

Calculations for electron-impact ionization of magnesium and calcium atoms in the method of interacting configurations in the complex number representation

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Abstract Next investigations in our program of transition from the He atom to the complex atoms description have been presented. The method of interacting configurations in the complex number representation is under consideration. The spectroscopic characteristics of the Mg and Ca atoms in the problem of the electron-impact ionization of these atoms are investigated. The energies and the widths of the lowest 1S , 1P , 1D , and 1F autoionizing states of Mg atom, and the lowest 1P autoionizing states of Ca atom, are calculated. Few results in the photoionization problem on the 1P autoionizing states above the $n=2$ threshold of helium-like Be^{++} ion are presented.

Keywords electron-impact ionization of atom, autoionizing states, quasistationary states, interacting configurations method

Our step by step transition from the He atom description to the complex atoms consideration has been realized via the problem of ionization of H^- , Li^+ ions [6, 7] up to the enough complex atoms (such as Be, Mg and Ca) investigations. The results were reported at the international conferences [6, 8–11] as some approbation of the method and found data. The complete description of the method formalism was given in [12], see, e. g., [13] as well. In [14] the choice of the ground state wave function for such precision calculations of the quasistationary states parameters has been considered and discussed. One of the goals of these investigations is to demonstrate that the ICCNR method can be useful for the complex atoms study on the level of popular R-matrix approach, see, e. g., [15]. The comparison with theoretical calculations in other methods has been considered as well.

Thus, the ICCNR method is applied here to the calculation of spectroscopic characteristics of autoionizing states (AIS) of Mg and Ca atoms in the problem of the electron-impact ionization of these atoms. In particular, the energies and the widths of the lowest (1S , 1P , 1D , and 1F) AIS of Mg atom, and the lowest 1P AIS of Ca atom, are calculated. Few results in the photoionization problem on the 1P AIS above the $n=2$ threshold of helium-like Be^{++} ion are presented as well. The first three 1P resonances above the $n=2$ threshold are considered. Found results are compared with [16, 17].

The exact quantum mechanical methods are welcome here because the experimental investigations of some atoms (e. g., beryllium atom) are complicated due to its chemical properties.

Some known results for Mg atom [18–20] are compared with our calculations in ICCNR method. Furthermore, our results (found in ICCNR method) for Ca atom are compared with experimental and theoretical investiga-

1 Introduction

We presented here next step in our last years program to apply the method of interacting configurations in the complex number representation (the ICCNR method) to the complex atoms description. The previous step was considered in [1, 2], where this method on the example of beryllium atom has been demonstrated.

The ICCNR method was suggested in papers [3–5] and successfully applied to the description of the quasistationary states of helium formed at its electron ionization in the energy interval above the threshold of excited ion formation. At the modern stage in the development of this method, a principal possibility is its application to the calculation of ionization processes in more complicated atomic structures.

tions [21–23].

Note that the analysis of the loss spectrum of ejected electrons made it possible to compare indirectly the obtained results with the results of studies of the scattering problem.

As one can see in the literature, beryllium [16, 17, 19, 24–44], magnesium [18–20, 24, 25, 45–58] and calcium [21–23, 59, 60] atoms turns out to be the promising objects for researches.

2 Some backgrounds of the method

The ICCNR method is a well-defined quantum-mechanical method for the calculation of parameters of atomic systems. This method is a development and a generalization of the known method of interacting configurations in the real number representation. It has some advantages in comparison with the standard method of interacting configurations in the real number representation and other calculation methods for the energies and widths of quasistationary atomic states. First, this is a capability of finding not only the energies, but also the widths of quasistationary states. Second, there are new possibilities for the resonance identification. The ICCNR method makes it possible, on the basis of the results of calculations, to estimate the contribution of each resonance state to the cross-section of the process and, if the resonance approximation is applicable, to introduce a set of parameters that determine the energies and the widths of quasistationary states, as well as the contours of resonance lines in the ionization cross-sections. In the concrete problems this approach also enables to investigate the applicability of approximate methods of cross-section estimation and to determine the limits of their validity. Those advantages make it possible to apply successfully the ICCNR method not only to scattering processes, but also to much more complicated processes such as ionization of atoms by electrons.

Consider the equation of the examined reaction

$$A(n_0L_0S_0) + e^-(\vec{k}_0) \rightarrow A^+(nl_1) + e^-(\vec{k}_1) + e^-(\vec{k}), \quad (1)$$

where $\vec{k}_0, \vec{k}_1, \vec{k}$ are the momenta of the incident, ejected, and scattered electrons, respectively. Then the generalized oscillator strength of the transition for the incident electron in the Born approximation is given by

$$\frac{df_{nl_1}}{dE}(Q) = \frac{E}{Q^2} \sum_{lL} |\langle nL_1El | \sum_{j=1}^n \exp(i\vec{Q}\vec{r}_j) | n_0L_0S_0 \rangle|^2. \quad (2)$$

In this formula $E = k_0^2 - k^2$ is the energy loss, $\vec{Q} = \vec{k}_0 - \vec{k}$ is the transmitted momentum, and $|nl_1El : LS_0\rangle$ is the wave function of an atom with total momentum L and spin S_0 provided that an electron with momentum l and energy E is in the field of ion A^+ , whose electron has the quantum numbers $|nl_1\rangle$. The function of the atomic ground state is given by $|n_0L_0S_0\rangle$.

Note that process (1) is a much more complicated physical phenomenon in comparison with the electron

scattering by an atom. Exact theoretical calculations of such processes constitute a problem for modern theoretical physics. Therefore, the consideration of this problem for multielectron atoms in the framework of the ICCNR method is an important and challenging scientific step.

More details of the ICCNR method formalism can be found in [12].

3 The results of calculations

Here the electron-impact ionizations of the Mg, Ca atoms in the interval of AIS excitation are considered. The corresponding results [1, 2] for beryllium atom are discussed briefly as well. Furthermore, some results for helium-like Be^{++} ion are given.

3.1 Energies and widths of helium-like Be^{++} ion below the $n=3$ threshold autoionizing states of Be atom

In articles [1, 2] energies and widths of the lowest AIS ($^1S, ^1P, ^1D$, and 1F) of a beryllium atom has been presented. These resonances were obtained in the ICCNR approximation in the problem of the electron-impact ionization of an atom. The indirect comparison with results of corresponding scattering problem has been fulfilled. Furthermore, the energies of 1P states, which are located between the first and second ionization thresholds of a beryllium atom, are found and compared with the results of calculations obtained by other authors (see, e. g., [5–10] in [2]). In calculations, the Coulomb wave functions were used as basis configurations. For every term, up to 25 basis configurations were taken into account.

Here we are able to add energies and the widths in the photoionization problem of the 1P AIS below the $n=3$ threshold of helium-like Be^{++} ion. The first three 1P resonances above the $n=2$ threshold are presented. The results are compared with theoretical calculations of [16, 17].

Table 1. Comparison of the energies and the widths obtained with the use of the ICCNR method for the AIS below the $n=3$ threshold of a helium-like Be^{++} ion with the theoretical results of other authors (the first three 1P resonances above the $n=2$ threshold are under consideration)

E, eV	Γ , eV	E, eV [16]	Γ , eV [16]	E, eV [17]	Γ , eV [17]
329.18	0.318	329.50	0.324	329.55	0.412
333.24	0.0081	333.35	0.086	333.69	0.088
337.47	0.0019	-	-	337.66	0.0023

3.2 Electron-impact ionization of a Mg atom in the interval of the excitation of autoionizing states

The investigation of the ionization of Mg atoms (and Mg^+ ions) by photons and electrons is a challenging problem. This assertion is proved by both experimental and theoretical papers of many authors (see, e.g., publications [24, 25, 45–58] cited here and papers [18–20], which are considered here directly). In brief publications

[9, 10], we started to study the electron-impact ionization of a Mg atom in the AIS excitation interval with the use of the ICCNR method. In Table 2, the results of our calculations for the energies and the widths of the lowest AIS (1S , 1P , 1D , and 1F) of a Mg atom (obtained in the electron-impact ionization problem in the ICCNR approximation) are presented.

First, our results are compared with similar states that are formed in the problem of electron scattering by Mg^+ ions [19] (see Table 2). Since another problem has been considered in article [19] – namely, the scattering one – such a comparison is indirect. In paper [19] the calculations were carried out in the diagonalization approximation. Second, in the framework of the problem of the electron-impact ionization of atoms, the energies of 1P -states must coincide with those obtained in the problem of photoionization of a Mg atom. Therefore, a direct comparison of our results with experimental ones [18] and with the results of calculations on the basis of the R-matrix method [20] can be made. In Table 3, the energy positions and the widths calculated for the 1P AIS of a magnesium atom with the use of the ICCNR method are directly compared with the experimental data of paper [18] and the theoretical data obtained with the help of the R-matrix formalism [20], as well as with the problem of electron scattering by a Mg^+ ion [19].

Thus, the original scientific results obtained with the help of the ICCNR method [3–5] for the energies and the widths of the lowest AIS (1S , 1P , 1D , and 1F) of a Mg atom in the problem of electron-impact ionization of this atom are presented (see Table 2). Their novelty consists in the application of the exact calculation method, namely, the method of interacting configurations and, moreover, the ICCNR method. The comparison with the calculations of corresponding energies and widths of AIS carried out in the diagonalization approximation in the problem of electron scattering by Mg^+ ions (Table 2) is indirect (a different object in a different problem), but really testifies to the reliability of the results obtained. Some of the results obtained here, namely, the energy positions of the 1P AIS of a Mg atom, can be directly compared with the experiment and the R-matrix calculations (see Table 3). The results of calculations carried out with the use of the ICCNR method are in good agreement with the corresponding calculations using the R-matrix method [20] and experimental results [18] (see Table 3).

3.3 Electron-impact ionization of a Ca atom in the interval of the excitation of autoionizing states

The application of ICCNR method to calculate the lowest AIS of calcium atom was started in paper [11]. The energies and the widths of the lowest 1P -states were calculated. The results were compared with the data obtained by other authors. In Table 4, besides the results of our calculations, the experimental data [21] and the results of theoretical calculations [22, 23] are shown. Analysis of the presented data testifies that the classification of AIS proposed in work [22] is possible. Thus, the results of our calculations agree well with the theo-

Table 2. Energies and widths of the lowest AIS (1S , 1P , 1D , and 1F) of a Mg atom obtained in the ICCNR approximation in the problem of electron-impact ionization of an atom. In paper [19], the energies of autoionizing states were calculated in the diagonalization approximation in the framework of the problem of electron scattering by a Mg^+ ion

1S	E, eV	Γ eV	E, eV [19]	Γ eV [19]
$4s^2$	13.08	0.0987	13.06	0.1010
$3d^2$	14.61	0.0480	14.66	0.0502
$4s5s$	14.92	0.0425	14.97	0.0473
$4s6s$	15.48	0.0196	15.53	0.0185
$3d4d$	15.59	0.0140	15.64	0.0129
$4s7s$	15.78	0.0115	15.80	0.0107
$4s8s$	15.80	0.0069	-	-
1P	E, eV	Γ eV	E, eV [19]	Γ eV [19]
$4s4p$	14.15	0.157	14.18	0.143
$3d4p$	15.01	0.172	14.95	0.162
$4s5p$	15.34	0.0324	15.29	0.0301
$4s6p$	15.68	0.0682	15.64	0.0667
$3d4f$	15.77	0.0481	15.74	0.0448
$4s7p$	15.85	0.0059	15.86	0.0048
$3s8p$	19.95	0.0140	19.93	0.0143
1D	E, eV	Γ eV	E, eV [19]	Γ eV [19]
$3d4s$	13.62	0.262	13.66	0.272
$3d^2$	14.31	0.253	14.38	0.269
$4d4s$	14.89	0.0192	14.96	0.0189
$3d5s$	15.28	0.0869	15.30	0.0951
$4p^2$	15.47	0.0570	15.49	0.0578
$3d4d$	15.58	0.0865	15.55	0.0876
$4s5d$	15.69	0.0258	15.66	0.0248
1F	E, eV	Γ eV	E, eV [19]	Γ eV [19]
$3d4p$	14.15	0.0225	14.66	0.0230
$4s4f$	15.01	0.0110	15.28	0.0113
$3d5p$	15.34	0.0540	15.53	0.0589
$3d4f$	15.53	0.0052	15.63	0.0053
$4s5f$	15.68	0.0201	15.71	0.0205
$3d6p$	15.77	0.0104	15.88	0.0109
$4s6f$	15.85	0.0125	15.90	0.0131

retical data obtained by other authors.

4 Conclusions

The method of interacting configurations in the complex number representation, which was applied earlier to the description of quasistationary states of a helium atom [3–5], is under consideration. The calculation of the ionization processes for more complicated atomic systems is suggested. The spectroscopic characteristics of the lowest AIS of Mg, Ca atoms were studied in the problem of the electron-impact ionization of these atoms (some results for helium-like Be^{++} ion are presented as well). The energies and the widths of the lowest AIS (1S , 1P , 1D , 1F) of Mg atom, and the lowest (1P) AIS of Ca atom, were calculated. The found results were compared with known experimental data and calculations on the basis of other methods. Hence, we may draw conclusion about a successful verification of the

Table 3. Comparison of the energies and the widths of the AIS of a magnesium atom found with the use of the ICCNR method with the experiment [18] and calculations for 1P -states [20] (paper [20]: the photoionization problem and the photoionization threshold; article [19]: the scattering problem)

1P	E, eV	Γ eV	E, eV [19]	Γ eV [19]
4s4p	14.15	0.157	14.18	0.143
3d4p	15.01	0.172	14.95	0.162
4s5p	15.34	0.0324	15.29	0.0301
3d5p	15.53	0.0775	15.56	0.0758
4s6p	15.68	0.00682	15.64	0.00667
3d4f	15.77	0.0481	15.74	0.0448
4s7p	15.85	0.00592	15.86	0.00476
4s8p	15.90	0.0087	-	-
3d6p	15.93	0.0295	-	-
4s9p	15.95	0.0011	-	-

1P	E, eV	Γ eV	E, eV [20]	Γ eV [20]	E, eV [18]
4s4p	14.15	0.157	14.2213	0.3921	14.18
3d4p	15.01	0.172	14.9048	0.6078	-
4s5p	15.34	0.0324	15.3133	0.0931	-
3d5p	15.53	0.0775	15.7264	0.0890	15.24
4s6p	15.68	0.00682	15.6653	0.0142	15.61
3d4f	15.77	0.0481	-	-	-
4s7p	15.85	0.00592	15.8675	0.0095	15.83
4s8p	15.90	0.0087	15.9802	0.0111	15.98
3d6p	15.93	0.0295	16.007	0.0417	-
4s9p	15.95	0.0011	16.065	0.0019	16.06

ICCNR method for the calculation of AIS of complex atoms and the processes of electron-impact ionization and excitation of such atoms.

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Table 4. Comparison of the energies and the widths obtained with the use of the ICCNR method for the AIS of a Ca atom with the theoretical results of other authors and the experiment [21]

1P	E, eV	E, eV [21]	E, eV [22]	E, eV [23]
3d5p	6.601	6.59	6.604	6.633
3d6p	7.033	7.02	7.038	7.080
3d7p	7.397	7.39	7.342	7.415
3d8p	7.465	7.47	7.471	7.502
3d9p	7.551	-	7.556	7.575
3d10p	7.610	-	7.614	7.624
4p5s	7.159	7.13	7.166	7.300
3d4f	6.937	-	6.938	6.960
3d5f	7.240	7.25	7.248	7.260
3d6f	7.425	-	7.427	7.427
3d7f	7.523	-	7.529	7.527
3d8f	7.591	-	7.596	7.593

1P	Γ eV	Γ eV [21]	Γ eV [22]	Γ eV [23]
3d5p	0.0801	0.21	0.0702	0.0846
3d6p	0.0059	0.17	0.0056	0.0067
3d7p	0.0451	-	0.0509	0.0399
3d8p	0.0261	0.14	0.0232	0.0315
3d9p	0.0163	-	0.0141	0.0282
3d10p	0.0140	-	0.0101	0.0207
4p5s	0.0129	0.15	0.0139	0.0132
3d4f	0.00006	-	0.000004	0.00001
3d5f	0.0059	-	0.0028	0.00003
3d6f	0.0019	0.17	0.0014	0.0024
3d7f	0.0009	-	0.0011	0.00007
3d8f	0.00007	-	0.00008	0.00006

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