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Oscillator strengths for 2 ^{2}P-n ^{2}D transitions of lithium-like systems with Z=11 to 20*

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The dipole-length, velocity and acceleration absorption oscillator strengths for the $1s^2 2p–1s^2 nd$ ($3 \leq n \leq 9$) transitions of the lithium-like systems with Z=11 to 20 are calculated using the energies and the multiconfiguration interaction wavefunctions obtained from a full core plus correlation method. The agreement between the f-values calculated from the length, velocity and acceleration formulae is excellent. Our results agree closely with the experimental data available in the literature. Combining these discrete oscillator strengths with the single-channel quantum defect theory, the discrete oscillator strengths for the transitions from $1s^2 2p$ state to highly excited states ($n \geq 10$) and the oscillator strength densities corresponding to the bound-free transitions are obtained.

Keywords: lithium-like system, full-core plus correlation, oscillator strength, quantum defect
PACC: 3110, 3130, 3270C

1. Introduction

The study of transition rates of highly ionized atomic systems is a subject of considerable interest for many fields. The transition rates are very important in astrophysical study because they play a significant role in the determination of atomic abundance. They are also essential to the study of controlled thermonuclear reactions, where the atomic radiation is one of the primary energy loss mechanisms. However, at present, information about the transition rates, or oscillator strengths, of highly ionized systems is far from adequate. First of all, their experimental measurements are usually very difficult so that these basic data needed in many fields have to be provided, to some extent, by accurate theoretical predictions. On the other hand, to obtain an accurate transition rate, accurate wavefunctions must be used for both the initial and final states. Especially, because three alternative forms of oscillator strength (e.g., the length, velocity and acceleration forms) are weighted towards different regions of electron configuration space,[1] the wavefunctions used in the calculations must be accurate enough in the whole configuration space to obtain satisfactory results where the values of oscillator strength from three formulae are in agreement with each other. All these facts mentioned above make a precision calculation of transition rate, or the oscillator strength, very challenging. For helium and helium-like ions, more accurate calculations of oscillator strengths have been carried out.[2,3] For lithium atom, the oscillator strength for 2 ^{2}S-2 ^{2}P transition has been calculated in the literature.[4] It is noted that only the f-values of the length form were given in most of these references. However, for the lithium-like ions with higher nuclear charge, there are few data previously available.

Recently, an elegant and complete variation approach, the full core plus correlation (FCPC) method, has been developed, and used successfully to calculate the ionization potentials for the ground states of lithium-like systems.[5,6] High-precision results for excitation energy and fine structure of lithium-like systems from Z=3 to 10 were also obtained by using this method.[7–9] Using the energies and wavefunctions obtained from the FCPC method, the dipole polarizabilities for the ground states of lithium-like systems with Z=3 to 50 were calculated.[10] Not long ago, this

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method was applied to the lowly excited states $1s^2nl$ (l=s, d, f; $n \leq 5$) of lithium-like systems with Z=11 to 20[11,12] and the ground states of lithium-like systems with Z=21 to 30.[13] By using this method we have also studied the electron density at the nucleus of the ground state for the lithium isoelectronic sequence from Z=3 to 10.[14] Lately, we have extended this method to the lithium-like systems with higher nuclear charge and in the higher energy region, and calculated the energy and fine structure for the highly excited states $1s^2np$ ($n \leq 9$) of lithium-like ions with Z=11 to 20.[15] In this paper, in order to testify the FCPC wavefunction thoroughly and get more reliable information of the dipole transition process, the dipole oscillator strengths for the $1s^22p$–$1s^2nd$ ($n \leq 9$) transitions of lithium-like ions with Z=11 to 20 are calculated using the energies and wavefunctions obtained from FCPC method. Combining these discrete oscillator strengths with the single-channel quantum defect theory (QDT), the oscillator strength for the $1s^22p$–$1s^2nd$ ($n \geq 10$) transitions and the oscillator strength densities corresponding to the bound-free transitions are predicted.

2. Theory

The FCPC method has been described in detail in Ref.[5], it will not be repeated here. The total wavefunctions of the three-electron system with $1s^2$ core is given by

$$\Psi(1,2,3) = A\left[\Phi_{1s1s}(1,2)\sum_i d_i r_3^i e^{-\beta r_3} Y_{l(i)}(3)\chi(3) + \sum_i C_i \Phi_{n(i),l(i)}(1,2,3)\right], \quad (1)$$

where A is the anti-symmetrization operator. In the first term in the right-hand side of Eq.(1), Φ_{1s1s} is a predetermined $1s^2$ core wavefunction, which is represented in terms of a CI basis set, and the factor multiplying with Φ_{1s1s} is a linear combination of the Slater orbital for the valence electron. The second term in the right-hand side of Eq.(1) accounts for the other possible correlation and the relaxation of the $1s^2$ core in the three electron system. The linear parameters in Eq.(1) are determined by solving the secular equation, and the nonlinear parameters are optimized in the energy minimization process. These wavefunctions and the transition energies obtained by the use of variation method [11,12,15] are used to calculate the dipole oscillator strength for the $1s^22p$–$1s^2nd$ ($3 \leq n \leq 9$) transitions with Z=11 to 20.

The dipole oscillator strength is given by any of the following three forms:[9]

$$f_L = \frac{2}{3}(E_j - E_i)\left|\langle \Psi_i \mid \boldsymbol{r} \mid \Psi_j\rangle\right|^2,$$
$$f_V = \frac{2}{3}(E_j - E_i)^{-1}\left|\langle \Psi_i \mid \nabla \mid \Psi_j\rangle\right|^2, \quad (2)$$

and

$$f_A = \frac{2}{3}(E_j - E_i)^{-3}\left|\left\langle \Psi_i \left| \frac{\boldsymbol{r}}{r^3} \right| \Psi_j \right\rangle\right|^2.$$

Here, E_i and E_j are the nonrelativistic energies of the initial and final states for the dipole transitions. These f-values should be calculated by summing over the final states and averaging over the initial states. These three alternatives are named the length, velocity and acceleration forms, respectively. They are equivalent when exact wavefunctions are used, but usually give rather different results when approximate wavefunctions are used, because the matrix elements in these three forms of oscillator strength are weighted towards different regions of electron configuration space. Therefore, whether the f-values obtained from the three formulae are in agreement with each other is a rigorous evaluation of the quality for the wavefunctions used in the calculation.

According to single channel quantum defect theory,[16–18] the quantum defect μ_n can be determined from the formula

$$E_n = -\frac{Z^2}{2(n-\mu_n)^2} \quad \text{(in a.u.)}, \quad (3)$$

with the energy term E_n obtained from the FCPC method for $n \leq 9$ as input. Here n is the principal quantum number. For highly excited states with $n \geq 10$, μ_n should be a smooth function of energy and approximated by a weakly varying function of energy in the form

$$\mu_n(E) = \mu_0 + h_1 E + h_2 E^2. \quad (4)$$

The coefficients μ_0, h_1, and h_2 for each series are determined by using the μ_n values obtained from Eq.(3). Treating Eqs.(3) and (4) as a system equation for E_n and μ_n, the quantum defect, μ_n, and energy term, E_n, for highly excited states ($n \geq 10$) are determined by the iteration method. At the beginning, we set $\mu_n \approx \mu_0$, and put it into Eq.(3). Then E_n and μ_n can be refined by iteration procedure. Finally, the quantum defect, μ_n, and the energy term, E_n, are obtained.

As is known, the oscillator strength densities corresponding to the final states in the continuum are associated with the discrete oscillator strength corresponding to the bound-bound transitions.[18] Thus the oscillator strength densities of the bound–bound transitions can be defined as

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} \quad \text{(in a.u.)}, \tag{5}$$

where Z is the charge of the ion core, E is the energy of the final state, f_{ij} is the discrete oscillator strength. n^* is the effective principal quantum number for the final state, which can be given by the quantum defect theory,[17,18]

$$n^* = n - \mu_n. \tag{6}$$

In the limit $E \to I$ (from below), where I is the ionization potential of the system, $\tau\ (E)$, as a function of E, will match to the oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon$, of continuum states, namely

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon}. \tag{7}$$

For the $1s^2 2p$–$1s^2 n$d transition of lithium-like systems under consideration, neither the Cooper minimum nor the following maximum is found in the near-threshold energy region. Hence, Eq.(7) can be used to extrapolate the discrete oscillator strength, f_{ij}, below the threshold to the oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon$, above the threshold. In the near-threshold region ($|E| \leq I/2$), the oscillator strength and the oscillator strength densities can be accurately approximated by the following form:[19]

$$\begin{aligned}\tau(E) =& \frac{(n^*)^3}{Z^2} f_{ij} = \frac{\mathrm{d}f}{\mathrm{d}\varepsilon} \\ =& \left(\frac{E_i}{E_i - E_j}\right)^s \left.\frac{\mathrm{d}f}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}.\end{aligned} \tag{8}$$

Using the discrete oscillator strengths obtained from the FCPC method, the coefficient s and the threshold oscillator strength densities, $\mathrm{d}f/\mathrm{d}\varepsilon|_{\varepsilon=0}$, can be determined. In this work, s is a fitting parameter and should be the function of nuclear charge Z. Equations (5) and (8) make it possible to determine the oscillator strength for transition from a certain initial state to all the final states of the Rydberg series.

3. Results and discussion

It is not difficult to find from Eq.(2), as mentioned above, that the length form of oscillator strength weights the integrand toward large r. The velocity form may give the best results when good variational wavefunctions are used, provided the transition energy is not small. In other words, the velocity expression emphasizes the wavefunctions at intermediate r values. The acceleration form tends to give poor results because the integrand is weighted toward small r, where the wavefunctions usually are poorly known. To a large extent, the agreement between the results of these three expressions becomes an indication of the accuracy of the wavefunction and the reliability of the calculated oscillator strength.

The calculated results of the oscillator strengths for the $1s^2 2p$–$1s^2 n$d ($3 \leq n \leq 9$) transitions of lithium-like systems with Z=11 to 20 are given in Table 1. The experimental data[20] available in the literature are also listed in this table. In most cases, as can be seen, the agreement between the oscillator strengths from the length and velocity formulae is up to four or five digits. Our acceleration f-values agree closely with the length and velocity results too. It appears that the agreement of our results for the oscillator strengths with the experimental data[20] available is fairly satisfactory. However, there are no experimental data for the $1s^2 2p$–$1s^2 n$d ($n > 7$) transitions available in the literature to compare with theory. We hope our predictions will be useful in making higher precision experimental measurements on these transitions. To the best of our knowledge, many approximate wavefunctions used in practice can be fairly accurate for the intermediate value of r, but are usually rather poor in the region near the nucleus. Thus it is difficult to obtain consistent f-values from using these three alternatives. The results in this paper show that our FCPC wavefunctions should be fairly accurate in the whole configuration space from the intermediate r to large r, even in the near-nucleus region they should also be accurate. Hence our f-values obtained by using them should be accurate.

Table 1. The oscillator strength of $1s^2 2p–1s^2 nd$ ($n \leq 9$) transitions for lithium-like systems from Z=10 to 20.

Z		3d	4d	5d	6d	7d	8d	9d
11	f_L	0.66547	0.12238	0.04527	0.02224	0.01273	0.00803	0.00541
	f_V	0.66560	0.12233	0.04530	0.02226	0.01275	0.00805	0.00542
	f_A	0.66401	0.12207	0.04516	0.02218	0.01270	0.00801	0.00540
	Exp.[20]	0.67	0.12	0.0460	0.0225	0.0131		
12	f_L	0.66786	0.12230	0.04521	0.02220	0.01271	0.00801	0.00541
	f_V	0.66796	0.12230	0.04523	0.02221	0.01271	0.00802	0.00541
	f_A	0.66585	0.12207	0.04517	0.02218	0.01270	0.00801	0.00540
	Exp.[20]	0.67	0.12	0.0459	0.0225	0.0130		
13	f_L	0.66988	0.12233	0.04514	0.02215	0.01267	0.00799	0.00541
	f_V	0.66998	0.12227	0.04517	0.02217	0.01269	0.00800	0.00542
	f_A	0.66903	0.12195	0.04506	0.02211	0.01266	0.00798	0.00541
	Exp.[20]	0.67	0.12	0.0457	0.0224	0.0130		
14	f_L	0.67166	0.12225	0.04510	0.02212	0.01266	0.00798	0.00539
	f_V	0.67173	0.12225	0.04512	0.02213	0.01266	0.00798	0.00539
	f_A	0.67028	0.12199	0.04503	0.02209	0.01264	0.00797	0.00538
	Exp.[20]	0.67	0.12	0.0456	0.0224	0.0130		
15	f_L	0.67320	0.12223	0.04505	0.02209	0.01263	0.00796	0.00536
	f_V	0.67326	0.12222	0.04507	0.02210	0.01264	0.00797	0.00536
	f_A	0.67202	0.12199	0.04499	0.02206	0.01262	0.00797	0.00535
	Exp.[20]	0.68	0.12	0.0455	0.0223	0.0129		
16	f_L	0.67457	0.12219	0.04502	0.02206	0.01262	0.00795	0.00538
	f_V	0.67461	0.12219	0.04503	0.02207	0.01262	0.00795	0.00538
	f_A	0.67345	0.12199	0.04496	0.02204	0.01262	0.00794	0.00538
	Exp.[20]	0.68	0.12	0.0455	0.0222	0.0129		
17	f_L	0.67577	0.12218	0.04496	0.02204	0.01260	0.00794	0.00536
	f_V	0.67581	0.12218	0.04499	0.02205	0.01261	0.00794	0.00537
	f_A	0.67477	0.12199	0.04493	0.02201	0.01259	0.00793	0.00537
	Exp.[20]	0.68	0.12	0.0455	0.0222	0.0128		
18	f_L	0.67685	0.12216	0.04493	0.02202	0.01259	0.00793	0.00537
	f_V	0.67688	0.12216	0.04496	0.02202	0.01259	0.00794	0.00537
	f_A	0.67591	0.12200	0.04490	0.02199	0.01258	0.00793	0.00537
	Exp.[20]	0.68	0.12	0.0454	0.0221	0.0128		
19	f_L	0.67782	0.12214	0.04491	0.02200	0.01258	0.00793	0.00537
	f_V	0.67785	0.12214	0.04493	0.02200	0.01258	0.00793	0.00537
	f_A	0.67695	0.12198	0.04488	0.02198	0.01258	0.00792	0.00537
	Exp.[20]	0.68	0.12	0.0453	0.0221	0.0127		
20	f_L	0.67869	0.12213	0.0449	0.02198	0.01256	0.00792	0.00534
	f_V	0.67872	0.12212	0.0449	0.02198	0.01256	0.00792	0.00535
	f_A	0.67786	0.12212	0.0449	0.02196	0.01255	0.00791	0.00535
	Exp.[20]	0.68	0.12	0.0452	0.0220	0.0127		

Table 2. The oscillator strength density, $df/d\varepsilon|_{\varepsilon=0}$ at the threshold and the s value in equation (8).

Z	11	12	13	14	15
$df/d\varepsilon\|_{\varepsilon=0}$	0.04328	0.03491	0.02879	0.02411	0.02049
s	2.86	2.87	2.87	2.88	2.88
Z	16	17	18	19	20
$df/d\varepsilon\|_{\varepsilon=0}$	0.01763	0.01533	0.01345	0.01189	0.01059
s	2.89	2.89	2.89	2.90	2.90

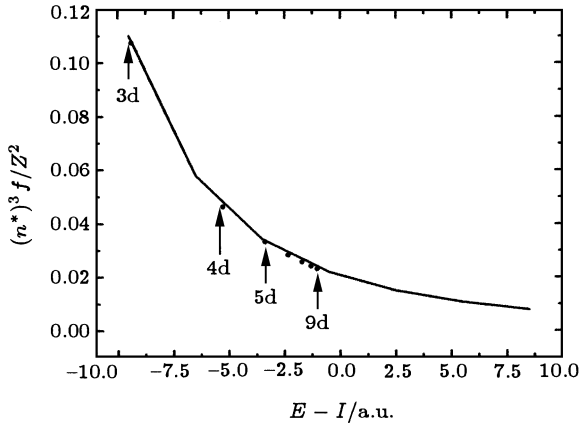


Fig.1. Oscillator strength of $1s^2 2p–1s^2 nd$ transitions in P XIII. The curve is obtained from Eqs.(5) and (8), and the dots represent the values calculated from Eq.(5). The discrete oscillator strengths are multiplied by factors $(n^*)^3/Z^2$. The continuous oscillator strengths above the threshold are $df/d\varepsilon$.

Equations (5) and (8) can be used to determine the oscillator strengths for transitions from a certain initial state to all states of the Rydberg series. The oscillator strength densities at threshold, $df/d\varepsilon|_{\varepsilon=0}$, and the values of fitting parameter s in Eq.(8) are listed in Table 2. As an example, Fig.1 depicts Eq.(8) corresponding to the $1s^2 2p–1s^2 nd$ transitions of P XIII. It is shown that the discrete oscillator strengths calculated from the FCPC energies and wavefunctions lie rather well along curve (8), and the discrete oscillator strength coincides with the oscillator strength density at the threshold $E=I$. These results seem to suggest that our extrapolation results should be reliable and accurate, and the procedure adopted in this paper should be reasonable.

4. Conclusion

In this paper, the dipole absorption oscillator strengths for $1s^2 2p–1s^2 nd$ transitions of the lithium-like systems with $Z=11$ to 20 are calculated by using the transition energies and wavefunctions obtained from the FCPC method. The close agreement between the oscillator strengths obtained from the length, velocity, and acceleration formulae indicates that our FCPC wavefunctions should be accurate in the whole configuration space from small r to large r, and the predicted f-values should also be accurate. Combining the calculated f-values with quantum defect theory, we have obtained accurate and reliable oscillator strengths for transitions from the initial state, $1s^2 2p$, to all the states of the Rydberg series, $1s^2 nd$, including the oscillator strength densities corresponding to the bound-free transitions.

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