

## Systematic trends in the line strengths and radial matrix elements of E1 transitions in the Be isoelectronic sequence

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**Abstract.** Line strength  $S$  and radial matrix element  $\sigma$  for the dipole allowed transitions within  $n=2$  complex of ions in the Be isoelectronic sequence have been fitted in the forms  $Z^2 S = A + B/(Z - C)$  and  $Z\sigma = A' + B'/(Z - C')$ . The constants  $A, B, C$  and  $A', B', C'$  have been calculated by employing a non-linear least square method. The relevant data for  $S$  and  $\sigma$  have been taken from calculations which includes correlation effects. It is shown that the fitted values of  $A$  and  $A'$  are in excellent accord with their hydrogenic values ( $Z \rightarrow \infty$ ) provided that we express the zeroth-order wavefunction of the ground state  $1s^2 2s^2 {}^1S$  as a quantum-mechanical admixture of the Hartree-Fock (HF) state  $1s^2 2s^2 {}^1S$  and the near-degenerate state  $1s^2 2p^2 {}^1S$ .

**Keywords.** Radial matrix elements; line strength; oscillator strength; Hartree-Fock; near-degeneracy; hydrogenic limit.

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### 1. Introduction

The optical oscillator strength between the two bound states of an atomic system is an important atomic quantity. This is related to the transition probability, refractive index, the dipole polarizability and the diamagnetic susceptibility. The optical oscillator strength can be used to test the accuracy of the generalized oscillator strength [1]. Its knowledge is useful in fields like astrophysics [2] to compute the opacity of the stellar envelopes [3]. It also finds application in fusion research [4].

Experimentally, the oscillator strength can be extracted from the measurements of transition probabilities by beam-foil [5] and beam-laser [6, 7] techniques. Various theoretical methods [8–11] which take into account the correlation effects can be employed for its calculations. The amount of correlation depends upon the size and nature of the basis function included in the calculation. If the values of oscillator strengths for few ions in an isoelectronic sequence of an atomic system are known, then an interpolation curve based on perturbation theory may be used to extract the information about other ions in the sequence. The perturbation theory is based upon  $1/Z$  expansion of oscillator strength, where  $Z$  is the nuclear charge of an ion. This method is valid only when there are no plunging configurations involved for an ion in an isoelectronic sequence. An interpolation curve based on the expansion of  $Z^2 S$  is more suitable as it does not involve the transition energy. In the limit of  $Z \rightarrow \infty$ , the value of  $Z^2 S$  approaches a finite hydrogenic value which can be trivially calculated. However, this limit is appropriate only when the near-degenerate effects [12], if

present, are included. This near-degenerate effect gives rise to the most important correlation effect. This effect is present in the ground state configuration of Be, B, C, N and O isoelectronic sequences within the  $n = 2$  complex. The  $Z^2S$  expansion has been studied for carbon [13] and oxygen [14] isoelectronic sequences which included the effects of near-degeneracy. The effect of  $2s-2p$  near-degeneracy was studied for these sequences and it was then shown that the correct value of  $Z^2S$  was obtained in the limit of infinite nuclear charge. In the present work, we have extended the  $Z^2S$  expansion for Be isoelectronic sequence. We have shown that the correct value of  $Z^2S$  is obtained in the limit  $Z \rightarrow \infty$  if we augment the HF ground state  $1s^2 2s^2 1S$  with its near-degenerate state  $1s^2 2p^2 1S$ . We have also expanded the dipole radial matrix elements based upon the perturbation expansion method for the dipole allowed transitions in the Be sequence.

## 2. Theory

The length form of line strength  $S$  between an initial bound state  $\phi$  and a final bound state  $\phi'$  is given by [15]

$$S = |\langle \phi(LS\pi) | \sum_{i=1}^N \mathbf{r}_i | \phi'(L'S'\pi') \rangle|^2 \quad (1)$$

where summation is taken over all the electrons of an atom,  $\mathbf{r}_i$  is the dipole operator for the  $i$ th electron,  $LS\pi(L'S'\pi')$  refer to the total angular momentum, spin angular momentum and parity of the initial (final) states. Because of the odd parity of the dipole operator, only states of opposite parity are connected by the dipole operator.

According to the perturbation theory the expansion for  $S$  is

$$Z^2 S = \sum_{i=0}^{\infty} S_i / Z^i. \quad (2)$$

In terms of the radial matrix elements, the perturbation expansion becomes

$$Z\sigma = \sum_{i=0}^{\infty} R_i / Z^i \quad (3)$$

where

$$S = \Lambda \sigma^2 \quad (4)$$

with  $\Lambda$  being an angular factor and  $\sigma$  is the dipole radial matrix element between an initial and the final bound states. The infinite series expansion of (2) and (3) can be written in a more compact fashion as

$$Z^2 S = A + \frac{B}{(Z - C)} \quad (5)$$

$$Z\sigma = A' + \frac{B'}{(Z - C)}. \quad (6)$$

It is trivial to note that  $S_0 = A, S_1 = B, S_j = B(C^{j-1})$  with  $j \geq 2$ . In other words, we have replaced the summation in (2) with a two-term expansion. The constant  $C$  may loosely be interpreted as a screening constant and  $B$  accounts for the residual correlation left over and above the HF correlation and the internal correlation. The same interpretation can

*Systematic trends in Be isoelectronic sequence*

be given to the constants  $B'$  and  $C'$ . Equation (5) was originally suggested by Edlen [16]. The constants  $A, B, C$  or  $A', B', C'$  were obtained by fitting the assumed forms given by (5) or (6) to the known values of  $Z^2S$  or  $Z\sigma$  by employing a non-linear least square method. The details of this procedure have already been given in [14]. In this reference there is a slight misprint in (8). There should be a minus sign in the denominator in front of the square brackets. Here we have studied the transitions  $1s^2 2s^2 1S^e \rightarrow 1s^2 2s 2p^1 P^0$ ,  $1s^2 2s 2p^3 P^0 \rightarrow 1s^2 2p^2 3P$  and  $1s^2 2p^2 1S \rightarrow 1s^2 2s 2p^1 P^0$  in the Be isoelectronic sequence for ions in the range  $Z = 6$  to 10, for which data for atomic opacity calculations was available [17]. These calculations involve correlation effects within and outside the  $n = 2$  complex. We have also used the data of Cheng *et al* [18] for the resonant transition  $1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0$  for ions up to  $Z = 26$  which includes only the internal correlations. These calculations were done in  $j-j$  coupling scheme by employing multi-configuration Dirac-Fock (MCDF) technique [18]. The MCDF wavefunctions are combinations of Slater determinants constructed from  $1s_{1/2}, 2s_{1/2}, 2p_{1/2}, 2p_{3/2}$  orbitals to form eigenfunctions of total angular momentum  $J$  and parity  $\pi$ . We truncated the data at  $Z = 26$  because for heavier ions relativistic effects begin to become appreciable.

The values of constants for the transitions studied here are presented in tables 1–3. We have also calculated the ab-initio values  $A_0$  and  $A'_0$ , which correspond to the values of  $Z^2S$  and  $Z\sigma$  respectively in the limit  $Z \rightarrow \infty$ . In this limit the nuclear term dominates over electron–electron repulsion term and the HF orbitals assume their hydrogenic character. For the  $1s^2 2s^2 1S$  ground state, near degenerate effects are present due to the promotion of two '2s' electrons into the two '2p' electrons giving rise to the near-degenerate state  $1s^2 2p^2 1S$  which strongly interacts with the HF state  $1s^2 2s^2 1S$ . In the limit  $Z \rightarrow \infty$  we can write the ground state wavefunction as a quantum mechanical admixture of the HF state  $\phi_1$  and the near-degenerate state  $\phi_2$  i.e.

$$\phi(1s^2 2s^2 1S) = c_1 \phi_1(1s^2 2s^2 1S) + c_2 \phi_2(1s^2 2p^2 1S). \quad (7)$$

The expansion coefficients  $c_1, c_2$  can be calculated trivially by diagonalizing the

**Table 1a.** The values of parameters of eq. (5).  $A_0$  is the ab-initio value of  $Z^2S$  with  $Z \rightarrow \infty$ .

Transition	$A_0$	$A$	$B$	$C$	$\chi^2$
$1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0$	38.495	38.714	145.418	2.353	1.0E-03

**Table 1b.** The values of parameters of eq. (6).  $A'_0$  is the ab-initio value of  $Z\sigma$  with  $Z \rightarrow \infty$ .

Transition	$A'_0$	$A'$	$B'$	$C'$	$\chi^2$
$1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0$	-4.242	-4.271	-7.561	1.788	2.2E-05

**Table 2a.** The values of parameters of eq. (5).  $A_0$  is the ab-initio value of  $Z^2S$  with  $Z \rightarrow \infty$ .

Transition	$A_0$	$A$	$B$	$C$	$\chi^2$
$1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0$	38.495	39.250	134.461	3.296	5.4E-15
$1s^2 2p^2 1S \rightarrow 1s^2 2s 2p^1 P^0$	33.504	34.194	102.529	3.318	1.7E-15

**Table 2b.** The values of parameters of eq. (6).  $A'_0$  is the ab-initio value of  $Z\sigma$  with  $Z \rightarrow \infty$ .

Transition	$A'_0$	$A'$	$B'$	$C'$	$\chi^2$
$1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0$	-4.242	-4.308	-6.929	2.765	1.0E-16
$1s^2 2p^2 1S \rightarrow 1s^2 2s 2p^1 P^0$	-4.242	-4.304	-6.127	2.836	4.7E-17

**Table 3a.** The values of parameters of eq. (5).  $A_0$  is the ab-initio value of  $Z^2S$  with  $Z \rightarrow \infty$ .

Transition	$A_0$	$A$	$B$	$C$	$\chi^2$
$1s^2 2s 2p^3 P \rightarrow 1s^2 2p^2 3P$	162.0	156.657	691.283	2.407	6.7E-15

**Table 3b.** The values of parameters of eq. (6).  $A'_0$  is the ab-initio value of  $Z\sigma$  with  $Z \rightarrow \infty$ .

Transition	$A'_0$	$A'$	$B'$	$C'$	$\chi^2$
$1s^2 2s 2p^3 P^0 \rightarrow 1s^2 2p^2 3P$	-5.196	-5.143	-10.597	1.733	2.53E-16

Hamiltonian in this two-basis set. We solve the secular equation

$$\sum_{i=1}^2 c_i (H_{ji} - E\delta_{ji}) = 0, \quad j = 1, 2 \quad (8)$$

where  $H_{ij}$  is a typical Hamiltonian matrix element; and

$$\frac{c_1}{c_2} = \frac{-2H_{12}}{(H_{11} - H_{22}) \pm \{(H_{11} - H_{22})^2 + 4H_{12}H_{21}\}^{1/2}} \quad (9)$$

with the normalization condition

$$c_1^2 + c_2^2 = 1. \quad (10)$$

*Systematic trends in Be isoelectronic sequence*

Using Slater's approach [17], we can write down

$$\begin{aligned}
 H_{11} - H_{22} &= 2I(2s, 2s) + 4F^0(1s, 2s) - 2G^0(1s, 2s) + F^0(2s, 2s) \\
 &\quad - 2I(2p, 2p) - 4F^0(1s, 2p) - F^0(2p, 2p) - 0.4F^2(2p, 2p) \\
 &\quad + 0.66666667G^1(1s, 2p) \\
 H_{12} = H_{21} &= (3)^{-1/2} G^1(2s, 2p).
 \end{aligned}$$

The  $I(nl, nl)$ ,  $F^k(nl, n'l')$  and  $G^k(nl, n'l')$  are the one- and two-electron Slater integrals [13]. Using the hydrogenic values of these integrals we get

$$\phi(1s^2 2s^2 1S) = -0.974321\phi_1(1s^2 2s^2 1S) + 0.225165\phi_2(1s^2 2p^2 1S) \quad (11)$$

and

$$\phi(1s^2 2p^2 1S) = 0.974321\phi_1(1s^2 2p^2 1S) + 0.225165\phi_2(1s^2 2s^2 1S). \quad (12)$$

It is now possible to write the line-strength  $S$  as

$$S_0(LS \rightarrow L'S') = c_1^2 S_1 + c_2^2 S_2 + 2c_1 c_2 \sqrt{S_1 S_2} \quad (13)$$

where

$$S_1 = |\langle \phi_1(1s^2 2s^2 1S) | r | \phi_3(1s^2 2s 2p^1 P^0) \rangle|^2 \quad (14)$$

$$S_2 = |\langle \phi_2(1s^2 2p^2 1S) | r | \phi_3(1s^2 2s 2p^1 P^0) \rangle|^2. \quad (15)$$

The angular factor  $\Lambda$  for each transition is calculated using the standard Racah algebra [19]. The angular factors for various transitions are

$$\Lambda(1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0) = 2$$

$$\Lambda(1s^2 2p^2 1S \rightarrow 1s^2 2s 2p^1 P^0) = 2/3$$

$$\Lambda(1s^2 2s 2p^3 P^0 \rightarrow 1s^2 2p^2 3P) = 6.$$

For the mixed state

$$\Lambda(c_1 \{1s^2 2s^2 1S\} + c_2 \{1s^2 2p^2 1S\} \rightarrow 1s^2 2s 2p^1 P^0) = 2.138636414$$

$$\Lambda(c_1 \{1s^2 2p^2 1S\} + c_2 \{1s^2 2s^2 1S\} \rightarrow 1s^2 2s 2p^1 P^0) = 1.861363589.$$

The radial matrix elements are given by

$$Z\sigma(2s \rightarrow 2p) = \int_0^\infty P_{2s}(r) P_{2p}(r) r dr = -\sqrt{27}. \quad (16)$$

The zeroth order multiplet strengths for various transitions in the hydrogenic limit are

$$Z^2 S_1(1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0) = 54$$

$$Z^2 S_2(1s^2 2p^2 1S \rightarrow 1s^2 2s 2p^1 P^0) = 18$$

$$Z^2 S_0(1s^2 2s 2p^3 P^0 \rightarrow 1s^2 2p^2 3P) = 162.0.$$

We finally get

$$Z^2 S_0(1s^2 2s^2 1S \rightarrow 1s^2 2s 2p^1 P^0) = 38.485$$

$$Z^2 S_0(1s^2 2p^2 1S \rightarrow 1s^2 2s 2p^1 P^0) = 33.504.$$

### 3. Results and discussion

We obtained excellent fits for  $Z^2S$  and  $Z\sigma$  data of Cheng *et al* [18] from their assumed forms given by (5) and (6) for the values of  $Z$  up to 26. From tables 1a and 1b, we notice that for the transition  $1s^22s^21S \rightarrow 1s^22s2p^1P^0$  the fitted value  $A (= 38.7146)$  is in excellent accord with the corresponding ab-initio value  $A_0 (= 38.495)$ . However, if the near-degeneracy effect is omitted, then the HF value ( $= 54.0$ ) for this transition becomes higher than the ab-initio value by about 40%. The value of  $A'$  which refers to the value of  $Z\sigma$  in the limit of  $Z \rightarrow \infty$  for this transition is  $-4.271$  which is again in excellent accord with the ab-initio value  $-4.242$ . Its corresponding HF value is  $-5.196$  which is higher than the ab-initio value by about 22%.

In table 2a, we have displayed the values of fitted and ab-initio constants for the resonant transition and the transition  $1s^22p^21S \rightarrow 1s^22s2p^1P^0$  where we have used the opacity data [17] which is given only up to  $Z = 10$ . For the resonant transition our fitted value is once again in good agreement with the ab-initio value. For the transition  $1s^22p^21S \rightarrow 1s^22s2p^1P^0$ , our fitted value of 34.194 differs from the ab-initio value of 33.504 by about 2%. These values (ab-initio and fitted) are almost twice the HF value which is 18. From table 2b, we notice that the agreement between  $A'_0$  and  $A'$  with their respective ab-initio values persist for both the transitions. These ab-initio values differ from their corresponding HF values of  $-5.196$  by 22%.

We have also carried out calculations for the transition  $1s^22s2p^3P^0 \rightarrow 1s^22p^23P$  using the opacity data [17]. In this transition there is no near-degeneracy effect present and so it is expected that the fitted value of  $A$  and  $A'$  would be in good agreement with the single-configuration value. From table 3a we notice that the fitted value of  $A$  is 156.657 which is in good agreement with the HF value of 162.0. Similarly, in table 3b the value of  $A'$  is  $-5.143$  which differs from its ab-initio value of  $-5.196$  by about 1%.

We conclude from our present study that both the fitted forms of  $Z^2S$  and  $Z\sigma$  give a good description of trends in  $S$  and  $\sigma$  along an isoelectronic sequence if the near-degenerate effects are included in the interpretation of  $A$  or  $A'$  values.

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*Systematic trends in Be isoelectronic sequence*

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