Calculations of Energy Levels Using the Weakest Bound Electron Potential Model Theory

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In this paper, we introduce a new method for calculation of energy levels in detail and give our results for several iso-spectrum-level series as examples: [He] $2s2p\ ^1P_1$, [He] $2s2p\ ^3P_0$, [He] $2s2p\ ^3P_2$, and [He] $2s3s\ ^3S_1$ series of Be-like sequence; [Ne] $3s^23d\ ^2D_{3/2}$ series and [Ne] $3s^23d\ ^2D_{5/2}$ series of Al-like sequences; [Ne] $4p\ ^2P_{1/2}$ series, [Ne] $5d\ ^2D_{5/2}$ series, and [Ne] $6f\ ^2F_{7/2}$ series of Na-like sequences. In the method $I(Z) = T_{\lim}(Z) - T(Z,n)$, where $I(Z)$, $T_{\lim}(Z)$, and $T(Z,n)$ denote ionization potential, series limit, and energy level of a given member, respectively. The expression of non-relativistic part of $I(Z)$ is derived from weakest bound election potential model theory and relativistic effects of $I(Z)$ are included by using a six-order polynomial in Z. Our results are compared with the experimental data and with those obtained by other theoretical method.

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1. Introduction

The energy levels are widely applied in many fields, such as plasma diagnosis, astrophysics, laser development, and analytical chemistry. Therefore, more and more attention has been paid on calculations of high--precision energy levels of atoms and ions. Many theoretical methods have been developed in this field: multiconfiguration Hartree–Fock (MCHF) method [1–3], multiconfiguration Dirac–Hartree–Fock (MCDHF) method [1–3], configuration interaction (CI) method [4–7], relativistic many-body perturbation theory (RMBPT) [8–14], and weakest bound election potential model (WBEPM) theory [15–23], etc.

In recent years, many excellent works have been done by theoretical researchers. The MCHF method has been widely used to calculate properties of atoms and ions including energy levels. Irimia and Fischer reported energy levels and transition probabilities of neutral argon using both MCHF method and MCDHF method [1]. Fischer and Tachiev also applied MCHF method to the study of energy levels and lifetimes for the Be-like to Ne-like sequences [2]. Two years later, the same group reported an extension of this work to the sequences with 11–18 electrons [3]. In their calculations, the MCHF approach was used for obtaining the "best" radial functions for the interacting terms and the relativistic effects were included through the Breit–Pauli approximation. Dzuba et al. used both Hartree–Fock (HF) and CI method to study the energy levels and lifetimes of Nd(IV), Pm(IV), Sm(IV), and Eu(IV) [4]. They also reported energy levels of Ge, Sn, Pb [5] and barium and radium [6, 7]. They started their calculations from the relativistic Hatree–Fock method and used CI method to treat the interaction between valence electrons. Another powerful method in this field is RMBPT. Yb-, Al-, Ga-like ions have been investigated by this method [8–10]. Energy levels of silver, beryllium, magnesium, francium and zinc isoelectronic sequences were also studied by this method [11–14]. The core–valence correlations are included beyond the second- or third-order of RMBPT. Since the WBEPM theory was proposed [15], many studies have been performed to calculate energy levels for atoms and ions [16–24]. In these works, the authors used the concept of the spectrum--level-like series and a new formula taking perturbation into account for calculation. Excellent results are obtained in those works. Deviations between the theoretical results and experimental values are generally smaller than 1 cm^{-1}.

The purpose of this paper is to introduce another new method to calculate energy levels proposed by one of authors (N.W.Z), recently [25]. After introducing the concept of iso-spectrum-level series, we give the results of several iso-spectrum-level series including Be-, Al-, and Na-like sequence as examples. According to the WBEPM theory, the expression of nonrelativistic ionization potential is written as a function with two-order in Z. The relativistic effects are included by using a six-order polynomial in Z. We compare our results with the experimental data and with those obtained by other theoretical method.

2. The conception of the iso-spectrum-level series

In our previous works, the conception of the iso--spectrum-level series has already been proposed and used to calculate the ionization potential [26–29]. In order to describe our method clearly, we introduce the conception of the iso-spectrum-level series first. The conception of iso-electronic series is usually used in the study

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for the ionization energies of ground state. All members (atom and ions) in an isoelectronic series have the same electron configuration. As a result, the conception of isoelectronic series is associated with the electron configuration and cannot provide the information relating to the terms or energy levels. However, for the study of ground state, all systems lie in the lowest energy state. Therefore, the conception of isoelectronic series is convenient to investigate the regularities of ionization energies of ground state. But for the atoms or ions with excited electrons, each electron configuration usually gives rise to several terms and each term splits into several spectral levels further. Under this situation, the conception of iso-electronic series is too rough to study the energies. Therefore, we introduce the conception of the iso--spectrum-level series study of the general regulations of excited states of atoms. An iso-spectrum-level series is a series of energy levels that is composed of energy levels with the same spectral level symbol in a given iso--electronic series. For example, Be(I) ([He] $2s3p\ ^3P_1$), B(II) ([He] $2s3p\ ^3P_1$), ..., O(V) ([He] $2s3p\ ^3P_1$), ..., make up an iso-spectrum-level series named Be(I) ([He] $2s3p\ ^3P_1$). From the definition, in a given iso-spectrum--level series, not only the electron configuration but also the spectrum energy levels is defined. The only variable parameter is the nuclear charge Z. Therefore, the ionization energy of WBE in a given iso-spectrum-level series could be approximate to a function of nuclear charge Z.

3. Theory and method

WBEPM theory is based on the consideration of the dynamic successive ionization, the choice of zero energy in quantum mechanics and the separation of the weakest bound electron (WBE) and non-weakest bound electrons (NWBE) [15, 16].

A free particle with N electrons and a nucleus of charge $+Ze$ in its ground state can give rise to N stages of ionization. The ionized species in N successive ionization stages are, respectively, neutral atom, unipositive ion, ..., $+(Z-1)$ ion. The conception of WBE is referred to the definition of the ionization of a free particle: the ionization potential for a free particle is defined as the energy required completely to move the WBE from the particle. Therefore, we classified the electrons in an atom or ion system into two types, WBE and NWBE. The WBE is the electron which is most weakly bound to the system and excited or ionized first, the rest electrons are called NWBE. In terms of excitation or ionization, the WBE in a given system differs from the rest of the electrons in behavior. We can separate the WBE and the NWBE, and the problem of the WBE can be treated as a one-electron problem. Each electron in the N-electrons system acts sooner or later as a WBE in the ionization procedure. By removing the first, the second, ... N-th WBE, an N-electrons atom can give N stages of ionization. Each stage of successive ionization processes corresponds to the removal of a WBE from the related subsystem. Accurate treatment of the WBE can provide accurate knowledge of atomic and ionic properties.

As the ionization energy is defined as the energy required completely removing the weakest bound electron from an atom or an ion in its ground or excited states, the energy of a level in spectrum-level-like series [17–24] can be written as

$$T(n) = T_{\rm lim} - I_{\rm exp}, \tag{1}$$

where $T_{\rm lim}$ is the ionization limit for a spectrum-level-like series. $I_{\rm exp}$ is the ionization energy of WBE. In order to get the value of $T(n)$ the value of $I_{\rm exp}$ is needed. In this work, we use the theoretical value of ionization energy, $I_{\rm cal}$, to replace the $I_{\rm exp}$. Therefore, we get

$$T(n) = T_{\rm lim} - I_{\rm cal}. \tag{2}$$

We divided approximately the ionization energy into non-relativistic part and relativistic part [30]

$$I_{\rm cal} = I_{\rm nr} + I_{\rm r}, \tag{3}$$

where $I_{\rm nr}$ represents the nonrelativistic energy and $I_{\rm r}$ represents relativistic energy.

Now we employ the WBEPM theory to calculate the nonrelativistic energy $I_{\rm nr}$.

According to WBEPM theory [15, 16], the Schrödinger equation of WBE is

$$\left[-\frac{1}{2}\nabla_i^2 + V(r_i)\right]\varphi_i = \varepsilon_i\varphi_i. \tag{4}$$

In WBEPM theory the potential function $V(r_i)$ in Eq. (4) may be written as (in atomic units)

$$V(r_i) = \frac{-Z'}{r_i} + \frac{d(d+1)+2dl}{2r_i^2}, \tag{5}$$

where Z' is the effective nuclear charge, l is the angular quantum number of WBE, and r_i is the distance between the WBEi and the nucleus. Parameter d is introduced to modify the integral quantum number n_i and angular quantum number l_i into nonintegral n_i' and l_i'.

Substituting Eq. (5) into Eq. (4) and solving the Schrödinger equation of the WBE, we can obtain the following expressions of energy eigenvalue and the radial function:

$$\varepsilon_i = -\frac{Z_i'^2}{2n_i'^2} \tag{6}$$

and

$$R = C\exp\left(-\frac{Z'r}{n'}\right) r^{l'} L_{n-l-1}^{2l'+1}\left(\frac{2Z'r}{n'}\right), \tag{7}$$

where n' is the effective principal quantum number with $n' = n + d$, l' is the effective angular quantum number with $l' = l + d$, C is the normalization factor, and $L_{n-l-1}^{2l'+1}\left(\frac{2Z'r}{n'}\right)$ is the generalized Laguerre polynomial.

Because Eq. (4) is the non-relativistic one-electron Schrödinger equation, the energy eigenvalue of WBE obtained from Eq. (4) negative value of the non-relativistic part of ionization energy, $I_{\rm nr}$:

$$I_{\rm nr} = -\varepsilon_i = \frac{Z_i'^2}{2n_i'^2}. \tag{8}$$

For an iso-spectrum-level series we can write Eq. (1)

into

$$T(Z,n) = T_{\rm lim}(Z) - I_{\rm exp}(Z), \tag{9}$$

and the effective nuclear charge Z' was proposed as a function concerning nuclear charge Z [15], that is

$$Z' = \sqrt{(Z-\sigma)^2 + g(Z-Z_0)}, \tag{10}$$

where Z_0 is the nuclear charge of the first member in an iso-spectrum-level series, for example, Z_0 is the nuclear charge of the Be atom for iso-spectrum-level series Be(I) ([He] $2s3p\ ^3P_1$), σ is the screening constant of the first member, and relatively increase factor g is a parameter that indicates the effect on the effective nuclear charge due to the increase in the nuclear charge in series.

The non-relativistic ionization energy can be written as

$$I_{\rm nr}(Z) = \frac{(Z-\sigma)^2 + g(Z-Z_0)}{2n'^2}. \tag{11}$$

In order to obtain the values of parameters n', σ, and g, we considered the first difference of the non-relativistic ionization potential. In an iso-spectrum-level series, the plot of the first difference of the ionization potential, $\Delta I_{\rm nr} = I_{\rm nr}(Z+1) - I_{\rm nr}(Z)$, vs. nuclear charge Z, would be a straight line. Because the relativistic part of ionization potential is quite small, the plot of the first differences of the experimental ionization potential $\Delta I_{\rm exp} = I_{\rm exp}(Z+1) - I_{\rm exp}(Z)$ vs. nuclear charge Z could be approximated to the plot of the first difference of the ionization potential, $\Delta I_{\rm nr} = I_{\rm nr}(Z+1) - I_{\rm nr}(Z)$, vs. nuclear charge Z. In this work, the experimental data are taken from Ref. [31]. Therefore, the effective principle quantum number n' can be treated as a constant approximately, and can be obtained from the plot of $\Delta I_{\rm exp}$ and nuclear charge Z. The screening constant of the first member σ and the relatively increase factor g can be calculated later. Therefore, the energy levels can be obtained from the following equation:

$$T(Z,n) \approx T_{\rm lim}(Z) - \frac{(Z-\sigma)^2 + g(Z-Z_0)}{2n'^2}. \tag{12}$$

As Z^2 is the highest power of Eq. (12), the relativistic effects such as mass velocity, the Darwin term, and the spin–orbit term cannot be included completely in Eq. (12). In order to get more accurate energies, the relativistic effects must be taken into account. As mentioned above, in a given iso-spectrum-level series, the only variable parameter is the nuclear charge Z. Therefore, in this work, the relativistic energies are presented as a univariant function of a six-order polynomial in nuclear charge

$$I_{\rm r}(Z) = \sum_0^6 a_i Z^i. \tag{13}$$

We considered the deviations between experimental ionization potential $I_{\rm exp}(Z)$ and the ionization potential $I_{\rm nr}(Z)$ calculated from Eq. (11) are equal to the relativistic part $I_{\rm r}(Z)$. Here experimental values of ionization potential are taken from NIST data base [31]. By fitting deviations $I_{\rm exp}(Z) - I_{\rm nr}(Z)$ to Eq. (13), we can obtain the values of coefficients a_i (i = 0–6). The theoretical value of ionization energy can be expressed as the following equation:

$$I_{\rm cal}(Z) = \frac{(Z-\sigma)^2 + g(Z-Z_0)}{2n'^2} + \sum_0^6 a_i Z^i. \tag{14}$$

Then for an iso-spectrum-level series, we obtain

$$T(n) = T_{\rm lim} - \left[\frac{(Z-\sigma)^2 + g(Z-Z_0)}{2n'^2} + \sum_0^6 a_i Z^i\right]. \tag{15}$$

As the Z is determined for a given member, Eq. (14) reduces as Eq. (2) and one can calculate $T(n)$ through $I_{\rm cal}$ and $T_{\rm lim}$.

4. Results and discussion

We studied the energy levels of iso-spectrum-level series along Be-, Al-, and Na-like sequences using the method mentioned above. The parameters needed in Eq. (15) are listed in Tables I–II, and the results of this work are listed in Tables III–IX.

TABLE I

Parameters of Eq. (14) for [He] $2s2p\ ^1P_1$; [He] $2s2p\ ^3P_0$; [He] $2s2p\ ^3P_2$; and [He] $2s3s\ ^3S_1$ series of Be-like sequences.

Parameters	[He] $2s2p\ ^1P_1$	[He] $2s2p\ ^3P_0$	[He] $2s2p\ ^3P_2$	[He] $2s3s\ ^3S_1$
σ	2.91379	2.61381	2.60991	2.62907
g	0.397358	0.295579	0.32755	0.338591
n'	1.99205	1.9906	1.99627	2.98728
a_0	73035.1	22114.3	24315.3	11693.9
a_1	−43659.7	−14188	−14082	−7217.97
a_2	9724.99	3392.89	2996.71	1634.36
a_3	−1062.34	−388.985	−310.527	−173.436
a_4	61.5715	22.9618	17.0618	9.2005
a_5	−1.81346	−0.679121	−0.475133	−0.236533
a_6	0.0212893	0.00817741	0.00520787	0.00243893

TABLE II

Parameters of Eq. (14) for [Ne] $3s^2 3d\ ^2D_{3/2}$ series, [Ne] $3s^2 3d\ ^2D_{5/2}$ series, and [Ne] $3s^2 3d\ ^2D_{5/2}$ series of Al-like sequences and [Ne] $4p\ ^2P_{1/2}$ series, [Ne] $5d\ ^2D_{5/2}$ series, and [Ne] $6f\ ^2F_{7/2}$ series of Na-like sequences.

Parameters	Al-like sequences			Na-like sequences	
	[Ne] $3s^2 3d\ ^2D_{3/2}$	[Ne] $3s^2 3d\ ^2D_{5/2}$	[Ne] $4p\ ^2P_{1/2}$	[Ne] $5d\ ^2D_{5/2}$	[Ne] $6f\ ^2F_{7/2}$
σ	11.9176	11.9172	9.76373	10.0198	10.0016
g	0.0958325	0.0994782	0.640162	−0.0152469	−0.00462789
n'	2.84873	2.84992	3.87277	4.88813	5.98929
a_0	20494300	17658700	646086	−93157	1920.37
a_1	6179120	5245450	199379	40195.8	−508.401
a_2	764622	638337	24607.5	−6764.28	38.3766
a_3	49786.7	40807.9	1561.9	570.524	0.785963
a_4	1801.3	1447.43	54.3212	−25.5031	−0.240012
a_5	34.3498	27.0199	0.994358	0.575745	0.0110767
a_6	0.269627	0.207276	0.00749563	−0.00520289	−0.000161941

TABLE III

Energy levels [cm^{-1}] for the [He] $2s2p\ ^1P_1$ series of Be-like sequences.

Z	Experimental results [31]	Present results	MBPT method [32]
4	42565.4	42566.8	38316
5	73396.5	73326.2	70046
6	102352	102472	99710
7	130694	130746	128534
8	158798	158722	156979
9	186844	186739	185279
10	214952	214950	213581
11	243208	243541	241993
12	271687	270861	270607
13	300490	300947	299511
14	329679	330319	328790
15	359343	359247	358537
16	389583	388965	388827
17	420501	419469	419799
18	452212	450993	451567
19	484800	486375	484250
20	518620	519007	517980
21	553440	546768	552911
22	589692	589446	589206
23	627500	626535	627054
24	667080	667130	666658

TABLE IV

Energy levels [cm^{-1}] for the [He] $2s2p\ ^3P_0$ series of Be-like sequences.

Z	Experimental results [31]	Present results	MBPT method [32]
4	21978.3	22008.5	20610
5	37335.5	37285.2	36624
6	52367.1	52354.3	51916
7	67209.2	67206.9	66898
8	81942.5	81946.8	81718
9	96590	96649.6	96447
10	111253	111347	111128
11	125880	126189	125785
12	140504	139525	140437
13	155148	155399	155095
14	169802	170310	169765
15	184478	184461	184456
16	199181	198973	199145
17	213913	213671	213877
18	228674	228580	228649
19	243520	246307	243460
20	258290	260020	258304
21	273200	267420	273185
22	288190	288209	288103
23	303100	301950	303062
24	318030	318023	318076

TABLE V

Energy levels [cm^{-1}] for the [He] $2s2p\ ^3P_2$ series of Be-like sequences.

Z	Experimental results [31]	Present results	MBPT method [32]
4	21981.3	22017.5	20614
5	37357.8	37293.4	36648
6	52447.1	52433.7	51997
7	67416.3	67424.9	67107
8	82385.3	82400.1	82164
9	97427	97486.8	97287
10	112702	112784	112578
11	128218	128514	128128
12	144091	143108	144030
13	160429	160691	160381
14	177318	177842	177281
15	194856	194855	194841
16	213182	212945	213157
17	232413	232050	232389
18	252683	252330	252668
19	274090	276562	274133
20	296950	298132	296932
21	321240	315023	321230
22	347260	347297	347198
23	375000	374979	375029
24	405020	408026	404922

Table I presents the parameters for the Be-like series including [He] $2s2p\ ^1P_1$; [He] $2s2p\ ^3P_0$; [He] $2s2p\ ^3P_2$; and [He] $2s3s\ ^3S_1$. For these series, the experimental data from $Z = 4$ to $Z = 16$ are used to obtain the parameters n', σ, and g. The experimental data are taken from Ref. [31]. The effective principle quantum number n' is obtained from the first differences of $I_{\rm exp}(Z)$. σ is the screening constant of the first member of a given iso--spectrum-level series, and we calculated it from Eq. (12). g is called relative increase factor which indicates the effect on the effective nuclear charge. Each member in a iso-spectrum-level series is used to obtain the relative g_i, and g is the arithmetical average of the g_i. When obtained the parameters a_i (i = 0–6) from the least--squares fitting, $Z = 20, 22, 24$ are added for [He] $2s2p\ ^1P_1$ series; $Z = 22, 24$ are added for [He] $2s2p\ ^3P_0$ series; $Z = 22, 23$ are added for [He] $2s2p\ ^3P_2$ series; and $Z = 22, 24$ are added for [He] $2s3s\ ^3S_1$ series. Results of these Be-like series are listed in Tables III–VI. All the energies are given in cm^{-1} unit. We compared our results with the experimental data and those obtained by Safronova et al. [32, 33]. In each table, column 1 is the nuclear charge of every member of a given iso-spectrum-level series. Column 2 lists the experimental data taken from the NIST data base [31]. The NIST collected accepted data were obtained by different authors all around the world and critically evaluated the reliability of those

TABLE VI

Energy levels [cm^{-1}] for the [He] $2s3s\ ^3S_1$ series of Be-like sequences.

Z	Experimental results [31]	Present results	MBPT method [33]
4	52080.9	52086	
5	129774	129765	
6	238213	238221	238878
7	377285	377274	377662
8	546973	546946	547283
9	747284	747290	747571
10	978300	978355	978538
11	1239974	1240330	1240225
12	1532450	1531590	1532687
13	1855760	1856250	1855990
14	2210700	2210810	2210204
15	2595600	2595510	2595410
16	3011500	3011470	3011652
17	3458700	3458540	3459100
18		3936770	3937848
19		4448800	4447996
20		4987890	4989632
21		5551910	5562939
22	6160800	6160810	6167992
23		6794530	6804958
24	7463000	7463000	7473998

TABLE VII

Energy levels [cm^{-1}] for the [Ne] $3s^2 3d\ ^2D_{3/2}$ series of Al-like sequences.

Z	Experimental results [31]	Present results	MBPT method [9]
13	32435.5	32402.5	
14	79338.5	79278.3	
15	116875	117487	
16	152133	151047	
17	185863	186753	
18	218593	217892	217980
19	250663	250834	
20	282356	283097	283270
21	313860	314016	
22	345315	343574	344199
23	376897	378044	
24	408640	408743	407623
25	440725	440180	
26	473223	473116	472279
27	506230	507436	
28	539839	539313	538960
29	574180	574190	

TABLE VIII

Energy levels [cm^{-1}] for the [Ne] $3s^2 3d\ ^2D_{5/2}$ series of Al-like sequences.

Z	Experimental results [31]	Present results	MBPT method [9]
13	32436.8	32443.4	
14	79355	79171.4	
15	116886	117548	
16	152147	151180	
17	185891	186808	
18	218653	217838	218030
19	250781	250792	
20	282577	283282	283288
21	314214	314627	
22	345859	344682	344726
23	377650	379521	
24	409741	410272	408710
25	442220	441401	
26	475202	473948	408710
27	508793	508611	
28	543107	543184	542192
29	578243	585846	

TABLE IX

Energy levels [cm^{-1}] for the [Ne] $4p\ ^2P_{1/2}$ series; [Ne] $5d\ ^2D_{5/2}$ series; and [Ne] $6f\ ^2F_{7/2}$ series of Na-like sequences.

Z	[Ne] $4p\ ^2P_{1/2}$		[Ne] $5d\ ^2D_{5/2}$		[Ne] $6f\ ^2F_{7/2}$	
	$T_{\rm exp}$[31]	$T_{\rm cal}$	$T_{\rm exp}$[31]	$T_{\rm cal}$	$T_{\rm exp}$[31]	$T_{\rm cal}$
11	30267	30277.8	37036.8	37033.9	38399.8	38399.1
12	80619.5	80580.9	103420	103431	109062	109064
13	143633	143666	188878	188866	201971	201970
14	218267	218289	291498	291495	315230	315228
15	304161	304140	410639	410649	448090	448090
16	401169	401134	546059	546058	600189	600194
17	509197	509228	697619	697616	771346	771343
18	628219	628386	865252	865294	961470	961431
19	758262	758597	1049130	1049130	1170440	1170430
20	899290	899775	1249030	1249080	1398440	1398280
21	1051640	1051640	1465130	1464910	1644980	1644730
22	1214390	1215030	1697480	1697480	1910650	1910650
23	1388410	1389190	1946500	1946010	2195100	2195300
24	1573840	1574350	2211080	2210730	2499260	2498930
25	1770400	1770440	2491700	2491540	2821800	2821490
26	1977650	1977630	2788610	2788610	3163190	3163140
27	2196500	2196500	3103000	3102610	3524500	3524500
28	2426100	2426760	3434600	3433420	3906100	3905340
29	2667490	2667620	3780600	3780600	4305000	4305000
30	2920300	2920300	4145000	4145940	4724800	4724920
31	3184600	3183920	4526100	4529430	5163500	5164580

data. Therefore, we took the data taken from the NIST data base for comparison. Column 3 lists the results obtained using WBEPM theory. The results obtained by Safronova et al. are contained in column 4. Using the RMBPT, Ref. [32] reported the energy levels of $n = 2$ states of berylium-like ions with nuclear charges ranging from $Z = 4$–100 [32]. In their calculations, both the Coulomb interaction and the Breit–Coulomb interaction are carried out to the second order. In the next year, the same group extended the theory to study the $2l3l'$ states of berylium-like ions. 16 even-parity ($2s3s$, $2p3p$, $2s3d$) excited states and 20 odd-parity ($2s3p$, $2p3s$, $2p3d$) excited states were studied in their work [33]. In general, their results are in good agreement with experimental data. Most deviations are smaller than 1000 cm^{-1}, when several of them are 1000–4000 cm^{-1} and only a few are more than 4000 cm^{-1}. The comparison shows that our results are at the same level with Safronova's ones. Table II gives the parameters for the two Al-like series and three Na-like series. The energy levels of these five series are listed in Tables VII–IX. For two Al-like series, the experimental data from $Z = 13$ to $Z = 22$ are used to obtain the parameters n', σ, and g. When we obtained the parameters a_i ($i = 0$–6) from the least-squares fitting, $Z = 23, 26, 29$ are added for [Ne] $3s^2 3d\ ^2D_{3/2}$ series and $Z = 24, 27, 28$ are added for [Ne] $3s^2 3d\ ^2D_{5/2}$ series. The results taken from Ref. [9] are given for comparison. For three Na-like series, the experimental data from $Z = 11$ to $Z = 17$ are used to obtain the parameters n', σ, and g. When obtained the parameters a_i ($i = 0$–6) from the least-squares fitting, $Z = 21, 27, 30$ are added for [Ne] $4p\ ^2P_{1/2}$ series; $Z = 22, 26, 29$ are added for [Ne] $5d\ ^2D_{5/2}$ series; and $Z = 22, 27, 29$ are added for [Ne] $6f\ ^2F_{7/2}$ series.

The main source of error in the present method is the incomplete treatment of relativistic effects. We find that the deviations between nonrelativistic energies and the experimental data show an increasing trend with the increase in Z along the iso-spectrum-level series. That is because the relativistic effects on the radial wave functions become more evident for high Z. Although the relative deviations caused by relativistic effects are very small, the absolute deviations will be little large ones. In present work, in order to improve the accuracy of our results, the relativistic corrections of an iso-spectrum-level series are included by a six-order polynomial in Z. By including the relativistic effects, deviations between our results and the experimental data become much smaller. However, this treatment is successful at present calculation. But for ions with much higher nuclear charge Z, the more precise consideration of relativistic effects is necessary.

In conclusion, employing the WBEPM theory, we calculated the energies for Be-, Al-, and Na-like sequence. Equation (11) is derived to calculate the non-relativistic energies, and the relativistic corrections are taken into account by a six-order polynomial in nuclear charge Z.

The present results are compared with available experimental data, and good agreements are obtained from the comparisons.

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