. J. H. McGuire, *Electron Correlation Dynamics in Atomic Collisions*, Cambridge University Press, Cambridge (1997).

8. J. Ullrich, R. Moshammer, R. O. Jagutzki, V. Mergel, H. Schmidt-Boking, and L. Spielberger, J. Phys. B **30**, 2917 (1997).

9. R. Krivec, M. Ya. Amusia, and V. B. Mandelzweig, Phys. Rev. A **62**, 064701 (2000).

10. R. Krivec, M. Ya. Amusia, and V. B. Mandelzweig, Phys. Rev. A **63**, 052708 (2001).

11. R. Krivec, M. Ya. Amusia, and V. B. Mandelzweig, Phys. Rev. A **67**(6), 62720-7 (2003).

12. E. G. Drukarev, M. Ya. Amusia, R. Krivec, and V. B. Mandelzweig, Few Body Systems **35**, 3 (2004).

13. M. Ya. Amusia, E. G. Drukarev, V. G. Gorshkov, and M. P. Kazachkov, J. Phys. B **8**, 1248 (1975).

14. M. Ya. Amusia, *Atomic Photoeffect*, Plenum Press, New York and London (1990).

15. M. I. Haftel and V. B. Mandelzweig, Phys. Rev. A **42**, 6324 (1990).

16. M. I. Haftel, R. Krivec, and V. B. Mandelzweig, J. Comp. Phys. **123**, 149 (1996).

17. R. Krivec, V. B. Mandelzweig, and K. Varga, Phys. Rev. A **61**, 062503 (2000).

18. M. Ya. Amusia, A. S. Baltenkov, private communication (1993).