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Oscillator strengths for 2 ^{2}S$-$n ^{2}P transitions of the lithium isoelectronic sequence

L. Qu[1,a], Z. Wang[2], and B. Li[3]

[1] Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics, Chinese Academy of Sciences, Wuhan 430071, P.R. China
[2] Institute of Atomic and Molecular Physics, Jilin University, Changchun 130021, P.R. China
[3] Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing, China and Wuhan Institute of Physics, Chinese Academy of Sciences, Wuhan 430071, P.R. China

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Abstract. The nonrelativistic dipole-length, -velocity and -acceleration absorption oscillator strengths for the $1s^22s$–$1s^2np$ $(3 \leq n \leq 9)$ transitions of the lithium isoelectronic sequence up to $Z = 10$ are calculated by using the energies and the multiconfiguration interaction wave functions obtained from a full core plus correlation (FCPC) method. In most cases, the agreement between the f-values from the length and velocity formulae is up to forth or fifth digit. Combining these discrete oscillator strengths with the single channel quantum defect theory (QDT), the discrete oscillator strengths for the transitions from the $1s^22s$ state to highly excited levels $(n \geq 10)$ and the oscillator strength densities corresponding to the bound-free transitions are obtained.

PACS. 31.25.-v Electron correlation calculations for atoms and molecules – 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

The study of transition rates is a subject of considerable interest for many fields. For example, the transition rates are very important in astrophysical studies, they play an important role in the determination of atomic abundance. They are also important in studies of controlled thermonuclear reactions, where the atomic radiation is one of the primary loss mechanisms. To obtain an accurate transition rate, accurate wave functions must be used for both the initial and final states. Unlike the calculation of energy where high precision results can be obtained, the lack of a bound property makes a precision calculation of transition rates, or the oscillator strengths very challenging. For helium and heliumlike ions, accurate nonrelativistic calculations of the oscillator strengths have been obtained by Cann and Thakkar [1], and by Kono and Hattori [2]. Much more accurate results are presented by Drake [3]. The less accurate, but much more extensive study was also carried out by Sanders and Knight [4]. For lithium, the oscillator strength for the $2s\ ^2S$–$2p\ ^2P$ transition was studied extensively in the literature [5–10] and high precision results have been obtained. The most accurate oscillator strengths for $2s\ ^2S$–$2p\ ^2P$ and $2p\ ^2P$–$3d\ ^2D$ transitions were given by Yan and Drake [5]. More recently, the oscillator strengths for the $2s\ ^2S$–$2p\ ^2P$ transitions of the lithium isoelectronic sequence up to $Z = 20$ are calculated [11], and the final lifetime for the $1s^22p\ ^2P$ state of lithium is in good agreement with the recent high-precision measurements [12,13]. But for other transitions, such as $2s\ ^2S$–$np\ ^2P$ $(n \geq 3)$ transition that the final states are in highly excited levels of the lithiumlike ions, there are not much accurate data previously available.

Recently, a full core plus correlation (FCPC) method has been developed [14], and used successfully to calculate the ionization potentials for the ground state of lithium-like systems [14,15]. The IP's of the ground states from Li I to Ne VIII are predicted to within 1 ppm [15]. Accurate excitation energies of lithiumlike systems were also obtained by using the FCPC method [16–18], and possible misidentifications in the observed optical spectra were pointed out [17]. Using the energies and wave functions obtained from the FCPC method, Wang and Chung [19] calculated the dipole polarizabilities for the ground states of lithiumlike systems from $Z = 3$ to 50.

A natural extension is to study the transition rates by using the FCPC method. In this work, the dipole absorption oscillator strengths for the $1s^22s$–$1s^2np$ $(3 \leq n \leq 9)$ transitions of the lithium isoelectronic sequence up to $Z = 10$ are calculated by using the energies and wave functions obtained from the FCPC method. Combining these reliable discrete oscillator strengths with the single channel quantum defect theory, the f-values for the

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[a] e-mail: `lhq@nmr.whcnc.ac.cn`

$1s^22s$–$1s^2np$ ($n \geq 10$) transitions and the oscillator strength densities for the corresponding bound-free transitions are obtained.

2 Theory

The FCPC method has been given in detail by Chung [14], they will not be repeated here. The wave function of the three electron system is given by

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

where A is the antisymmetrization operator, Φ_{1s1s} (1,2) is the $1s^2$ core wave function. The second term on the right hand side of equation (1) accounts for other possible correlations and the relaxation of the $1s^2$ core. The linear parameters are determined by solving the secular equation, and the non-linear parameters are optimized in the energy minimization process. These wave functions are used to calculate the oscillator strengths.

It can be shown that the dipole oscillator strength is given by any of the following three forms [20]

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

Here, E_i and E_j are the nonrelativistic energies of the initial and final states for the dipole transition, respectively. These f-values should be calculated by summing over the final states and averaging over the initial states. These three alternatives are called the length, velocity, and acceleration forms, respectively.

As is known, the oscillator strength densities corresponding to the final states in continuum are associated with the discrete oscillator strengths corresponding to the bound-bound transitions [21]. We define the oscillator strength densities of the bound-bound transitions by:

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

where Z is the charge of the ion core, E is the energy of the final state, and f_{ij} is the discrete oscillator strength. n^* is the effective principle quantum number of the final state which is defined in the quantum defect theory [22] by:

$$n^* = n - \mu_n \quad (4)$$

where n is the principle quantum number. According to the quantum defect theory [22], the quantum defect, μ_n can be determined from the following formula

$$E_n = -\frac{Z^2}{2(n-\mu_n)^2} \text{ (in a.u.)} \quad (5)$$

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

$$\mu_n(E) = \mu_0 + h_1 E + h_2 E^2. \quad (6)$$

The coefficients, μ_0, h_1 and h_2 for each series are determined by using the μ_n values obtained from equation (5). Treating equations (5, 6) as a system equation for E_n and μ_n, one can use the interaction method to determine the quantum defect, μ_n and the term energy, E_n for highly excited states ($n \geq 10$). First, we let $\mu_n \approx \mu_0$, and put it into equation (5). Then E_n and μ_n can be refined by interaction procedure. Finally, the quantum defect, μ_n and term energy, E_n can be obtained.

In the limit $E \longrightarrow I$ (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, $df/d\varepsilon$ of continuum states, namely

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} = \frac{df}{d\varepsilon}\,. \quad (7)$$

For the $1s^22s$–$1s^2np$ transitions of lithiumlike systems (except lithium atom) under consideration, neither the Cooper minimum nor the following maximum is found in the near threshold energy region. Hence, equation (7) can be used to extrapolate the discrete oscillator strength, f_{ij}, below the threshold, and the oscillator strength densities, $df/d\varepsilon$, above the threshold. The oscillator strength and oscillator strength densities can be accurately approximated by the following formula in the near-threshold region ($|E| \leq I/2$)

$$\tau(E) = \frac{(n^*)^3}{Z^2} f_{ij} = \frac{df}{d\varepsilon} = \left(\frac{E_i}{E_i - E_j}\right)^s \frac{df}{d\varepsilon}\Big|_{\varepsilon=0} \quad (8)$$

where s and the threshold oscillator strength density, $df/d\varepsilon|_{\varepsilon=0}$ can be determined from our predicted discrete oscillator strengths. The f-values of some lithiumlike ions from S^{13+} to Yb^{67+} were calculated [23], and a formula very similar to equation (8), employing $s = 2$, was used to extrapolate the cross section to highly excited states. As is known, for highly charged lithiumlike ions, such as in reference [23], the spectrum is dominated by the ionic coulomb field. However for neutral atoms and low charged ions, such as in our work, the short-range core effects play a relatively more important role, and the influence of nuclear charge on the short-range core effects is sensitive. For this reason, $s = 2$ is a good approximation in reference [23], but in our work, s is a fitting parameter, and should be the function of nuclear charge Z. Equations (3, 8) make it possible to determined the oscillator strengths easily for transitions from a certain initial state to all the final states of the Rydberg series.

Table 1. The nonrelativistic oscillator strength for $1s^22s$–$1s^2np$ ($n \leq 9$) transitions of lithiumlike systems from Li I to Ne VIII.

Z		$2s$–$3p$	$2s$–$4p$	$2s$–$5p$	$2s$–$6p$	$2s$–$7p$	$2s$–$8p$	$2s$–$9p$
3	f_L	0.004819	0.004284	0.002599	0.001581	0.001012	0.000687	0.000445
	f_V	0.004822	0.004278	0.002597	0.001576	0.001011	0.000688	0.000443
4	f_L	0.08316	0.03123	0.01487	0.008196	0.004799	0.003373	0.001969
	f_V	0.08315	0.03126	0.01487	0.008193	0.004797	0.003370	0.001964
5	f_L	0.15376	0.04981	0.02256	0.01223	0.007364	0.004803	0.003222
	f_V	0.15375	0.04982	0.02256	0.01222	0.007362	0.004795	0.003208
6	f_L	0.20344	0.06128	0.02708	0.01447	0.008691	0.005664	0.003902
	f_V	0.20344	0.06128	0.02708	0.01441	0.008691	0.005660	0.003897
7	f_L	0.23894	0.06884	0.02997	0.01588	0.009562	0.006185	0.004270
	f_V	0.23890	0.06883	0.02997	0.01589	0.009562	0.006189	0.004264
8	f_L	0.26526	0.07413	0.03196	0.01691	0.01012	0.006543	0.004489
	f_V	0.26525	0.07413	0.03196	0.01691	0.01013	0.006544	0.004490
9	f_L	0.28547	0.07802	0.03342	0.01761	0.01050	0.006794	0.006308
	f_V	0.28545	0.07802	0.03340	0.01761	0.01050	0.006793	0.006308
10	f_L	0.30142	0.08011	0.03447	0.01813	0.01080	0.006974	0.004781
	f_V	0.30142	0.08010	0.03447	0.01814	0.01081	0.006971	0.004779

Table 2. Comparison of our oscillator strengths with those of Peach *et al.* [8] for $2s\ ^2S$–$np\ ^2P$ transitions of lithium.

Transition	This work	Peach *et al.* [8]*	
$2s$–$3p$	0.00482	0.00488	(0.00481)
$2s$–$4p$	0.00428	0.00435	(0.00430)
$2s$–$5p$	0.00260	0.00260	(0.00257)
$2s$–$6p$	0.00158	0.00160	(0.00158)

* The values in this column are the nonrelativistic oscillator strengths by using the Model potential method, and the values in parentheses are obtained from the close-coupling method.

3 Results and discussion

In most cases, a transition only involves the participation of one and two electrons, the rest of the electrons act as spectators. In principle, we may compromise on the accuracy of the part of the wave function for the spectator as long as they are the same in the initial and final state. However, one must make sure that the part of the wave function for the active electrons is sufficiently accurate in such an approximation. For the lithiumlike systems, the $1s^2$ core behaves like a spectator for the $1s^2nl$–$1s2n'l'$ transitions, and the FCPC method could be very useful in obtaining the transition rates.

As is known, the length formula emphasizes the wave functions at large distance, the gradient operator (the velocity expression) emphasizes the wave functions at intermediate r values, and the acceleration formula emphasizes the wave functions at small values of r. If we use exact wave functions the three expressions are identical, but if we evaluate the oscillator strengths using only approximate wave functions the results should differ from each other. In most cases, the agreement between the results of these three expressions becomes an indication on the accuracy of the wave functions and the reliability of the calculated oscillator strength.

In Table 1, we present our oscillator strengths for the $1s^22s$–$1s^2np$ ($3 \leq n \leq 9$) transitions of lithiumlike systems from Li I to Ne VIII. As can be seen, in most cases, the agreement between the oscillator strengths from the length and velocity formulae is up to four or five digits. As an example, for the $2s$–$3p$ transition of N V, the length and velocity f-values are 0.238 94 and 0.238 90 respectively. We know that, many approximate wave functions used in practice are most accurate for the intermediate value of r, thus the velocity formula is usually the most reliable form. The length formula results are often more accurate by using the variation wave function. Our results seem to suggest that the FCPC wave functions should be accurate in the configuration space from intermediate r to large r. Although the length and velocity results agree quiet well, there are still rooms for improvement for the acceleration results. Since variation principle is used in the FCPC method, the length formula results are probably more accurate. The acceleration formula emphasize the region near the nucleus where the contribution of the wavefunction to the energy is small. The wave function in that region is probably less accurate. For example, the length and velocity f-values for $2s$–$3p$ transition of O VI are 0.265 26 and 0.265 25 respectively, however, the acceleration f-value is 0.264 65.

The oscillator strengths for the $2s$–$2p$ transition of the lithium isoelectronic sequence with $Z = 3$–10 have been calculate [24], and the results are in good agreement with

Table 3. The fitted values of the QDT parameters of equation (6), the oscillator strength densities at threshold $df/d\varepsilon\ |_{\varepsilon}= 0$, and the s values in equation (8).

	Li I	Be II	B III	C IV	N V	O VI	F VII	Ne VIII
μ_0	4.7144(−2)	5.0338(−2)	4.4291(−2)	3.8379(−2)	3.3451(−2)	2.9425(−2)	2.6186(−2)	2.3667(−2)
h_1	−4.601(−2)	−7.997(−3)	−2.082(−3)	−8.709(−4)	−3.421(−4)	−1.455(−4)	−5.233(−5)	−3.612(−5)
h_2	−3.006(−2)	−1.075(−3)	−1.206(−4)	3.581(−5)	1.085(−5)	4.032(−6)	7.875(−7)	4.540(−7)
$df/d\varepsilon\ \|_{\varepsilon}= 0$	0.3639	0.1221	0.0828	0.0549	0.0384	0.0281	0.0211	0.166
s	−1.30	1.52	1.58	1.64	1.70	1.76	1.82	1.86

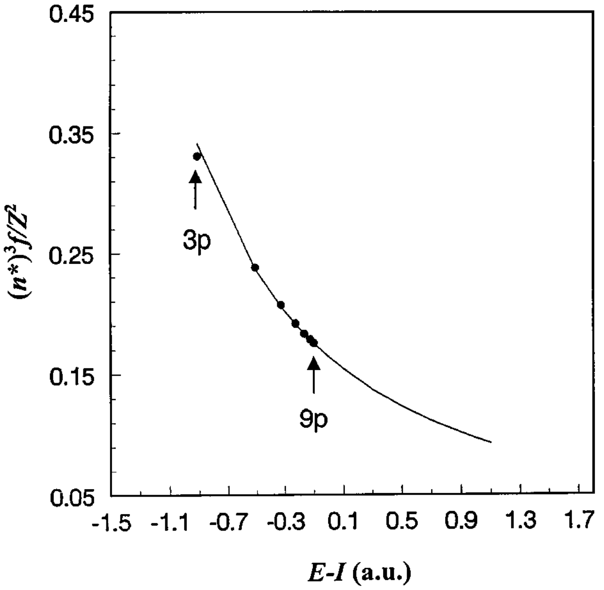

Fig. 1. Oscillator strengths of $1s^22s$–$1s^2np$ transitions in C IV. The solid curves are obtained according to equations (3, 8), the dots represent the values computed from equation (3). The discrete oscillator strengths are multiplied by respective factors $(n^*)^3/Z^2$. The continuous oscillator strengths above the threshold are $df/d\varepsilon$.

the recent accurate theoretical ones of Yan and Drake [5] and Yan *et al.* [11]. In this work, our main purpose is to extend the FCPC method to calculate the f-values for transitions that the final states are in higher excited levels. For the lithium atom, The oscillator strengths for $2\ ^2S$–$n\ ^2P$ ($n \geq 3$) transitions have been calculated by several authors [8,10,25], and the most accurate nonrelativistic results are probably those of Peach *et al.* [8]. In Table 2 we present a comparison of our nonrelativistic oscillator strengths for $2s\ ^2S$–$np\ ^2\mathrm{P}$ transitions of lithium with the accurate nonrelativistic results of Peach *et al.* [8]. Earlier work on this subject are not included in this table, for example, it may be found in references [10,25]. It appears that our nonrelativistic oscillator strengths are in close agreement with those of Peach *et al.* [8]. Above discussion suggests that the FCPC method is useful in calculating the transition processes where the participation of the core is weak in the optical transitions of $1s^2nl$–$1s^2$ $n'l'$, and the cancelation of the error in the core wave function will likely assist in obtaining a more accurate result [14].

In this work, the main calculation error is from the relativistic effects. For Ne VIII, it is about 0.2%. The error from the energy convergence is less than 1 ppm, and the error in the core wavefunction can cancel out in the calculating the transition energies [14]. The total error of Ne VIII is about 0.2%, For other members of the isoelectronic sequence ($Z < 10$), the calculation error is less than 0.2%.

Equations (3, 8) make it possible to determine easily the oscillator strengths for transitions from a certain initial state to all the states of the Rydberg series. The oscillator strength density at threshold, $df/d\varepsilon|_{\varepsilon=0}$, the s values of equation (8), and the fitted values of the QDT parameters of equation (6) are listed in Table 3. As an example, Figure 1 depicts the function (8) corresponding to the $1s^22s$–$1s^2np$ transitions of C IV. It is seen that the oscillator strengths calculated from the FCPC energies and wave functions lie rather well along curve (8), and the discrete oscillator strength coincides with the oscillator strength density at the threshold $E = I$. This indicates that, our procedure should be reasonable and the extrapolation results are reliable and accurate.

4 Conclusion

In this work, the nonrelativistic dipole absorption oscillator strengths of the lithium isoelectronic sequence up to $Z = 10$ are calculated by using the energies and wave functions obtained from the FCPC method. The close agreement between the oscillator strengths from the length and velocity formulae seems to suggest that the FCPC wave functions should be accurate in the configuration space from intermediate r to large r, and the predicted oscillator strengths could be accurate. Combining the calculated f-values with the quantum defect theory, the reliable and accurate oscillator strengths for transitions from a certain initial state to all the states of the Rydberg series can be obtained.

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