ATOMS, MOLECULES,
OPTICS

Calculation of the Photoionization with Deexcitation Cross Sections of He and Helium-Like Ions[¶]

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Received October 31, 2005

Abstract—We discuss the results of the calculation of the photoionization with deexcitation 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 deexcitation, $\sigma_d^{+*}(\omega)$, 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.
PACS numbers: 32.80.Fb, 31.15.Ja
DOI: 10.1134/S1063776106040042

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 in 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 wavefunction 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 two-electron systems such as the He atom and helium-like ions. Therefore, 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 references therein).

In the high photon energy region, the cross sections of two-electron processes can be expressed via the initial-state wavefunctions. 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 the initial state correlations. Both exhibit the same dependence on ω at high ω. The contribution of the final-state interaction, 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 deexcitation.

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 deexcitation. As far as we are aware, the deexcitation 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 deexcitation. 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 wavefunction using the correlation function hyperspherical harmonic method (CFHHM). The local accuracy of this wavefunction

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[¶] The text was submitted by author in English.

was previously studied for the ground and the 2^1S state of the He atom in [15], where it was shown that the local deviation of the CFHHM wavefunction from the exact value is extremely small. Very accurate nonvariational CFHHM wavefunctions of the He atom and the 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 via the initial-state two-electron wavefunctions $\Psi_i(\mathbf{r}_1, \mathbf{r}_2)$.

In this work, we use these nonvariational wavefunctions 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 deexcitation. 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. In this work, we use atomic units.

Unfortunately, until now, only the double- and single-charged ions have been counted in the absolute majority of experiments. Therefore, the excitation and deexcitation processes have 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

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

where

$$I_{n_f n_i} = 4\pi\left|\int_0^\infty \Psi_i(0, r)R_{n_f 0}(r)r^2 dr\right|^2 \qquad (2)$$

is 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 wavefunctions with the principal quantum number n_f and an angular momentum of zero. 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

$$\sigma_i^+(\omega) = \frac{128Z^2\sqrt{2}\pi^3}{3c\omega^{7/2}}\left|\int_0^\infty \Psi_i(0, r)R_{n_i 0}(r)r^2 dr\right|^2. \qquad (3)$$

The cross section $\sigma_{(d)}^{+*}$ of the photoionization with deexcitation 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 excitation principal quantum number n_i, the wavefunction approaches a symmetrized product of two pure Coulomb wavefunctions. One of these is an ^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 $n_f < n_i$.

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 wavefunction $\Psi_i(0, r)$.

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 hyper spherical 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 wavefunction and the hydrogen single-electron ones of higher orders. Very precise calculations of the CFHHM wavefunction $\Psi_i(0, r)$ at the first electron–

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

nucleus distance zero arid for large values of r arc required. The precision of the CFHHM wavefunction, including its values for large r, increases slowly with increasing K_m, while the calculation time increases considerably as K_m grows. We here used the hyperspherical harmonic basis with $K_m = 100$ for the excited $2S – 7S$ of both singlet and triplet states of He atom and the one with $K_m = 64$ for the other ions in the excited states, which make the calculation quite difficult. This gives data with an accuracy well above those that will be experimentally obtainable in the foreseeable future.

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

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

4. DISCUSSION AND CONCLUSIONS

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

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

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 that the initially excited electron will 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 deexcitation and the cross section of the ionization with excitation presents a rather complex function of the initial state and is completely determined by its wavefunction. Observation of this process could serve as an additional (to studies of ionization with excitation) verification of the quality of the wavefunctions used in describing the initial state of the target atoms or ions.

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

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

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.

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

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

The development of an experimental technique and growth in intensity of available high photon beams will without a doubt lead to experiments in which, for a given photon frequency, the outgoing photoelectron energy will be detected with sufficient accuracy. This will make it possible to study ionization with excitation and deexcitation. A good object for deexcitation studies would be the 2^3S state of He, whose lifetime is about 8 min. Experimental detection of ionization with deexcitation 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, et al., 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 Univ. Press, Cambridge, 1997).

8. J. Ullrich, R. Moshammer, R. O. Jagutzki, et al., 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**, 62720 (2003).

12. E. G. Drukarev, M. Ya. Amusia, R. Krivec, and V. B. Mandelzweig, Few-Body Syst. **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, in *Atomic Photoeffect*, Ed. by K. T. Taylor (Plenum, New York, 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. Comput. 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).

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