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APPLICATION OF THE METHOD OF INTERACTING CONFIGURATIONS IN THE COMPLEX NUMBER REPRESENTATION TO CALCULATING THE SPECTROSCOPIC CHARACTERISTICS OF THE AUTOIONIZING STATES OF Be, Mg, AND Ca ATOMS

The method of interacting configurations in the complex number representation, which was earlier applied to describe helium quasistationary states, has been used for the calculation of ionization processes in more complicated atomic systems. The spectroscopic characteristics of the lowest quasistationary states of the Be, 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 Be and Mg atoms, and the lowest ^1P autoionizing state of a Ca one are calculated.

Keywords: autoionizing states, quasistationary states, configuration superposition.

1. Introduction

Researches of autoionization phenomena in the framework of the problems dealing with the ionization and the electron scattering by atoms and ions were separated in the last decades into an independent branch of theoretical atomic physics. The scientific interest to the description of the processes of excitation and decay of quasistationary states is associated with a necessity to specify the parameters of elementary processes, which are used in theoretical estimations and calculations in plasma physics, laser spectroscopy, solid state physics, and crystallography, at the development of technological methods of isotope separation at the atomic level, the designing of coherent ultra-violet and x-ray radiation generators, as well as in other physical domains.

The results of experimental researches concerning the autoionizing states (AISs) located between the first and second ionization thresholds for helium and helium-like ions were qualitatively explained on the basis of the theory of isolated Fano resonance and in the diagonalization approximation. The appearance of new experimental data on resonance structures in partial cross-sections of helium photoionization above the threshold of excited ion formation (more exactly, in the interval between the second and third thresholds, to which the AIS energies converge in the atomic ionization problem) brought about a number of theoretical issues dealing, first of all, with the description of the interaction of a considerable number of overlapping quasistationary states, which decay through several open channels. Theoretical calculations and the analysis of resonance structures decaying into several states of a residual ion should be carried out, in the general case, with regard for all interconfiguration interactions.

One of the first theoretical methods that made it possible to obtain results coinciding with experimental data was the method of configuration superposition or the method of interacting configurations. In the terminology adopted in this work, this formalism is called the method of interacting configurations in the real number representation (see Section 3). An important step of the theory became the method of interacting configurations in the complex number representation (ICCNR). The ICCNR method was developed in works [1–5] 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 advantage is its application to the calculation of ionization processes in more complicated atomic structures [6–9]. As one can see in the literature [10–26], beryllium, magnesium, and calcium atoms turn out the most promising objects for researches. In our work, the ICCNR method is applied to the calculation of spectroscopic characteristics of AIS of Be, 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) AISs of Be and Mg atoms, and the lowest (^1P) AIS of a Ca one were calculated.

2. General Characteristic of the Method

The ICCNR method is used to calculate the energies and the widths of quasistationary states in the problem of electron impact ionization of Be, Mg, and Ca atoms. In this section, the fundamentals and the formalism of the method are briefly described.

The ICCNR method is an exact 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 a number of 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. This approach also enables the applicability of approximate methods to the estimation of cross-sections in specific problems to be studied and the limits of their validity to be determined. Those advantages make it possible to successfully apply the ICCNR method not only to scattering processes, but also to much more complicated processes of atomic ionization by electrons.

Our research was aimed at illustrating the capabilities of the ICCNR method in the determination of spectroscopic characteristics of complicated atoms. Quasistationary states were studied in such multielectron atomic systems as Be, Mg, and Ca atoms [6–9]. The capabilities of the method were illustrated by the example of the atomic ionization by the electron impact [6–9], which are challenging for researches. The analysis of the loss spectrum of knocked out electrons made it possible to indirectly compare the obtained results with the results of studies of the scattering problem. The results were reported at a number of international scientific conferences [6–9].

3. Fundamentals of the Method of Interacting Configurations in the Complex Number Representation Applied to the Calculation of Processes of Electron-Impact Ionization of Atoms

Let us recall the fundamentals of the ICCNR method for the study of the processes of atomic ionization by the electron impact. Let the equation of the examined reaction read

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

where $\mathbf{k}_0$, $\mathbf{k}_1$, and $\mathbf{k}$ are the momenta of the incident, knocked out, and scattered electrons, respectively. Then the generalized oscillator strength of the transition for the incident electron in the Born approximation looks like

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

In this formula, $E = k_0^2 - k^2$ is the energy loss, $\mathbf{Q} = \mathbf{k}_0 - \mathbf{k}$ is the transmitted momentum, and $|nl_1El:LS_0\rangle$ is the wave function of an atom with total momentum L and spin S, 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 looks like $|n_0LS_0\rangle$.

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.

The choice of the wave function for the ground state is dictated by a desirable accuracy of the final results of calculations. In the case of two-electron systems, this is a multiparametric Hylleraas-type wave function, and, in the case of Be, Mg, and Ca atoms, this is, as a rule, a Hartree–Fock wave function obtained in the multiconfigurational approximation. The system of equations in the ICCNR method has the following form:

$$\begin{aligned}&(E_n - E)a^{Ei}_{\lambda n} + \sum_{\lambda'} \int_0^\infty b^{Ei}_{\lambda\lambda'}(E')V_{n\lambda'}(E')dE',\\&\sum_m a^{Ei}_{\lambda m} V^*_{m\lambda'}(E') + (E' - E)b^{Ei}_{\lambda\lambda'}(E') = 0.\end{aligned} \tag{3}$$

The multipliers $a^{Ei}_{\lambda m}$ and $b^{Ei}_{\lambda\lambda'}(E')$ are the coefficients of expansion of the wave function $\Psi^E_\lambda(\mathbf{r}_1, \mathbf{r}_2)$ in the basis

$$\begin{aligned}&\Psi^E_\lambda(\mathbf{r}_1, \mathbf{r}_2) = \sum_m a^{Ei}_{\lambda m}|m\rangle +\\&+\sum_{\lambda'} \int_0^\infty b^{Ei}_{\lambda\lambda'}(E')|\lambda' E'\rangle dE'.\end{aligned} \tag{4}$$

The basis wave functions satisfy the conditions

$$\langle m|\widehat{H}|n\rangle = E_n\delta_{nm}, \quad \langle\lambda' E'|\widehat{H}|\lambda E\rangle = E\delta_{\lambda\lambda'}\delta(E-E'), \tag{5}$$

where $\widehat{H}$ is the total Hamiltonian of the system.

The formal solution for $b^{Ei}_{\lambda\lambda'}(E')$ is selected in the form

$$\begin{aligned}&b^{Ei}_{\lambda\lambda'}(E') = P\frac{\sum_m a^{Ei}_{\lambda m} V_{m\lambda}(E)}{E - E'} + [A_{\lambda\lambda'} \pm\\&\pm i\pi \sum_m a^{Ei}_{\lambda m} V_{m\lambda'}(E)]\delta(E - E'),\end{aligned} \tag{6}$$

where $V_{m\lambda}(E) = \langle m|\widehat{H}|\lambda E\rangle$. The matrix $A_{\lambda\lambda'}$ depends on the asymptotic properties of the basis functions $|\lambda E\rangle$. Substituting Eq. (6) into Eq. (3) transforms the system of equations obtained in the ICCNR method into a system of linear algebraic equations for the coefficients $a^{Ei}_{\lambda m}$,

$$\begin{aligned}&(E_n - E)a^{Ei}_{\lambda n} + \sum_m [F_{nm}(E) - i\gamma_{nm}(E)]a^{Ei}_{\lambda m} =\\&= -\sum_{\lambda'} A_{\lambda\lambda'} V_{\lambda' n}(E).\end{aligned} \tag{7}$$

The latter can be expressed in terms of eigenvectors and eigenvalues of the complex matrix

$$W_{nm}(E) = E_n\delta_{nm} + F_{nm}(E) - i\gamma_{nm}(E), \tag{8}$$

where

$$\begin{aligned}&\gamma_{nm}(E) = \pi \sum_\lambda V_{n\lambda}(E)V_{\lambda m}(E);\\&F_{nm}(E) = \frac{1}{\pi} \int_0^\infty \frac{\gamma_{nm}(E)}{E - E'} dE'.\end{aligned} \tag{9}$$

The analysis of formulas (8) and (9) allows one to compare various approximations, which can be done in the ICCNR method. One can see that, in the framework of this method, the following approximations are possible:

1) the method of interacting configurations in the real number representation; this approximation corresponds to the neglect of complex components $i\gamma_{nm}(E)$ in matrix (8);

2) the diagonalization approximation in the real number representation consists in that the sum of all non-diagonal members $F_{nm}(E) - i\gamma_{nm}(E)$ in the matrix $W_{nm}(E)$ is neglected;

3) the diagonalization approximation involving the transitions outside the energy surface (or the diagonalization approximation in the complex number representation) arises if the term $F_{nm}(E)$ is neglected in calculations.

The account for all members in matrix (8) is, in essence, the ICCNR method, the advantages of which over the indicated approximations are obvious.

After determining the eigenvectors and eigenvalues of the matrix $W_{nm}(E)$, we can calculate the energies and widths of quasistationary states that are located above the threshold of excited ion formation [1–5]. The partial amplitudes of the resonance ionization can be determined as follows:

$$T_{|0\rangle\to|\lambda E\rangle}(E) = t^{\mathrm{dir}}_\lambda(E) + \sum_m \frac{H_{m\lambda(E)}}{\varepsilon_m(E) + 1}. \tag{10}$$

The quantities in formula (10) are defined by the relations

$$\begin{aligned}&t^{\mathrm{dir}}_\lambda(E) = \sqrt{C(E)}\langle\lambda E|\hat{t}|0\rangle,\\&H_{m\lambda}(E) = 2\widetilde{V}_{m\lambda}(E)[t_m(E) - i\tau_m(E)]\Gamma^{-1}_m(E),\end{aligned} \tag{11}$$

where

$$\begin{aligned}&t_m(E) = \sqrt{C(E)}\langle\widetilde{F}^E_m|\hat{t}|0\rangle,\\&\tau_m(E) = \sqrt{C(E)}\langle\chi^E_m|\hat{t}|0\rangle.\end{aligned} \tag{12}$$

Hence, the expressions for the cross-sections become parametrized,

$$\sigma_\lambda(E) = \sigma_\lambda^{\mathrm{dir}}(E) + \\ + \sum_m \frac{\Gamma_m(E) P_{m\lambda}(E) + \varepsilon_m(E) Q_{m\lambda}(E)}{\varepsilon_m^2(E) + 1}. \quad (13)$$

The real functions $P_{m\lambda}(E)$ and $Q_{m\lambda}(E)$ of the total energy E are the doubled real and imaginary, respectively, parts of the complex function $N_{m\lambda}(E)$, which looks like

$$N_{\alpha m}(E) = \sum_{\lambda\varepsilon\alpha} H_{m\lambda}(E)(t_\lambda^{\mathrm{dir}}(E) + \\ + \sum_n \frac{H_{m\lambda}(E)}{\varepsilon_n(E) - \varepsilon_m(E) + 2i})^*. \quad (14)$$

Hence, the resonance ionization cross-section is determined by a collection of the following functions of the total energy E: $\sigma_\lambda^{dir}(E)$, $N_{\alpha m}(E)$, $\varepsilon_m(E)$, and $\Gamma_m(E)$ [5]. See more details about the formalism of the method in work [5].

4. Electron Impact Ionization of a Be Atom in the Interval of the Excitation of Autoionizing States

In work [8], using the ICCNR method, the research of the ionization of a Be atom by the electron impact in the AIS excitation interval was started, and the spectra of energy loss were analyzed. The photoionization of this atom was studied as well. The autoionizing states that arise at that can be compared with the AISs that are formed in the problem of electron scattering at the corresponding ion. In calculations, the Coulomb wave functions were used as basis configurations. For every term, up to 25 basis configurations were taken into account.

Table 1 contains the results of our calculations for the energies and the widths of the lowest AISs of a Be atom (^1S, ^1P, ^1D, and ^1F) obtained in the problem of the ionization of this atom by the electron impact with the use of the ICCNR method [8]. The results are compared with the energies and the widths of AISs obtained in the problem of electron scattering by a Be^+ ion in work [13]. Therefore, this comparison is indirect. In addition, in Table 2, the energies of ^1P states, which are located between the first and second ionization thresholds of a beryllium atom, are compared with the results of calculations obtained by other authors [10–15].

In the literature, there are no similar results obtained on the basis of exact computational methods, in particular, on the basis of the method of interacting configurations and, the more so, on the basis of the ICCNR one. The comparison with the results of calculations of corresponding autoionizing state ener-

Table 1. **Energies and widths of the lowest AISs (^1S, ^1P, ^1D, and ^1F) of a beryllium atom obtained in the ICCNR approximation in the problem of the electron impact ionization of an atom. In work [13], the energies of autoionizing states were calculated in the diagonalization approximation in the framework of the problem of electron scattering by a Be^+ ion**

^1S	E, eV	Γ, eV	E, eV [13]	Γ, eV [13]
$3s^2$	16.42	0.0803	16.40	0.0818
$3p^2$	18.65	0.0110	18.57	0.0116
$3s4s$	18.82	0.0351	18.74	0.0358
$3s5s$	19.48	0.0163	19.45	0.0167
$3s6s$	19.77	0.00869	19.75	0.00884
$3s7s$	19.96	0.00518	19.92	0.00527
^1P	E, eV	Γ, eV	E, eV [13]	Γ, eV [13]
$3s3p$	17.70	0.157	17.68	0.169
$3s4p$	18.85	0.0318	18.83	0.0321
$3s5p$	19.45	0.00601	19.41	0.0062
$3s6p$	19.73	0.0157	19.68	0.0161
$3p4s$	19.81	0.00328	19.77	0.0033
$3s7p$	19.89	0.0274	19.82	0.0282
$3s8p$	19.95	0.0140	19.93	0.0143
^1D	E, eV	Γ, eV	E, eV [13]	Γ, eV [13]
$3s3d$	17.62	0.0214	17.56	0.0220
$3p^2$	18.31	0.0224	18.67	0.0230
$3s4d$	19.09	0.0378	19.09	0.0389
$3s5d$	19.60	0.0121	19.56	0.0128
$3d^2$	19.67	0.00789	19.63	0.0796
$3s6d$	19.81	0.00331	19.79	0.0034
^1F	E, eV	Γ, eV	E, eV [13]	Γ, eV [13]
$3p3d$	18.96	0.0203	18.95	0.0214
$3s4f$	19.43	0.0149	19.43	0.0155
$3s5f$	19.72	0.0070	19.70	0.00717
$3s6f$	19.88	0.0023	19.85	0.00235
$3s7f$	19.95	0.00021	19.94	0.00023
$3s8f$	19.97	0.0019	–	–

gies in the problem of electron scattering by Be^+ ions performed in work [13] in the diagonalization approximation (see Table 1) is indirect, because it deals with a different object in a different problem. Nevertheless, it really evidences the reliability of the results obtained here.

5. Electron Impact Ionization of a Mg Atom in the Interval of the Excitation of Autoionizing States

The research of the ionization of Mg atoms (and Mg^+ ions) by photons and electrons is a challenging problem, which is proved by both experimental and theoretical works of many authors (see, e.g., publications [13, 16–23]). In works [6, 7], 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 3, the results of our calculations for the energies and the widths of the lowest AISs (^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 analogous states that are formed in the problem of electron scattering by Mg^+ ions [13] (see Table 3). Since a different problem was considered in work [13] – namely, the scattering one – such a comparison is indirect. In work [13], 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 [16] and with the results of calculations on the basis of the R-matrix method [17] can be made. In Table 4, the energy positions and the widths calculated for the ^1P autoionizing states

Table 2. **Comparison of the energies obtained with the use of the ICCNR method for the AISs of a Be atom, which are located between the corresponding first and second ionization thresholds, with the results of other authors**

^1P	E, eV	E, eV [10]	E, eV [11]	E, eV [12]
$2p3s$	10.71	10.71	10.93	10.77
$2p3d$	10.84	11.86	11.86	11.86
$2p4s$	12.03	11.97	12.10	12.07
$2p4d$	12.42	12.47	12.50	12.49
^1P	E, eV	E, eV [13]	E, eV [14]	E, eV [15]
$2p3s$	10.71	10.73	10.63	10.91
$2p3d$	10.84	11.85	12.03	11.83
$2p4s$	12.03	12.09	12.09	12.09
$2p4d$	12.42	12.49	12.61	12.44

Table 3. **Energies and widths of the lowest AISs (^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 work [13], 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 [13]	Γ, eV [13]
$4s^2$	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 [13]	Γ, eV [13]
$4s4p$	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 [13]	Γ, eV [13]
$3d4s$	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 [13]	Γ, eV [13]
$3d4p$	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

of a magnesium atom with the use of the ICCNR method are directly compared with the experimental data of work [16] and the theoretical data obtained with the help of the R-matrix formalism [17], as well as with the problem of electron scattering by a Mg^+ ion [13].

The original scientific results obtained with the help of the ICCNR method [1–5] for the energies and the widths of the lowest AISs (^1S, ^1P, ^1D, and ^1F) of a Mg atom in the problem of electron impact ionization of this atom are presented (see Table 3). Their novelty consists in the application of the exact calculation method, namely, the method of interacting configurations and, the more so, the ICCNR method. The comparison with the calculations of corresponding energies and widths of AISs carried out in the diagonalization approximation in the problem of electron scattering by Mg^+ ions (Table 3) 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 AISs of a Mg atom, can be directly compared with the experiment and the R-matrix calculations (see Table 4). 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 [17] and experimental results [16] (see Table 4).

Table 4. **Comparison of the energies and the widths of the AISs of a magnesium atom obtained with the use of the ICCNR method with the experiment [16] and calculations for ^1P-states [17] (work [17]: the photoionization problem and the photoionization threshold; work [13]: the scattering problem)**

^1P	E, eV	Γ, eV	E, eV [13]	Γ, eV [13]
$4s4p$	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 [17]	Γ, eV [17]	E, eV [16]
$4s4p$	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

6. Electron Impact Ionization of a Ca Atom in the Interval of the Exctation of Autoionizing States

The application of ICCNR method to calculate the lowest AISs of calcium atom was begun in work [9]. The energies and the widths of the lowest ^1P-

Table 5. **Comparison of the energies and the widths obtained with the use of the ICCNR method for the AISs of a Be atom with the theoretical results of other authors and the experiment [24]**

^1P	E, eV	E, eV [24]	E, eV [25]	E, eV [26]
$3d5p$	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 [24]	Γ, eV [25]	Γ, eV [26]
$3d5p$	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

states were calculated. The results were compared with the data obtained by other authors. In Table 5, besides the results of our calculations [9], experimental data [24] and the results of theoretical calculations [25, 26] are shown. Their analysis testifies that the classification of AISs proposed in work [25] is possible. The results of our calculations agree well with the theoretical data obtained by other authors.

7. 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, was used to calculate the ionization processes of more complicated atomic systems. The spectroscopic characteristics of the lowest AISs of the Be, Mg, and Ca atoms were studied in the problem of the electron impact ionization of these atoms. The energies and the widths of the lowest autoionizing states (^1S, ^1P, ^1D, and ^1F) of Be and Mg atoms and the lowest (^1P) autoionizing states of a Ca atom were calculated. The calculation 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 method proposed for the calculation of autoionizing states of multielectron atoms and the processes of electron ionization and excitation of atoms.

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ЗАСТОСУВАННЯ МЕТОДУ ВЗАЄМОДІЮЧИХ КОНФІГУРАЦІЙ У ЗОБРАЖЕННІ КОМПЛЕКСНИХ ЧИСЕЛ ДО РОЗРАХУНКІВ СПЕКТРОСКОПІЧНИХ ХАРАКТЕРИСТИК АВТОІОНІЗАЦІЙНИХ СТАНІВ АТОМІВ Be, Mg, Ca

Р е з ю м е

Метод взаємодіючих конфігурацій у зображенні комплексних чисел, який раніше застосовувався до опису квазістаціонарних станів атому гелію, використовується для розрахунку процесів іонізації більш складних атомних структур. Досліджено спектроскопічні характеристики найнижчих квазістаціонарних станів атомів Be, Mg, Ca в задачі іонізації цих атомів електронним ударом. Виконано розрахунки енергетичних положень та ширин найнижчих ^1S, ^1P, ^1D, ^1F автоіонізаційних станів атомів Be, Mg та найнижчих ^1P автоіонізаційних станів атома Ca.