COMPARISON OF TWO THEORETICAL METHODS FOR STUDYING 2–2 TRANSITIONS IN BERYLLIUM ISOELECTRONIC SEQUENCE

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Theoretical investigation of characteristics of allowed dipole 2–2 transitions in beryllium isoelectronic sequence is performed applying two different theoretical methods: the relativistic many-body perturbation theory and the configuration interaction method. The data on oscillator strengths are obtained for ions with nucleus charge ranging from 4 till 29. The calculated data reveal a very good coincidence of these two methods almost for all investigated ions. The comparison of results of the present work with experimental and theoretical data of other authors for N III and Fe XXIII shows that the level of accuracy of the obtained oscillator strength values is high enough for interpretation of the experimental data as well as for modelling of the different types of plasma.

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1. Introduction

Few-electron systems are simple objects allowing one to perform the wide computations of spectral characteristics with rather an exact account of the correlation and relativistic effects. One of such kind of systems is the four-electron ions of the beryllium isoelectronic sequence. They constantly attract attention of both experimentalists and theorists. Numerous publications devoted to investigations of both the energy spectra and the transition characteristics confirm this. The data for the particular ions are presented in papers [1–12] and references therein. The aim of the present work is to investigate the allowed 2–2 transitions in the long ($Z = 4, \ldots, 29$) beryllium isoelectronic sequence calculated within two different approaches: the relativistic many-body perturbation theory (PT) and the configuration interaction method (CI).

In the following section a short description of two applied methods is presented. An explicit description of the configuration interaction method on the basis of transformed radial orbitals is available in papers [13–21]. A detailed specification of the relativistic many-body perturbation theory used in this work is presented in [22]. In the third section the obtained results are discussed and compared with the data presented in the NIST database. In addition, the data for N IV and Fe XXIII are widely compared with results obtained from literature. The main conclusions are made at the end of the paper.

2. The methods of calculations

2.1. Configuration interaction

The transition probabilities were calculated by the configuration interaction method on the basis of transformed radial orbitals with a variable parameter (TRO) [13]. First of all the Hartree–Fock equations were solved for the configuration $1s^2 2s 2p$. Further these radial orbitals (RO) were used to obtain TROs which described the virtual excitations of electrons to the shells with $3 \leq n \leq 10$ and $l \leq 6$. TROs are formed out of the Hartree–Fock functions as follows:

$$P_{\text{TRO}}(nl|r) =$$

$$N \left(f(k, m, B|r) \, P_{\text{HF}}(n_0 l_0|r) - \sum_{n' < n} P(n'l|r) \times \right.$$

$$\left. \int_0^\infty P(n'l|r) \, f(k, m, B|r) \, P_{\text{HF}}(n_0 l_0|r) \, \mathrm{d}r \right). \quad (1)$$

Here N is a normalization factor. The first term in the brackets represents the transformation itself and the second one is necessary to ensure the orthogonality of the radial orbitals. An exponential transformation of the form

$$f(k, m, B|r) = r^k \exp\left(-Br^m\right),$$

$$\text{where } k \geq l - l_0, \quad k > 0, \quad m > 0, \quad B > 0, \quad (2)$$

was used as the transforming function. The criterion in determining the optimal values of the integer parameters k and m and the real parameter B is the maximum of the averaged energy correction, expressed in the second order of perturbation theory:

$$\Delta E(K_0, K') = \quad (3)$$

$$\frac{\sum\limits_{TLST'} (2L+1)(2S+1)\langle K_0 TLS \| H \| K'T'LS \rangle^2}{g(K_0)\left[\bar{E}(K') - \bar{E}(K_0)\right]}.$$

The analytical expressions of the mean values presented in the numerator and the denominator in (3) are available in [14, 15].

The basis of 46 TROs was set. Using TROs one may obtain high precision results for both the energy spectra and the transition characteristics (see for example the results of calculations for highly charged ions: Cl X [23], K XI [24], S X, [25], Ca IX [26], Ar X [27], Fe XXII [28]). TROs were also successfully applied investigating the two-electron transitions in the boron isoelectronic sequence [29] studied in the present work as well. These radial orbitals are not inferior to the best orbitals for CI, i. e. the solutions of the multiconfiguration Hartree–Fock–Jucys equations [30], in respect of their effectiveness. We gave these equations the name of Adolfas Jucys traditionally, as he was the first to obtain the general form of the equations used today. A detailed comparison of the properties of TROs to the solutions of Hartree–Fock–Jucys equations has been performed in [19].

The obtained basis of ROs is used to describe both the even and the odd configurations. Naturally the initial Hartree–Fock radial orbitals are not quite adequate for the even configurations ($1s^2 2s^2$ and $1s^2 2p^2$) as the Hartree–Fock equations have been solved for the configuration $1s^2 2s 2p$. However, this incorrectness is rapidly removed when the configuration superposition is performed. Moreover, when calculating the transition characteristics, the same RO basis for the description of both the initial and final configurations enables one to avoid problems concerned with the need for ac-

count of the non-orthogonality of the basis in the case when they are not the same.

The one-electron and two-electron virtual excitations of all electrons from the investigated configurations to all possible states within the predetermined RO basis were used to obtain the admixed configurations. Then 1321 even and 991 odd admixed configurations were formed. However, there is no necessity to take into account all possible admixed configurations as their importance is far from being the same. In order to evaluate the input of the particular admixed configurations K' to the wave function of the adjusted configuration K_0 [14, 15, 18] the averaged weight coefficients are used:

$$W(K_0, K') = \quad (4)$$

$$\frac{\sum\limits_{TLST'} (2L+1)(2S+1)\langle K_0 TLS \| H \| K'T'LS \rangle^2}{g(K_0)\left[\bar{E}(K') - \bar{E}(K_0)\right]^2}.$$

Only those configurations with averaged weight exceeding 10^{-8} are used in this calculation. As follows from our experience [20, 21], the value of the selection criterion allows us to take into account all necessary configurations. It is known that the correlation effects decrease together with the growth of the ionization degree. Correspondingly, the number of the selected admixed configurations is changing along the investigated isoelectronic sequence. Thus the number has decreased to 862 for the even admixed configurations and to 634 for the odd ones, when $Z = 4$. That is, in both cases the number of configurations is reduced by a third approximately. In the case when $Z = 29$ the number of the admixed configurations decreased to 540 and 357 correspondingly after selection. It is seen that the number of accounted even admixed configurations for this degree of ionization amounts to approximately one third of the number for neutral beryllium and even more for the odd ones. The number of the even admixed configurations is greater than that of the odd ones in all cases. It is caused by the fact that two even configurations and only one odd configuration are adjusted. It is necessary to mention that a part of the admixed configurations for the $1s^2 2s^2$ adjusted configuration coincides with the admixed configurations for the configuration $1s^2 2p^2$. At the same time, taking into account the corrections to both these configurations enables one to consider not only the two-electron excitations, but also the excitations of a higher order, due to the strong mixing of $1s^2 2s^2$ and $1s^2 2p^2$.

The selected configurations contain a big number of terms. This causes a necessity to calculate and to diago-

nalize huge matrices of the energy operator. In the case $Z = 4$ all even configurations contain 26010 terms and all odd ones 18140 terms. The number of terms can be reduced to 5695 and 4059 correspondingly if one takes into consideration the fact that the operator of electron Coulomb interaction used for account of the correlation effects is diagonal not only with respect to the total momentum J, but also with respect to the total orbital and spin momenta LS. The number of the accounted terms can be reduced by approximately two times down to 2693 and 2084 after rearranging the virtual electrons by moving them to the beginning of the list of active shells as it is described in [16, 17]. In this way the amount of the accounted terms decreases by almost ten times comparing to the initial one. The analogous reduction of the number of terms was performed for all degrees of ionization.

The reduced system of terms was used to form the energy operator matrix within the Breit–Pauli approach. The methods described in [16, 20] were used to reduce the order of matrices and to accelerate their formation and diagonalization. The eigenenergies and eigenfunctions obtained after diagonalization were used for calculating the characteristics of the electric dipole transitions between the investigated configurations. In calculations the computer programs from the complex [31] were used along with our own codes.

2.2. Perturbation theory

The atomic systems satisfy the Schrödinger equation

$$H |\Psi\rangle = E |\Psi\rangle \,, \tag{5}$$

where H is the "no-pair" Hamiltonian given by

$$H = H_0 + V_{\mathrm{I}} \,, \tag{6}$$

Here the model Hamiltonian H_0 is given by

$$H_0 = \sum_i h(i) \,, \tag{7}$$

with

$$h = c\,\boldsymbol{\alpha} \cdot \boldsymbol{p} + (\beta - 1)mc^2 + V_{\mathrm{nuc}}(r) + U(r) \,. \tag{8}$$

In Eq. (8), the nuclear Coulomb potential, $V_{\mathrm{nuc}}(r)$, in general includes the effect of the finite size of the nucleus. The model potential $U(r)$ accounts approximately for the effect of the electron–electron interactions. In the present calculations, we choose to be the frozen-core Hartree–Fock potential. In Eq. (6), the perturbation V_{I} is given by

$$V_{\mathrm{I}} = \sum_{i<j} \Lambda_+ \frac{1}{r_{ij}} \Lambda_+ - \sum_i \Lambda_+ U(r_i) \Lambda_+ \,, \tag{9}$$

where Λ_+ is the positive-energy projection operator.

We expand the exact wave function $|\Psi\rangle$ and the exact energy E in powers of V_{I}:

$$E = E^{(0)} + E^{(1)} + \dots \,, \tag{10}$$

$$|\Psi\rangle = |\Psi^{(0)}\rangle + |\Psi^{(1)}\rangle + \dots \,. \tag{11}$$

Substituting Eqs. (10) and (11) into (5) one gets

$$\left(H_0 - E^{(0)}\right)|\Psi^{(0)}\rangle \tag{12}$$

and

$$\left(H_0 - E^{(0)}\right)|\Psi^{(1)}\rangle = \left(E^{(1)} - V_{\mathrm{I}}\right)|\Psi^{(0)}\rangle \,. \tag{13}$$

We now limit the discussion to atoms with two valence electrons outside a closed core. A zeroth-order wave function describing an atomic state with angular momentum JM may be written as

$$|\Psi_{JM}^{(0)}\rangle = \sum_{(vw)\in P} C_{vw}|\Phi_{vw}^{(0)}\rangle \,, \tag{14}$$

where C_{vw} and $|\Phi_{vw}^{(0)}\rangle$ are the configuration weight coefficients and the configuration wave functions, respectively. The configurations included in the zeroth-order wave function span the model space P. In the present calculations, we include all possible configurations within the $n = 2$ complex in the model space. The reference states are described by multiconfiguration wave functions that take account of the valence–valence correlations. The core–valence and core–core correlations are treated by perturbation. It is possible in this way to take into account strongly interacting configurations to all orders and treat the weakly interacting ones by means of low-order perturbation.

The transition amplitude is the reduced matrix element of the transition operator

$$T(\omega) = -c\,\boldsymbol{\alpha} \cdot \boldsymbol{A}(\omega) \,, \tag{15}$$

where ω is the photon energy. The photon energy can also be expanded in powers of V_{I}:

$$\omega = \omega^{(0)} + \delta\omega^{(1)} + \dots \,, \tag{16}$$

where $\omega^{(0)}$ is the zeroth-order photon energy, while $\delta\omega^{(1)}$ is the first-order correction to the photon energy.

Consequently, the transition operator can also be expanded in powers of V_I:

$$T(\omega) = T^{(0)}(\omega) + T^{(1)}(\omega) + \dots, \qquad (17)$$

where

$$T^{(0)}(\omega) = T(\omega^{(0)}) \qquad (18)$$

and

$$T^{(1)}(\omega) = \delta\omega^{(1)} \frac{\mathrm{d}T(\omega^{(0)})}{\mathrm{d}\omega}. \qquad (19)$$

The first-order transition amplitude is given by

$$\langle F\|T(\omega)\|I\rangle^{(1)} = \langle \Psi_F^{(0)}\|T(\omega^{(0)})\|\Psi_I^{(0)}\rangle. \qquad (20)$$

The second-order transition amplitude is

$$\langle F\|T(\omega)\|I\rangle^{(2)} = \langle \Psi_F^{(1)}\|T(\omega^{(0)})\|\Psi_I^{(0)}\rangle$$

$$+ \langle \Psi_F^{(0)}\|T(\omega^{(0)})\|\Psi_I^{(1)}\rangle$$

$$+ \delta\omega^{(1)} \left\langle \Psi_F^{(0)} \left\| \frac{\mathrm{d}T(\omega^{(0)})}{\mathrm{d}\omega} \right\| \Psi_I^{(0)} \right\rangle, \quad (21)$$

The detailed description of the used method is available in [22]. The absorption oscillator strength is

$$f_{FI} = \frac{6c^2}{\omega(2J_I + 1)} |\langle F\|T(\omega)\|I\rangle|^2, \qquad (22)$$

where I and F are the lower and upper levels, respectively. The Einstein A coefficient for the emission process from F to I is

$$A = \frac{2\omega^2}{c^3} \frac{2J_I + 1}{2J_F + 1} f_{FI}. \qquad (23)$$

The analogous definitions of the physical values have been used within the CI method as well.

3. Discussion of the results

The symmetrized oscillator strengths gf (the absolute values of oscillator strengths f multiplied by the statistical weight g) of the allowed transitions $2s^2$–$2s2p$ and $2s2p$–$2p^2$ of the beryllium isoelectronic sequence for ions with the nucleus charge from 4 to 29, obtained by the described calculations, are presented in Table 1. As seen from the table the results of both methods are in good coincidence for the vast majority of the nuclear charges. In most cases the mean deviations do not exceed a few tenths of a percent. An essential difference of values of the oscillator strengths appears only for some transitions between the levels of singlet terms ($2s2p\ ^1P_1 - 2s^2\ ^1S_0$, $2p^2\ ^1S_0 - 2s2p\ ^1P_1$, $2p^2\ ^1D_2 -$

$2s2p\ ^1P_1$) from the neutral beryllium to doubly ionized carbon. It happens because taking into account the correlation effects is much more complicated in such systems both for the perturbation theory method and for the configuration interaction. It is necessary to perform appreciably more extensive and complex calculations to get the more precise values of the mentioned oscillator strengths. In the case of the CI method one can make the results more accurate by using the solutions of the Hartree–Fock–Jucys equations but not the Hartree–Fock functions to describe the adjusted configurations themselves. The mentioned deviations vanish rapidly as the ionization degree grows.

Table 1 also contains the oscillator strengths taken from the NIST [32] database when they are available there. The deviations of the NIST data from the results of theoretical calculations do not exceed few percent for the majority of lines. Here the deviations are less than 1% in many cases. Only some lines of the ions B II, F VI, and Ne VII are exceptional in this context. These values of the oscillator strengths of the ions are marked out in bold italic in the table. The values are not only essentially different from the data of the present work, but also obviously out of the isoelectronic sequence, as it is clearly seen from Table 1. Most likely the mentioned deviations are caused by the fact that the data on these transition characteristics are not renewed for a long period as it follows from [32].

The transition probabilities data are not presented in the table in order to shorten it. However the comparison of those values was performed as well. The mean deviations of the transition probabilities almost coincide in their values with the corresponding deviations of the oscillator strengths starting from the doubly ionized carbon. Yet the tendency of the increase of mismatch between the transition probabilities calculated by two different methods springs up starting from the nucleus charges exceeding 20. These mismatches can reach few percent whereas the oscillator strengths remain in a much better coincidence when $Z = 29$. The noted behaviour is connected to a difference of dependence of the oscillator strengths and transition probabilities on transition energy. The experimental energy values were used while performing the calculations within the PT approach. Consequently, the increase of mismatches of the transition probability values is caused by the errors when calculating the energy differences within the Breit–Pauli approximation. It is quite natural, as the relativistic corrections are determined up to the second order of the fine structure constant on the basis of non-relativistic ROs within this approach. Moreover, the

Table 1. Oscillator strengths (gf) of the 2–2 transitions in the beryllium isoelectronic sequence.

Z	PT	CI	NIST	PT	CI	NIST	PT	CI	NIST
	$2s2p\ ^1P_1 - 2s^2\ ^1S_0$			$2p^2\ ^1S_0 - 2s2p\ ^1P_1$			$2p^2\ ^1D_2 - 2s2p\ ^1P_1$		
4	1.200	1.394	1.380	0.786	0.901		0.381	0.213	
5	0.926	0.999	*1.100*	0.603	0.646	*0.360*	0.585	0.541	*1.980*
6	0.725	0.759	0.759	0.492	0.486	0.486	0.573	0.592	0.545
7	0.592	0.611	0.611	0.408	0.400	0.399	0.525	0.522	0.514
8	0.500	0.511	0.512	0.348	0.342	0.342	0.474	0.472	0.470
9		0.441	*0.620*	0.306	0.299	*0.165*	0.432	0.429	*0.810*
10	0.382	0.388	*0.056*		0.267			0.392	
11		0.347	0.335	0.244	0.241	0.240	0.360	0.361	0.360
12	0.310	0.314	0.314	0.222	0.219	0.219	0.333	0.334	0.333
13		0.287	0.278	0.203	0.201	0.200	0.312	0.311	0.312
14	0.262	0.265	0.266	0.188	0.186	0.193	0.291	0.291	0.300
15	0.244	0.247	0.240	0.175	0.173		0.274	0.274	0.294
16	0.229	0.231		0.164	0.162		0.259	0.259	
17	0.216	0.218			0.153		0.246	0.246	
18	0.204	0.206		0.145	0.144			0.234	
19	0.195	0.196		0.137	0.137		0.223	0.222	
20	0.186	0.188		0.131	0.130		0.213	0.212	
21	0.179	0.180	0.182	0.125	0.124	0.135	0.204	0.203	0.214
22	0.172	0.173	0.175	0.119	0.119	0.129	0.195	0.193	0.204
23	0.166	0.168	0.169	0.115	0.114	0.123	0.186	0.185	0.194
24	0.161	0.163	0.164	0.110	0.110	0.118	0.178	0.177	0.185
25	0.157	0.158	0.159	0.107	0.106	0.113	0.171	0.169	0.177
26	0.153	0.154	0.155	0.103	0.103	0.109	0.164	0.163	0.169
27	0.150	0.151	0.152	0.100	0.100	0.105	0.158	0.157	0.162
28	0.147	0.148	0.149	0.097	0.097	0.103	0.153	0.152	0.157
29	0.144	0.145		0.095	0.095		0.149	0.148	
	$2p^2\ ^3P_0 - 2s2p\ ^3P_1$			$2p^2\ ^3P_1 - 2s2p\ ^3P_2$			$2p^2\ ^3P_1 - 2s2p\ ^3P_1$		
4	0.450	0.454	0.453	0.560	0.568	0.570	0.336	0.341	0.342
5	0.342	0.345	0.330	0.429	0.431	0.415	0.257	0.258	0.237
6	0.272	0.273	0.272	0.340	0.341	0.340	0.204	0.205	0.204
7	0.225	0.225	0.225	0.281	0.281	0.281	0.169	0.169	0.169
8	0.191	0.191	0.191	0.238	0.238	0.238	0.143	0.143	0.143
9	0.166	0.166	0.156	0.207	0.207	*0.190*	0.125	0.125	0.117
10	0.146	0.147	0.151	0.182	0.183	0.188	0.110	0.110	0.113
11	0.131	0.131	0.131	0.163	0.164	0.163	0.0987	0.0989	0.0984
12	0.119	0.119	0.118	0.148	0.148	0.147	0.0897	0.0898	0.0894
13	0.109	0.109	0.108	0.135	0.135	0.135	0.0822	0.0823	0.0819
14	0.100	0.100	0.102	0.124	0.124	0.126	0.0759	0.0761	0.0771
15	0.0930	0.0933		0.115	0.115		0.0708	0.0708	
16	0.0867	0.0872		0.107	0.107		0.0663	0.0664	
17		0.0819			0.101			0.0625	
18	0.0768	0.0773		0.0940	0.0946		0.0591	0.0592	
19	0.0729	0.0732		0.0885	0.0893		0.0561	0.0563	
20	0.0690	0.0697		0.0835	0.0846		0.0537	0.0538	
21	0.0660	0.0665	0.0678	0.0795	0.0804	0.0820	0.0516	0.0516	0.0528
22	0.0630	0.0637	0.0660	0.0755	0.0765	0.0775	0.0495	0.0497	0.0507
23	0.0606	0.0611	0.0624	0.0720	0.0731	0.0740	0.0477	0.0480	0.0489
24	0.0582	0.0589	0.0597	0.0690	0.0700	0.0705	0.0462	0.0465	0.0474
25	0.0561	0.0568	0.0573	0.0660	0.0671	0.0675	0.0450	0.0451	0.0459
26	0.0543	0.0550	0.0555	0.0635	0.0645	0.0650	0.0438	0.0439	0.0447
27	0.0525	0.0533	0.0540	0.0610	0.0621	0.0620	0.0426	0.0429	0.0435
28	0.0507	0.0518	0.0522	0.0585	0.0598	0.0600	0.0417	0.0420	0.0426
29	0.0492	0.0504		0.0565	0.0578		0.0411	0.0411	

Table 1 (continued).

Z	PT	CI	NIST	PT	CI	NIST	PT	CI	NIST
	$2p^2\,{}^3\mathrm{P}_1 - 2s2p\,{}^3\mathrm{P}_0$			$2p^2\,{}^3\mathrm{P}_2 - 2s2p\,{}^3\mathrm{P}_2$			$2p^2\,{}^3\mathrm{P}_2 - 2s2p\,{}^3\mathrm{P}_1$		
4	0.450	0.454	0.455	1.685	1.703	1.700	0.561	0.568	0.570
5	0.343	0.345	0.330	1.285	1.292	1.250	0.429	0.431	0.420
6	0.273	0.273	0.272	1.020	1.024	1.021	0.342	0.342	0.341
7	0.225	0.225	0.225		0.844	0.843	0.281	0.282	0.281
8	0.191	0.191	0.191	0.715	0.716	0.716	0.239	0.239	0.239
9	0.166	0.166	0.160	0.620	0.622	***0.550***	0.209	0.208	0.198
10	0.147	0.147	0.151	0.550	0.550	0.565	0.185	0.185	***0.201***
11	0.132	0.132	0.132	0.493	0.493	0.491	0.166	0.166	0.165
12	0.120	0.120	0.120	0.447	0.447	0.445	0.151	0.151	0.150
13	0.110	0.110	0.110	0.409	0.409	0.408	0.139	0.139	0.139
14	0.102	0.102	0.104	0.377	0.377	0.382	0.129	0.129	0.131
15	0.0955	0.0955		0.350	0.349	0.360	0.121	0.121	0.120
16	0.0898	0.0898		0.326	0.325		0.114	0.114	
17		0.0849			0.303			0.108	
18		0.0807		0.285	0.284		0.103	0.102	
19	0.0771	0.0771		0.267	0.265		0.0987	0.0981	
20	0.0740	0.0740		0.249	0.247		0.0951	0.0943	
21	0.0713	0.0714	0.0733	0.232	0.230	0.238	0.0918	0.0911	0.0945
22	0.0691	0.0691	0.0709	0.216	0.214	0.221	0.0891	0.0883	0.0918
23	0.0671	0.0671	0.0688	0.200	0.198	0.204	0.0870	0.0860	0.0894
24	0.0655	0.0655	0.0670	0.184	0.182	0.188	0.0852	0.0841	0.0873
25	0.0641	0.0641	0.0656	0.169	0.168	0.175	0.0837	0.0827	0.0858
26	0.0630	0.0629	0.0643	0.155	0.154	0.158	0.0828	0.0817	0.0849
27		0.0620	0.0633	0.142	0.142	0.145	0.0822	0.0812	0.0843
28	0.0613	0.0612	0.0625	0.131	0.131	0.133	0.0822	0.0812	0.0843
29	0.0607	0.0606		0.120	0.121		0.0822	0.0816	

obtained data corroborate the fact that the Breit–Pauli approach in conjunction with the CI method can be successfully used for the calculations of the transition characteristics of atoms ionized 20 and more times.

As mentioned earlier, there are numerous publications devoted to the theoretical and experimental investigations of particular transitions in the ions of beryllium isoelectronic sequence found in the literature. A consistent comparison of all available data would have increased the size of this work substantially and it would obviously exceed the framework of the task. Therefore we content ourselves with a comparison of results of the present work with the data obtained in literature only for the cases of two widely investigated ions: N IV from the beginning of the investigated sequence and Fe XXIII from the end of it.

The oscillator strengths and probabilities of the emissive transitions for the nitrogen ion are presented in Table 2. In the table these values are compared with the results of calculations obtained within the multiconfiguration Hartree–Fock approach (MCHF), i. e. using the Hartree–Fock–Jucys equations, the configuration interaction method performed by the computer code CIV3 [33], the multiconfiguration Dirac–Fock approximation

(MCDF), and the relativistic many-body perturbation theory (RMBPT) from paper [9]. The experimental data are also presented [2, 3]. The values from this work are in a very good coincidence with the results presented in [6] for all the transitions $2p^2\,{}^3\mathrm{P}_J - 2s2p\,{}^3\mathrm{P}_{J'}$, therefore they are only partially presented in the table. As seen from the table, the results of this work agree well with the CIV3, MCHF, MCDF, and the experimental data. Then the CI approach demonstrates a little higher precision of the results. It happens because the correlation corrections are taken into account more accurately due to the higher number of interacting configurations within the approach. The reasons of the existing deviations from the results of perturbation theory presented in [9] are explained in [35].

The data on transition characteristics within the Fe XXIII ion are presented in Table 3. In this case the investigated theoretical methods are in a quite good coincidence among them and with the experimental data. At the same time it is seen that the deviations of values of the transition probabilities between CI and PT are higher than the corresponding deviations of the oscillator strengths. The reason of this mismatch has been discussed earlier. The comparison of data for other ions

Table 2. Characteristics of electron transitions in N IV.

gf	A (10^9 s^{-1})	Method	Ref.
$2s2p\ ^1P_1 - 2s^2\ ^1S_0$
0.5920	2.25	PT	Present work
0.6107	2.32	CI	Present work
0.609	2.31	CIV3	[6]
0.609	2.13	MCHF	[6]
0.6099		MCDF	[34]
0.6117		MCDF	[8]
	1.94	RMBPT	[9]
0.619±0.022		exp.	[2]
	2.4±0.1	exp.	[3]
$2p^2\ ^1S_0 - 2s2p\ ^1P_1$
0.4080	2.99	PT	Present work
0.3997	2.92	CI	Present work
0.400	2.93	CIV3	[6]
0.396	2.89	MCHF	[6]
	2.84	RMBPT	[9]
	2.9±0.2	exp.	[3]
0.390±0.033		exp.	[2]
$2p^2\ ^1D_2 - 2s2p\ ^1P_1$
0.5250	0.237	PT	Present work
0.5217	0.236	CI	Present work
	0.229	RMBPT	[9]
	0.24±0.2	exp.	[3]
0.540±0.027		exp.	[2]
$2p^2\ ^3P_1 - 2s2p\ ^3P_2$
0.281	0.730	PT	Present work
0.281	0.730	CI	Present work
0.281	0.731	CIV3	[6]
0.280	0.729	MCHF	[6]
$2p^2\ ^3P_0 - 2s2p\ ^3P_1$
0.225	1.76	PT	Present work
0.225	1.76	CI	Present work
0.223	1.76	CIV3	[6]
0.224	1.75	MCHF	[6]
$2p^2\ ^3P_1 - 2s2p\ ^3P_1$
0.169	0.440	PT	Present work
0.169	0.440	CI	Present work
0.169	0.440	CIV3	[6]
0.168	0.439	MCHF	[6]

Table 3. Characteristics of electron transitions in Fe XXIII.

gf	A (10^9 s^{-1})	Method	Ref.
$2s2p\ ^1P_1 - 2s^2\ ^1S_0$
0.1530	19.3	PT	Present work
0.1541	19.0	CI	Present work
0.1539		MCDF	[8]
	19.0jh	RMBPT	[9]
0.156±0.015		exp.	[3]
$2p^2\ ^1S_0 - 2s2p\ ^1P_1$
0.1029	30.9	PT	Present work
0.1028	30.2	CI	Present work
	30.8	RMBPT	[9]
0.096±0.014		exp	[3]
$2p^2\ ^1D_2 - 2s2p\ ^1P_1$
0.1638	44.6	PT	Present work
0.1627	43.6	CI	Present work
	45.0	RMBPT	[9]

the nucleus charges. In addition, the applied configuration interaction method enables one to obtain a little more precise results for the neutral beryllium and first ions. At the same time the reliability of results obtained using the perturbation theory is higher when the charge of the nucleus approaches 30. It is caused by a more precise account of the relativistic effects within this theory.

The performed comparison showed that the results are in a quite good coincidence with the experimental and theoretical data of other authors. All these facts and the mutual agreement of the output of two methods enable us to assert that the applied methods are reliable enough and the obtained results can be used for interpretation of the experimental data as well as for modelling of the different types of plasma.

found in the literature but not presented in the paper in order to make it shorter reveals the same behaviour.

4. Conclusion

The performed calculations of characteristics of the allowed 2–2 transitions in the ions of beryllium isoelectronic sequence revealed, that both approximations used in the paper (relativistic many-body perturbation method and configuration interaction method on the basis of the transformed radial orbitals) produce the results in a very good coincidence within a wide range of

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DVIEJŲ TEORINIŲ METODŲ LYGINIMAS NAGRINĖJANT 2–2 ŠUOLIUS BERILIO IZOELEKTRONINĖJE SEKOJE

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Santrauka

Atliktas teorinis leistinų elektrinių dipolinių šuolių 2–2 tyrimas berilio izoelektroninei sekai. Branduolių krūviams nuo 4 iki 29 tyrimas atliktas dviem artiniais – konfigūracijų superpozicija ir trikdžių teorija. Gautas geras šuolių tikimybių ir osciliatorių stiprių, gautų skirtingais teoriniais metodais, tarpusavio sutapimas esant

įvairiems jonizacijos laipsniams. Literatūros duomenų N III ir Fe XXIII jonams palyginimas su šio darbo rezultatais patvirtina pakankamai aukštą pastarųjų patikimumą.

Taip pat nurodytas esminis gautų osciliatorių stiprių nesutapimas su NIST duomenų bazės duomenimis kai kurioms B II, F VI ir Ne VII jonų linijoms.