

# The Beryllium Atom Lowest Autoionizing States in the Method of Interacting Configurations in the Complex Number Representation

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**Abstract** The beginning of the application of the method of interacting configurations in the complex number representation to the compound atomic systems has been presented. The spectroscopic characteristics of the Be atom in the problem of the electron impact ionization of this atom are investigated. The energies and the widths of the lowest  $^1S$ ,  $^1P$ ,  $^1D$ , and  $^1F$  autoionizing states of Be atom are calculated.

**Keywords** Quasistationary states, Autoionizing states, Interacting configurations

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## 1. Introduction

The method of interacting configurations in the complex number representation (ICCNr method) is applied to the calculation of spectroscopic characteristics of autoionizing states (AIS) of Be atom in the problem of the electron impact ionization of this atom. In particular, the energies and the widths of the lowest ( $^1S$ ,  $^1P$ ,  $^1D$ , and  $^1F$ ) AIS of Be atom are calculated.

The exact quantum mechanical methods are welcome here because the experimental investigations of beryllium are complicated due to its chemical properties. Furthermore, the atomic shell of Be atom is not simple and is not very complex. Therefore, this atom is enough suitable object for the beginning of the application of the ICCNR method to the compound atomic systems investigations.

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 AIS 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 ICCNR method. This method was developed in works [1-3] 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.

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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, see, e. g., [4]. As one can see in the literature [5-14], beryllium atom turns out to be the promising objects for researches.

Here some results from [5-10] are compared with the calculations on the basis of ICCNR method. Further analysis of literature shows that beryllium atom until today is the interesting experimental and theoretical problem, see, e. g., [11-15]. The authors of [11-15] prefer to approbate their experimental and theoretical methods in the investigations of processes in the beryllium atomic shell.

## 2. General Description of the Method

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

Since we deal with the quantum-mechanical three body problem (see the reaction (1) below) let us consider briefly the main methods for studying the three-particle quantummechanical scattering phenomena.

The first well-defined mathematical method is based on Faddeev equations, see, e. g., [16-18]. Indeed, some times the three body problem in quantum mechanics can be solved with the help of Faddeev equations. Nevertheless, this method is applied rarely for the calculations in atomic problems. The reason is in the long-range property of Coulomb potential and, as a consequence, in the slow convergence of the corresponding series. Therefore, usually the method is applied for the simplest atomic systems [16-18]. As an example, the method was applied for the (e, H) system, in which the H<sup>-</sup> bound state and the lowest members of the resonances in both the singlet and the triplet  $J=0$  series were calculated [16]. Further, in [17] the AIS of He atom were calculated. The resonance ionization by fast protons was studied, which was possible for the short-range nuclear potential. In [18] the scattering of electrons and positrons on hydrogen atom below the  $n=2$  threshold was investigated. Thus, the Faddeev equations are not applied for the complex atoms AIS calculations.

On the other hand both the Faddeev and ICCNR methods are based on the Lippmann-Schwinger-“type” equations. Indeed, the Faddeev formalism is started from the indication of the absence of uniqueness in the Lippmann-Schwinger solutions. This fact indicates some similarity between methods. However, the difference appears in T-operator analysis. Moreover, we do not appeal to three particle potential.

Another well-defined mathematical method, which has some similarity to Faddeev approach, is the method of hyperspherical functions (hyperspherical coordinates). The success of this method is evident from [19, 20]. However,

this method is working good only for few body systems (here with Coulomb interaction too) and is not applied for the complex atoms AIS investigations as well.

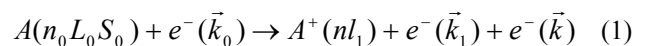
Note that the R-matrix method is the most spread in the complex atoms AIS investigations [21, 22]. This method is widely applied for the scattering of photons and electrons on the complex atoms both in ordinary [21] and B-spline [22] formalism.

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. 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.

The goal of our research is to illustrate 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 atom [4]. The capabilities of the method were illustrated briefly by the example of the atomic ionization by the electron impact [4], which are challenging for researches. 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. The results were reported at the international conference [4]. This paper is the expanded presentation of [4].

## 3. Formalism of the Method

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



Here  $\vec{k}_0$ ,  $\vec{k}_1$ , and  $\vec{k}$  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 looks like

$$\frac{\partial f_{nl_1}}{\partial E}(Q) = \frac{E}{Q^2} \sum_L \left| \langle nl_1 EI | \sum_{j=1}^n \exp(i\vec{Q}\vec{r}_j) | n_0 L_0 S_0 \rangle \right|^2 \quad (2)$$

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  $|nl_1 EI; LS_0\rangle$  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  $|n_0 LS_0\rangle$ .

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 [23], and, in the case of Be atom, this is, as a rule, a Hartree-Fock wave function obtained in the multiconfiguration approximation [24]. The system of equations in the ICCNR method has the following form:

$$\begin{cases} (E_n - E)a_{\lambda n}^{Ei} + \sum_{\lambda'} \int_0^\infty b_{\lambda\lambda'}^{Ei}(E') \cdot V_{n\lambda'}(E') dE' = 0, \\ \sum_m a_{\lambda m}^{Ei} V_{m\lambda'}^*(E') + (E' - E)b_{\lambda\lambda'}^{Ei}(E') = 0. \end{cases} \quad (3)$$

The multipliers

$$a_{\lambda m}^{Ei}, b_{\lambda\lambda'}^{Ei}(E') \quad (4)$$

are the coefficients of expansion of the wave function  $\Psi_\lambda^E(\vec{r}_1, \vec{r}_2)$  in the basis

$$\Psi_\lambda^E(\vec{r}_1, \vec{r}_2) = \sum_m a_{\lambda m}^{Ei} |m\rangle + \sum_{\lambda'} \int_0^\infty b_{\lambda\lambda'}^{Ei}(E') |\lambda' E'\rangle dE' \quad (5)$$

The basis wave functions satisfy the conditions

$$\langle m | \hat{H} | n \rangle = E_n \delta_{nm}, \quad \langle \lambda' E' | \hat{H} | \lambda E \rangle = E \delta_{\lambda\lambda'} \delta(E - E'), \quad (6)$$

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

The formal solution for the second multiplier from (4) is selected in the form

$$b_{\lambda\lambda'}^{Ei}(E') = P \frac{\sum_m a_{\lambda m}^{Ei} V_{m\lambda'}(E)}{E - E'} + \left[ A_{\lambda\lambda'} \pm i\pi \sum_m a_{\lambda m}^{Ei} V_{m\lambda'}(E) \right] \delta(E - E'), \quad (7)$$

where

$$V_{m\lambda}(E) = \langle m | \hat{H} | \lambda E \rangle. \quad (8)$$

The matrix  $A_{\lambda\lambda'}$  depends on the asymptotic properties of the basis functions  $|\lambda E\rangle$ . Substitution of Eq. (7) into Eq. (3) transforms the system of equations obtained in the ICCNR method into a system of linear algebraic equations for the first coefficient from (4)

$$(E_n - E)a_{\lambda n}^{Ei} + \sum_m [F_{nm}(E) - i\gamma_{nm}(E)] a_{\lambda m}^{Ei} = -\sum_{\lambda'} A_{\lambda\lambda'} V_{\lambda n}(E) \quad (9)$$

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

$$W_{nm}(E) = E_n \delta_{nm} + F_{nm}(E) - i\gamma_{nm}(E) \quad (10)$$

where

$$\begin{aligned} \gamma_{nm}(E) &= \pi \sum_\lambda V_{n\lambda}(E) \cdot V_{\lambda m}(E), \\ F_{nm}(E) &= \frac{1}{\pi} \int_0^\infty \frac{\gamma_{nm}(E')}{E - E'} dE'. \end{aligned} \quad (11)$$

The analysis of formulas (10) and (11) 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 (10);
- 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 (10) 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, 2]. The partial amplitudes of the resonance ionization can be determined as follows:

$$T_{|0\rangle \rightarrow |\lambda E\rangle}(E) = t_{\lambda}^{dir}(E) + \sum_m \frac{H_{m\lambda}(E)}{\varepsilon_m(E) + 1}. \quad (12)$$

The quantities in formula (12) are defined by the relations

$$\begin{aligned} t_{\lambda}^{dir}(E) &= \sqrt{C(E)} \langle \lambda E | \hat{t} | 0 \rangle, \\ H_{m\lambda}(E) &= 2\tilde{V}_{m\lambda}(E) [t_m(E) - i\tau_m(E)] \Gamma_m^{-1}(E), \end{aligned} \quad (13)$$

where

$$t_m(E) = \sqrt{C(E)} \langle \tilde{F}_m^E | \hat{t} | 0 \rangle, \quad \tau_m(E) = \sqrt{C(E)} \langle \chi_m^E | \hat{t} | 0 \rangle. \quad (14)$$

Hence, the expressions for the cross-sections become parametrized

$$\sigma_{\lambda}(E) = \sigma_{\lambda}^{dir}(E) + \sum_m \frac{\Gamma_m(E) P_{m\lambda}(E) + \varepsilon_m(E) Q_{m\lambda}(E)}{\varepsilon_m^2(E) + 1}. \quad (15)$$

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

$$N_{am}(E) = \sum_{\lambda \in \alpha} H_{m\lambda}(E) (t_{\lambda}^{dir}(E) + \sum_n \frac{H_{m\lambda}(E)}{\varepsilon_n(E) - \varepsilon_m(E) + 2i})^*. \quad (16)$$

Hence, the resonance ionization cross-section is determined by a collection of the following functions of the total energy  $E$ :  $\sigma_{\lambda}^{dir}(E)$ ,  $N_{am}(E)$ ,  $\varepsilon_m(E)$ , and  $\Gamma_m(E)$ . See more details about the formalism of the method (for two electron systems) in the article [25].

## 4. The Results of the Calculations

Here the electron impact ionization of the Be atom in the interval of AIS excitation is considered.

In work [4], 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 AIS 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 AIS 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 [4]. The results are compared with the energies and the widths of AIS obtained in the problem of electron scattering by a  $\text{Be}^+$  ion in work [8]. 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 [5-10].

**Table 1.** Energies and widths of the lowest AIS ( $^1S$ ,  $^1P$ ,  $^1D$ , and  $^1F$ ) of a beryllium atom obtained in the ICCNR approximation in the problem of the electron-impact ionization of an atom. In work [8], the energies of autoionizing states were calculated in the diagonalization approximation in the framework of the problem of electron scattering by a  $\text{Be}^+$  ion

$^1S$	$E$ , eV	$\Gamma$ , eV	$E$ , eV [8]	$\Gamma$ , eV [8]
$3s^2$	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	$\Gamma$ , eV	$E$ , eV [8]	$\Gamma$ , eV [8]
$3s3p$	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	$\Gamma$ , eV	$E$ , eV [8]	$\Gamma$ , eV [8]
$3s3d$	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	$\Gamma$ , eV	$E$ , eV [8]	$\Gamma$ , eV [8]
$3p3d$	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	-	-

**Table 2.** Comparison of the energies obtained with the use of the ICCNR method for the AIS 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 [5]	$E$ , eV [6]	$E$ , eV [7]
$2p3s$	10.71	10.71	10.93	10.77
$2p3d$	11.84	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 [8]	$E$ , eV [9]	$E$ , eV [10]
$2p3s$	10.71	10.73	10.63	10.91
$2p3d$	11.84	11.85	12.03	11.83
$2p4s$	12.03	12.09	12.09	12.09
$2p4d$	12.42	12.49	12.61	12.44

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 energies in the problem of electron scattering by  $\text{Be}^+$  ions performed in work [8] 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. 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 [1-3], was used to calculate the ionization processes of more complicated atomic systems. The spectroscopic characteristics of the lowest AIS of the Be atom were studied in the problem of the electron-impact ionization of these atom. The energies and the widths of the lowest autoionizing states ( $^1S$ ,  $^1P$ ,  $^1D$ , and  $^1F$ ) of Be 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 AIS of multielectron atoms and the processes of electron ionization and excitation of atoms.

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