Oscillator strengths for Na-like ions

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Abstract   We have calculated the optical oscillator strengths, of both the length and velocity forms, for the inner-shell excitation $1s^2 2s^2 2p^6 3s\ ^2S_{1/2} \to 1s^2 2s^2 2p^6 3s^2\ ^2p^0_{1/2}$ and $1s^2 2s^2 2p^6 3s\ ^2S_{1/2} \to 1s^2 2s^2 2p^5 3s^2\ ^2p^0_{1/2}$ transitions in Ca^{9+}, Sc^{10+}, Ti^{11+}, Cu^{18+} and Zn^{19+} ions of the sodium isoelectronic sequence employing the Tiwary approach in the intermediate coupling scheme. Our present theoretical results demonstrate that the Tiwary approach is capable of yielding encouraging results.

1. Introduction

The study of ionized atoms has attracted special interest in modern atomic physics and other related fields such as astrophysics and plasma physics. Lines emitted from ionized atoms such as the first transition elements immersed in solar, stellar, and laboratory plasmas have been playing a very important role in modelling these matters. Development of experimental techniques such as electron-beam ion sources or ion accelerators has helped to study the spectroscopic properties and scattering cross-sections of various ion-collision processes with high accuracy. In the analysis of the spectra observed in these experiments, accurate level structures and optical oscillator strengths for an atom in various charged states are required.

There has been a growing interest in the inner-shell excitation of alkali metal atoms and alkali-like ions from both experimentalists and theorists, because inner-shell excitation may lead to autoionization which has an important role in explaining the structure observed in the integrated ionization cross-section curves for electron impact. Consequently, the reliable theoretical calculation of position of the autoionizing level and hence the theoretical estimate of the excitation threshold, which is used in the calculation of the oscillator strengths, of both length and velocity forms, is of special interest. The oscillator strength information is important to know the electronic probabilities for both valence and inner-shell excitation and ionization processes in many areas of application including plasmas, fusion research, lithography, aeronomy, astrophysics, space chemistry and physics, laser development, radiation biology,

dosimetry, health physics and radiation protection. Such information is also a crucial requirement for the development and evaluation of quantum-mechanical theoretical methods and for the modelling procedures and for various phenomenon involving electronic transitions induced by energetic radiation.

We have calculated the optical oscillator strengths, of both length and velocity forms, for several transitions in the sodium and sodium-like ions using the HF as well as CI wave functions for both initial and final states in exactly same manner as in the case of the potassium isoelectronic sequence by Tiwary *et al* [1-5] and Tiwary [6-11]. In our earlier work we have reported the oscillator strengths for the inner-shell excitation $1s^2 2s^2 2p^6 3s\ ^2S^e \rightarrow 1s^2 2s^2 2p^5 3s^2$ $^2P^0$ transition in P^{4+} ion using non-relativistic HF and CI wave functions for both initial and final states involved in the transition. However, there is a considerable discrepancy between the length and velocity forms of the oscillator strengths.

It is well known that the relativistic effects play an extremely important role in obtaining accurate results. Consequently, it is indispensable to incorporate the relativistic effects into the study of atomic structure in order to generate reliable results. In our earlier work we have calculated the oscillator strengths using the non-relativistic CI wave function. In this work we have taken into account of the relativistic effects which may then be used to calculate transitions which are forbidden in pure LS coupling scheme.

In the present paper, we have calculated the optical oscillator strengths, of both the length and velocity forms, for the inner-shell excitation $1s^2 2s^2 2p^6 3s\ ^2S^e\ _{1/2} \rightarrow 1s^2 2s^2 2p^5 3s^2$ $^2P^0\ _{1/2}$ and $1s^2 2s^2 2p^6 3s\ ^2S^e\ _{1/2} \rightarrow 1s^2 2s^2 2p^5 3s^2\ ^2P^0\ _{3/2}$ transitions in $Ca^{9+}, Sc^{10+}, Ti^{11+}, Cu^{18+}$, and Zn^{19+} ions of the sodium isoelectronic sequence employing the Tiwary approach in the intermediate coupling scheme.

2. Theory

We have performed our relativistic calculation using the general configuration interaction code CIV3 of Hibbert [12] and Glass and Hibbert [13]. The LS wave functions are written in the form:

$$\Psi(LS) = \sum_{i=1}^{M} a_i \phi_i (\alpha, LS).$$

(1)

The coefficients a_i are eigenvectors components of the Hamiltonian matrix with typical elements

$$H_{ij} = <\phi_i |H|\phi_j >,$$

(2)

ϕ are single configuration functions constructed from one-electron functions, whose orbital and spin angular momenta are coupled to form the common total angular momentum quantum numbers L and S according to a prescription denoted in (1) by α_i.

We express the radial parts of the one-electron functions in analytic form as a sum of Slater type orbitals, following Clementi and Roetti [14]

$$P_{nl} = \sum_{j=1}^{k} c_{jnl}\ r^{I_{jnl}}\ e^{-\xi_{jnl} r}.$$

(3)

The parameters in (3) can be varied to optimize the energy of any state, subject to the orthonormality condition

$$\int_0^\infty P_{nl}(r) \, P_{n'l}(r) = \delta_n \tag{4}$$

Once the radial functions are determined, effects may be added to the Hamiltonian in the form of the Breit-Pauli interaction, of which we include the spin-orbit, spin-other-spin, spin-spin, mass correction, and one-body Darwin term. The first three terms split LS states into J-dependent levels while the last two affect the overall energy of each term. The expansion (1) is then replaced by

$$\Psi(J) = \sum_{i=1}^{M} a_i \phi_i (\alpha_i \, LSJ) , \tag{5}$$

where the summation now includes single-configuration with different L and S (which can couple to form a common J value). The matrix which is diagonalized to give the eigenenergies and eigenvectors components a_i now contain the Breit-Pauli operators as well as the previous nonrelativistic terms in the Hamiltonian.

The length and velocity forms of the electric dipole oscillator strengths, for transition between initial and final states Ψ_i and Ψ_f respectively (assuming $e = \hbar = m = c = 1$) are

$$f_L = \frac{2\Delta E}{3g_i} \sum \Psi_i \sum_{k=1}^{N} r_k \, \Psi_f . \tag{6}$$

$$f_V = \frac{2}{3 \Delta E} \frac{1}{g_i} \sum \left| \left\langle \Psi_f \left| \sum_{k=1}^{N} p_k \right| \Psi_i \right\rangle \right| \tag{7}$$

where the outer sum is over the M_L, M_S degeneracies of the two states, and

$$\Delta E = E_f - E_i . \tag{8}$$

$$g_i = (2L_i + 1)(2S_i + 1). \tag{9}$$

When summations of the form (5) are used for the wavefunctions of the two states, then for example, the matrix element in (6) becomes

$$\sum \sum a_s^i a_t^f \qquad \sum r_p \tag{10}$$

The determination of the CI wave functions and oscillator strengths described in this paper has been performed with the general configuration interaction code CIV3.

3. Results and discussion

We have calculated the optical oscillator strengths, of both the length and velocity forms, for the inner-shell excitation $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2P^0{}_{1/2}$ and $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2P^0{}_{3/2}$ transitions in Ca^{9+}, Sc^{10+}, Ti^{11+}, Cu^{18+}, and Zn^{19+} ions of the sodium isoelectronic sequence employing the Tiwary approach in the intermediate coupling scheme.

Table 1 displays the J-dependent HF and CI optical oscillator strengths, of both length and velocity forms, of the inner-shell excitation $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2P^0{}_{1/2}$ transitions in Ca^{9+}, Sc^{10+}, Ti^{11+}, Cu^{18+}, and Zn^{19+} ions of the sodium isoelectronic sequence. Table 2 shows exactly the same quantities as in table 1 but for the transition $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2P^0{}_{3/2}$.

Table 1. Oscillator strengths for the inner-shell excitation $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2}$ $1s^2\,2s^2\,2p^5\,3s^2\,{}^2p^0{}_{1/2}$ transition in the sodium isoelectronic sequence.

Systems	HF		CI	
	f_L	f_V	f_L	f_V
Ca^{9+}	0 0240	0.0215	0.0317	0 0307
Sc^{10+}	0 0235	0 0212	0 0315	0 0303
Ti^{11+}	0 0231	0 0209	0 0312	0 0298
Cu^{18+}	0.0210	0.0190	0.0296	0.0262
Zn^{19+}	0 0208	0 0188	0.0295	0.0258

Several features of importance emerge from Table 1-2. first, the optical oscillator strengths, of both length and velocity forms, increase with increase of atomic number (Z) for both transitions $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2P^0{}_{1/2}$ and $1s^2\,2s^2\,2p^6\,3s\,{}^2S^e{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2P^0{}_{3/2}$ in all ions of our present consideration. Second, the values of $CI\,f_L$ and f_V are larger than $HF\,f_L$ and f_V for both transitions given in Tables 1 and 2 in all ions which reflect that the correlation enhances the oscillator strengths. Third, the disagreement between $CI\ f_L$ and f_V decreases with increase of Z which shows that the effect of correlation increases in all ions of our present consideration. Fourth, the disagreement between $HF\,f_L$ and f_V values for $\Delta J = 0$ are significantly smaller compared to the f_L and f_V values for the $\Delta J = 1$ transition. Finally, our present investigation indicates that it is indispensable to incorporate the relativistic and correlation effects simultaneously in order to obtain accurate results.

Table 2. Oscillator strengths for the inner-shell excitation $1s^2\,2s^2\,2p^6\,3s\,{}^2S{}_{1/2} \rightarrow 1s^2\,2s^2\,2p^5\,3s^2\,{}^2p^0{}_{1/2}$ transition in the sodium isoelectronic sequence.

Systems	HF		CI	
	f_L	f_V	f_L	f_V
Ca^{9+}	0.0476	0.0435	0.0625	0 0617
Sc^{10+}	0.0466	0.0429	0.0619	0.0608
Ti^{11+}	0 0457	0.0423	0.0613	0.0598
Cu^{18+}	0.0412	0.0388	0.0573	0.0526
Zn^{19+}	0.0407	0.0384	0.0569	0.0518

4. Conclusion

Our present theoretical investigation of J-dependent oscillator strengths (f_L and f_V) demonstrates that the Tiwary approach is very compact, convenient, economic from computational point of view and capable of yielding encouraging results for the complex inner-shell excitation transition in the medium ionized atoms of the sodium isoelectronic sequence. This approach may provide significant advantage also in the case of CI calculations in molecules, clusters and solids. The present CI wave functions may be of use in calculations of scattering cross sections for the inner-shell excitation process in Ca^{9+}, Sc^{10+}, Ti^{11+}, Cu^{18+}, and Zn^{19+} ions. However, there is disagreement between the length and velocity forms of oscillator strengths which may be probably due to the lack of inseparable way of including correlation and relativity, quantum electrodynamic and nuclear size effect. Our theoretical results suggest that the reliable theoretical predictions of oscillator strengths require methods that account for correlation, relativity, QED and nuclear size effects in a systematic and coherent manner. At present we do not have a comprehensive and practical method that accounts for all effects mentioned above on equal footing. We hope that this work will stimulate reliable experimental as well as other accurate theoretical investigations.

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