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Theoretical studies of the atomic transitions in boron-like ions: Mg VIII, Si X and S XII

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Abstract
In this paper, we have carried out the calculations of the weighted oscillator strengths and the transition probabilities for a few low-lying transitions of boron-like ions: Mg VIII, Si X and S XII, which are astrophysically important, particularly in the atmosphere of the solar corona. We have employed an all-order relativistic many-body theory called the relativistic coupled-cluster theory to calculate very precisely these atomic quantities of astrophysical interest. We have reported for the first time the transition probabilities for some forbidden transitions which are unavailable in the literature, either theoretically or experimentally. We also discuss the physical effects associated with these transitions. Our data can be used for the identification of spectral lines arising from the coronal atmospheres of the Sun and Sun-like stars having an extended corona.

1. Introduction

With the remarkable advances in the field of observational astronomy such as the deployment of satellite probes for data acquisition, there is considerable interest in accurate calculations of the oscillator strengths and the transition probabilities for highly stripped ions which are very important in astrophysics, mainly in the identification of spectral lines [1–5]. Various electromagnetic transitions from the low-lying single-valence excited states, $2s^2\,2p_{3/2}(^2P_{3/2})$, $2s^2\,3s(^2S_{1/2})$, $2s^2\,3d_{3/2}(^2D_{3/2})$, and $2s^2\,3d_{5/2}(^2D_{5/2})$ to the ground state in the highly ionized boron-like ions such as Mg^{7+}, Si^{9+} and S^{11+} are observed in the solar atmosphere [6, 7]. Most of the lines correspond to the soft x-ray waveband and have the potential to probe the chromosphere–corona transition region and possibly the coronal hole regions of the solar atmosphere [7–9], where the temperatures would be of the order of a million Kelvin. The relative line intensity ratios in Mg VIII and Si X line emission spectrum have been found to be density sensitive [10, 11]. The EUV line intensity ratios of these ions have been studied [12] to infer the electron density in different solar features such as active region, quiet sun and off-limb. Therefore, lines emitted from boron-like ions can be used as a powerful tool in the diagnostics of the electron density [13] and the temperature in the solar atmosphere. Interestingly, the soft x-ray coronal emission lines of S XII in the stellar binary Capella, which is one of the nearby Sun-like stars, have been observed by Audard *et al* [14] using the high resolution RGS XMM-Newton satellite.

There are a few calculations of certain transition probabilities of the considered boron-like ions available in the literature; some of them are completely non-relativistic and based on the multi-configuration Hartree–Fock (MCHF) method [15–17]; some others are based on MCHF calculations with Breit–Pauli corrections (MCHF+BP) [18–20] and there are a few calculations based on the relativistic many-body perturbation theory (MBPT) [21] and the relativistic multi-reference configuration interaction (MRCI) method [22]. Often the theoretical calculations are scaled to match the observed transition energies [6, 20]. Given the increasing need for accurate spectroscopic data in astrophysics, it is necessary to use all-order relativistic many-body methods like the relativistic coupled-cluster (RCC) theory [23] to calculate the principal atomic quantities of astrophysical interest such as the energy levels, the oscillator strengths, the transition probabilities and the lifetimes of the excited states.

The study of boron-like ions is interesting from the point of view of the strong core–valence electron correlation effects and also because the transition energies are in reach of current laboratory astrophysics experimental facilities such as the electron beam ion trap (eBIT) [24]. In this paper, we present both the allowed and forbidden transition amplitudes and the corresponding transition probabilities of a few low-lying states in the boron-like ions. We also discuss the behaviour of correlation effects associated with these calculations.

The organization of the paper is as follows. In section 2, we give the working formulae for the transition probabilities and the oscillator strengths and briefly discuss the RCC method employed in calculating these quantities. In section 3, we present the results and compare them with those available in the literature and the conclusions are drawn in the last section.

2. Theory and method of calculation

The spontaneous transition probabilities due to E1, E2, M1 and M2 operators from a state $|J_f M_f\rangle$ to the state $|J_i M_i\rangle$ are given by [25],

$$A^{\mathrm{E1}}_{J_f J_i} = \frac{64\pi^4 e^2 a_0^2}{3h\lambda^3(2J_f+1)} S^{\mathrm{E1}} = \frac{2.0261\times 10^{-6}}{\lambda^3(2J_f+1)} S^{\mathrm{E1}}, \tag{2.1}$$

$$A^{\mathrm{E2}}_{J_f J_i} = \frac{64\pi^6 e^2 a_0^4}{15h\lambda^5(2J_f+1)} S^{\mathrm{E2}} = \frac{1.12\times 10^{-22}}{\lambda^5(2J_f+1)} S^{\mathrm{E2}}, \tag{2.2}$$

$$A^{\mathrm{M1}}_{J_f J_i} = \frac{64\pi^4 e^2 a_0^2(\alpha/2)^2}{3h\lambda^3(2J_f+1)} S^{\mathrm{M1}} = \frac{2.6971\times 10^{-11}}{\lambda^3(2J_f+1)} S^{\mathrm{M1}}, \tag{2.3}$$

and

$$A^{\mathrm{M2}}_{J_f J_i} = \frac{64\pi^6 e^2 a_0^4(\alpha/2)^2}{15h\lambda^5(2J_f+1)} S^{\mathrm{M2}} = \frac{1.491\times 10^{-27}}{\lambda^5(2J_f+1)} S^{\mathrm{M2}}, \tag{2.4}$$

respectively, where, the numerical factor applies for the wavelength λ in cm and the transition line strength S^O, defined as the absolute square of the transition matrix element, i.e.

$$S^O_{(J_f;J_i)} = |\langle J_f \| O \| J_i\rangle|^2, \tag{2.5}$$

where $\langle J_f \| O \| J_i \rangle$ is the reduced-matrix element for the appropriate multipole operator O, in atomic units (au). Here, J is the total angular momentum quantum number.

The single-particle reduced-matrix elements for the E1 and E2 operators in length gauge and the gauge-independent M1 and M2 operators are, respectively, given by [26],

$$\langle \kappa_f \| e1 \| \kappa_i \rangle = \frac{3}{k} \langle \kappa_f \| C_q^{(1)} \| \kappa_i \rangle \int_0^\infty \Big\{ j_1(kr)[P_f(r)P_i(r) + Q_f(r)Q_i(r)] + j_2(kr) \times \left[\frac{\kappa_f - \kappa_i}{2} [P_f(r)Q_i(r) + Q_f(r)P_i(r)] + [P_f(r)Q_i(r) - Q_f(r)P_i(r)] \right] \Big\} \,\mathrm{d}r, \tag{2.6}$$

$$\langle \kappa_f \| e2 \| \kappa_i \rangle = \frac{15}{k^2} \langle \kappa_f \| C^{(2)} \| \kappa_i \rangle \int_0^\infty \Big\{ j_2(kr)[P_f(r)P_i(r) + Q_f(r)Q_i(r)] + j_3(kr) \times \left[\frac{\kappa_f - \kappa_i}{3} [P_f(r)Q_i(r) + Q_f(r)P_i(r)] + [P_f(r)Q_i(r) - Q_f(r)P_i(r)] \right] \Big\} \,\mathrm{d}r, \tag{2.7}$$

$$\langle \kappa_f \| m1 \| \kappa_i \rangle = \frac{6}{\alpha k} \langle -\kappa_f \| C^{(1)} \| \kappa_i \rangle \int_0^\infty \frac{\kappa_f + \kappa_i}{2} j_1(kr)[P_f(r)Q_i(r) + Q_f(r)P_i(r)] \,\mathrm{d}r, \tag{2.8}$$

and

$$\langle \kappa_f \| m2 \| \kappa_i \rangle = \frac{30}{\alpha k^2} \langle -\kappa_f \| C^{(2)} \| \kappa_i \rangle \int_0^\infty \frac{\kappa_f + \kappa_i}{3} j_2(kr)[P_f(r)Q_i(r) + Q_f(r)P_i(r)] \,\mathrm{d}r, \tag{2.9}$$

where κ is the relativistic angular momentum quantum number. The radial functions $P_i(r)$ and $Q_i(r)$ are the large and small components of the ith single-particle Dirac orbital, respectively. The coefficients of the Racah tensor are given by

$$\langle \kappa_f \| C^{(\gamma)} \| \kappa_i \rangle = (-1)^{j_f + 1/2} \sqrt{(2j_f + 1)(2j_i + 1)} \begin{pmatrix} j_f & \gamma & j_i \\ 1/2 & 0 & -1/2 \end{pmatrix} \pi(l_f, \gamma, l_i), \tag{2.10}$$

where j is the single-particle angular momentum quantum number. The parity selection rule is given by

$$\pi(l1, l2, l3) = \begin{cases} 1 & \text{for } l1 + l2 + l3 = \text{even} \\ 0 & \text{otherwise.} \end{cases} \tag{2.11}$$

In equations (2.6) through (2.9), we define the wave vector k as $k = w\alpha$, where $w = \epsilon_i - \epsilon_j$ is the excitation energy at the single-particle level, α is the fine structure constant, l is the orbital angular momentum quantum number and $j_n(kr)$ is a spherical Bessel function of order n. Since kr is sufficiently small, we apply the following approximation to calculate the above matrix elements:

$$j_n(z) \approx \frac{z^n}{1.3.5 \ldots (2n+1)}. \tag{2.12}$$

The oscillator strength and the corresponding transition probability for a transition of any multipole type are related by the general formula

$$f_{(J_f;J_i)} = 1.4992 \times 10^{-16} A_{(J_f;J_i)} \frac{g_f}{g_i} \lambda^2, \tag{2.13}$$

where g_f and g_i are the degeneracies associated with the final and initial states, respectively, λ is the wavelength in Å and $A_{(J_f;J_i)}$ is the transition probability in s^{-1}.

Generally, in the astrophysical context, one uses the weighted oscillator strength which is the product of the degeneracy of the initial state and the oscillator strength and is symmetric with respect to the initial and final states, i.e.

$$gf = (2J_i + 1) f_{if} = -(2J_f + 1) f_{fi}. \tag{2.14}$$

As can be inferred from the above equations, there is a great need for precise values of the transition wavelengths and the transition line strengths for the accurate determination of the oscillator strengths and the transition probabilities. This demands a highly powerful many-body method which would include fully relativistic effects and the electron correlation effects that are sufficiently large especially in many-electron systems. So we employ the RCC theory, which is briefly discussed below, to calculate these quantities of interest.

The starting point of our method is the relativistic generalization of the valence universal coupled-cluster (CC) theory introduced by Mukherjee *et al* [27, 28] which was put later in a more compact form by Lindgren [23, 29]. In this approach, first we obtain the closed-shell Dirac–Fock (DF) wavefunction ($|\Phi_0\rangle$) which corresponds to the electronic configuration $1s^2\,2s^2$. This amounts to solving the DF equations for $N-1$ electrons where N is the total number of electrons in the system. These equations can be expressed as

$$[c\vec{\alpha}_i \cdot \vec{\mathrm{p}}_i + (\beta_i - 1)c^2 + V_{\mathrm{Nuc}}(r_i) + U_{\mathrm{DF}}(r_i)]|\phi_i\rangle = \epsilon_i|\phi_i\rangle, \tag{2.15}$$

where c is the speed of light in vacuum, $\vec{\alpha}$ and β are the Dirac matrices, $V_{\mathrm{Nuc}}(r_i)$ is the nuclear potential and $U_{\mathrm{DF}}(r_i)$ is the effective average potential called the Dirac–Fock potential, which is given by

$$U_{\mathrm{DF}}(r_i)|\phi_i\rangle = \sum_{j=1}^{N-1}\left[\langle\phi_j|\frac{1}{r_{12}}|\phi_j\rangle|\phi_i\rangle - \langle\phi_j|\frac{1}{r_{12}}|\phi_i\rangle|\phi_j\rangle\right]. \tag{2.16}$$

The large and small radial components of the single-particle relativistic wavefunctions are expanded in terms of the Gaussian-type orbitals (GTOs) of the form [30, 31],

$$g_{\kappa_i}^L(r) = N^L r^{n_{\kappa_i}} \mathrm{e}^{-\zeta_i r^2} \tag{2.17}$$

and

$$g_{\kappa_i}^S(r) = N^S\left[\frac{\mathrm{d}}{\mathrm{d}r} + \frac{k}{r}\right] g_{\kappa_i}^L(r), \tag{2.18}$$

where N^L and N^S are the normalization factors for the large and small radial components, respectively, of the one-electron orbitals, n_{κ_i} varies for each relativistic symmetry and takes an integer value as 1 for $\mathrm{s}_{1/2}$, 2 for $\mathrm{p}_{1/2}$ and so on.

In equation (2.17) we have used the even tempering condition for the exponents, i.e,

$$\zeta_i = \zeta_0 \eta^{i-1} \qquad \text{where} \quad i = 1, 2, 3, \ldots, n, \tag{2.19}$$

where ζ_0 and η are the user-defined parameters and n is the size of the basis set. In equation (2.18), the kinetic balance condition is imposed on the small-radial components to avoid the variational collapse of the wavefunctions into the negative energy continuum [30].

The differential equations (2.15) become matrix eigenvalue equations of the form [32],

$$FC = SC\epsilon \tag{2.20}$$

where F, S, C and ϵ are the Fock matrix, overlap matrix, eigenvector and eigenvalue matrix, respectively. This is then transformed to a true eigenvalue problem and diagonalized to get the energies (eigenvalues) and the mixing coefficients (eigenvectors) for both the occupied and the virtual orbitals. The virtual orbitals (including the $2\mathrm{p}_{1/2}$ valence orbital) obtained by this procedure are clearly generated in the V^{N-1} potential of the frozen core orbitals. The details of this method can be found elsewhere [32, 33].

The exact wavefunction ($|\Psi_0\rangle$) for the corresponding closed-shell system is calculated in the RCC theory using

$$|\Psi_0\rangle = e^T|\Phi_0\rangle, \tag{2.21}$$

where T is the excitation operator for the core orbitals. It is the sum of all single, double, triple and higher order excitations of occupied electrons. The open-shell reference state for the desired valence electron, v, can be written as $|\Phi_v\rangle = a_v^\dagger|\Phi_0\rangle$, where $a_v^\dagger$ is the creation operator for the valence electron and $|\Phi_0\rangle$ is a closed-shell reference state which is the Slater determinant representing the $1s^2\,2s^2$ configuration, whereas $|\Phi_v\rangle$ is the Slater determinant representing, for example, the $1s^2\,2s^2\,2p_{1/2}$ configuration.

The exact wavefunction for the open-shell atomic system can be expressed in the RCC theory as

$$|\Psi_v\rangle = e^T\{e^{S_v}\}|\Phi_v\rangle, \tag{2.22}$$

where S_v corresponds to the excitation operator for the valence and valence-core orbitals. Since the systems considered in the present case contain a single-valence electron in their electronic configurations, the nonlinear terms in the expansion of the exponential function of S_v will not exist and the above wavefunction ultimately reduces to the form

$$|\Psi_v\rangle = e^T\{1 + S_v\}|\Phi_v\rangle, \tag{2.23}$$

where { } indicates that the operator is normal ordered.

Even in the few-electron systems, it is not possible to consider all correlated excitations due to huge requirement of the computer memory. In fact, it has been found that the CC theory with both single and double excitations (CCSD) is quite successful in incorporating the maximum correlation effects. However, we have considered the CCSD method along with the important triple excitations (CCSD(T) method). The electron affinity energy (ΔE_v) for the valence electron v and the RCC operator amplitudes are calculated self-consistently using the following coupled equations:

$$\langle\Phi_L|\{\widehat{He^T}\}|\Phi_0\rangle = \Delta E_0\delta_{L,0} \tag{2.24}$$

$$\langle\Phi_K|\{\widehat{He^T}\}S_v|\Phi_v\rangle = -\langle\Phi_K|\{\widehat{He^T}\}|\Phi_v\rangle + [\langle\Phi_K|S_v|\Phi_v\rangle + \delta_{K,v}]\Delta E_v, \tag{2.25}$$

where $|\Phi_L\rangle$ with $L(=1, 2)$ represents the singly or doubly excited state from the closed-shell reference (DF) wavefunction ($L = 0$) and ΔE_0 is the correlation energy for the closed-shell system and $|\Phi_K\rangle$ with $K(=1, 2)$ denotes the singly or doubly excited state from the single-valence reference state ($K = v$). The excitation energies (EE) between different states are calculated from the electron affinity energies.

We calculate the transition matrix elements of any physical operator O by using

$$\begin{aligned}\langle O\rangle_{i\to f} &= \frac{\langle\Psi_f|O|\Psi_i\rangle}{\sqrt{\langle\Psi_f|\Psi_f\rangle\langle\Psi_i|\Psi_i\rangle}}\\ &= \frac{\langle\Phi_f|\left\{1+S_f^\dagger\right\}\overline{O}\{1+S_i\}|\Phi_i\rangle}{\sqrt{\langle\Phi_f|\left\{1+S_f^\dagger\right\}e^{T^\dagger}e^T\{1+S_f\}|\Phi_f\rangle\langle\Phi_i|\left\{1+S_i^\dagger\right\}e^{T^\dagger}e^T\{1+S_i\}|\Phi_i\rangle}},\end{aligned} \tag{2.26}$$

where $\overline{O} = e^{T^\dagger}Oe^T$. First, we compute the operator $\overline{O}$ as the effective one-body and two-body operators using the generalized Wick theorem [23] and later sandwich this between the necessary S_v operators. It has to be noticed that the fully contracted $\overline{O}$ does not contribute

Table 1. Comparison of the calculated excitation energies with the tabulated NIST data. The ground state is $1s^2 2s^2 2p_{1/2}$.

		EE (cm^{-1})	
Atomic system	Upper states	This work	NIST [34]
Mg VIII	$2s^2\,3d_{5/2}$	1 339 798	1 336 030
	$2s^2\,3d_{3/2}$	1 339 584	1 335 860
	$2s^2\,3p_{3/2}$	1 276 642	
	$2s^2\,3p_{1/2}$	1 275 753	
	$2s^2\,3s_{1/2}$	1 210 608	1 210 690
	$2s^2\,2p_{3/2}$	3 433	3 302
Si X	$2s^2\,3d_{5/2}$	1 980 585	1 979 730
	$2s^2\,3d_{3/2}$	1 980 086	1 979 260
	$2s^2\,3p_{3/2}$	1 904 870	
	$2s^2\,3p_{1/2}$	1 902 937	
	$2s^2\,3s_{1/2}$	1 821 314	1 822 000
	$2s^2\,2p_{3/2}$	7 261	6 990
S XII	$2s^2\,3d_{5/2}$	2 753 686	2 748 100
	$2s^2\,3d_{3/2}$	2 752 714	2 747 400
	$2s^2\,3p_{3/2}$	2 659 966	
	$2s^2\,3p_{1/2}$	2 656 319	
	$2s^2\,3s_{1/2}$	2 559 004	
	$2s^2\,2p_{3/2}$	13 465	13 135

in the present calculations. The contribution from the normalization of the wavefunctions (Norm) is given by

$$\text{Norm} = \langle \Psi_f | O | \Psi_i \rangle \left\{ \frac{1}{\sqrt{\mathcal{N}_f \mathcal{N}_i}} - 1 \right\}, \tag{2.27}$$

where $\mathcal{N}_v = \langle \Phi_v | e^{T^\dagger} e^T | \Phi_v \rangle + \langle \Phi_v | S_v^\dagger e^{T^\dagger} e^T S_v | \Phi_v \rangle$ for the valence electron $v(= i, f)$.

3. Results and discussion

In table 1, we present our calculated EEs for the $2s^2\,2p_{3/2}$, $2s^2\,3s_{1/2}$, $2s^2\,3p_{1/2}$, $2s^2\,3p_{3/2}$, $2s^2\,3d_{3/2}$ and $2s^2\,3d_{5/2}$ states from the ground state $2s^2\,2p_{1/2}$ for all the considered systems and compared our results with the available National Institute of Standards and Technology (NIST) database [34]. Our results, in general, agree very well with the measured NIST energies except for the fine structure level of the ground states, i.e. $2s^2\,2p_{3/2}$ states. This shows that the higher order relativistic effects are important for these states and also the quantum electrodynamics (QED) corrections may be required to match the observed results. In all the systems considered, EEs were not known for the $2s^2\,3p_{3/2}$ and $2s^2\,3p_{1/2}$ states, and here we have presented them for the first time that can be used in the astrophysical observations for the identification of spectral lines.

We have used the length gauge in the calculation of the transition properties of E1 and E2. In table 2, we have reported the weighted oscillator strengths and the transition probabilities of a few allowed electric dipole transitions obtained from the RCC calculations. We observe that the transition probabilities for $2s^2\,3d_{3/2} \rightarrow 2s^2\,2p_{1/2}$ transitions are larger than those of $2s^2\,3s \rightarrow 2s^2\,2p_{1/2}$ transitions, maybe because the overlap of radial wavefunctions of the

Table 2. Weighted oscillator strengths and transition probabilities for the allowed E1 transitions to the ground state.

		Weighted oscillator strength (au)		Transition probability (10^{11} s^{-1})	
Atomic system	Upper state	This work	Others	This work	Others
Mg VIII	$2s^2\,3s_{1/2}$	0.051	0.052 [20]	0.251	0.255 [20]
	$2s^2\,3d_{3/2}$	1.188	1.205 [20]	3.555	3.589 [20]
Si X	$2s^2\,3s_{1/2}$	0.048	0.049 [20]	0.529	0.541 [20]
			0.044 [18]		0.481 [18]
			0.051 [15]		0.585 [15]
	$2s^2\,3d_{3/2}$	1.234	1.247 [20]	8.066	8.149 [20]
			1.232 [18]		8.010 [18]
			1.234 [15]		8.310 [15]
S XII	$2s^2\,3s_{1/2}$	0.045	0.047 [15]	0.987	1.06 [15]
	$2s^2\,3d_{3/2}$	1.260	1.256 [15]	15.932	16.2 [15]

Table 3. Contribution from the individual terms for E1 transition amplitude (in au) of $2s^2\,3s \rightarrow 2s^2\,2p_{1/2}$ and $2s^2\,3d_{3/2} \rightarrow 2s^2\,2p_{1/2}$ transitions.

RCC terms	Mg VIII	Si X	S XII
	$2s^2\,3s \rightarrow 2s^2\,2p_{1/2}$ transition amplitudes		
$\overline{O}$	1.28×10^{-1}	9.84×10^{-2}	7.93×10^{-2}
$\overline{O}S_i$	-6.52×10^{-3}	-4.09×10^{-3}	-3.04×10^{-3}
$S_f^{\dagger}\overline{O}$	-5.38×10^{-3}	-2.68×10^{-3}	-1.10×10^{-3}
$S_f^{\dagger}\overline{O}S_i$	1.90×10^{-3}	1.27×10^{-3}	9.12×10^{-4}
Norm	6.14×10^{-5}	1.04×10^{-4}	1.03×10^{-4}
Total	1.18×10^{-1}	9.30×10^{-2}	7.62×10^{-2}
DF	1.28×10^{-1}	9.89×10^{-2}	7.99×10^{-2}
	$2s^2\,3d_{3/2} \rightarrow 2s^2\,2p_{1/2}$ transition amplitudes		
$\overline{O}$	-5.21×10^{-1}	-4.36×10^{-1}	-3.75×10^{-1}
$\overline{O}S_i$	1.73×10^{-2}	1.20×10^{-2}	9.28×10^{-3}
$S_f^{\dagger}\overline{O}$	-3.03×10^{-2}	-2.36×10^{-2}	-1.87×10^{-2}
$S_f^{\dagger}\overline{O}S_i$	-3.66×10^{-3}	-3.06×10^{-3}	-1.51×10^{-3}
Norm	-2.54×10^{-3}	-2.34×10^{-3}	-2.09×10^{-3}
Total	-5.40×10^{-1}	-4.53×10^{-1}	-3.88×10^{-1}
DF	-5.32×10^{-1}	-4.45×10^{-1}	-3.83×10^{-1}

former two states is larger than that of the latter two states. We compare our results with the MCHF+BP results of [20] in which the calculated energies are scaled to match the observed transition energies and with a few non-relativistic results available in the literature [18, 15]. Their methods are less powerful than the all-order RCC theory in incorporating the electron correlation effects and rigourous relativistic effects, and also the RCC method has distinct advantages over the former two [23, 35, 36]. Here, we have used the unscaled computed wavelengths in calculating the transition probabilities.

In order to understand the correlation effects, we have given explicitly the individual contributions to the electric dipole transition amplitudes, in table 3, for the

Table 4. Computed transition amplitudes and transition probabilities for selected forbidden transitions.

Atomic system	Upper state	Multipole	Transition amplitude (au) DF	CCSD(T)	Δ (in %)	Transition probability (s^{-1}) Present	[20]	[22]
Mg VIII	$2s^2\,3d_{5/2}$	M2	1.34×10^{0}	1.33×10^{0}	−1.13	1.90×10^{3}		
	$2s^2\,3d_{3/2}$	M2	-4.12×10^{-1}	-4.01×10^{-1}	−2.76	2.58×10^{2}		
	$2s^2\,3p_{3/2}$	E2	-2.54×10^{-1}	-2.67×10^{-1}	4.98	6.78×10^{6}		
	$2s^2\,3p_{3/2}$	M1	1.24×10^{-3}	-2.86×10^{-3}	143.21	1.15×10^{2}		
	$2s^2\,3p_{1/2}$	M1	2.62×10^{-4}	5.76×10^{-4}	54.44	9.28×10^{0}		
	$2s^2\,2p_{3/2}$	E2	-2.96×10^{-1}	-2.70×10^{-1}	−9.96	9.85×10^{-7}	8.8804×10^{-7}	9.61×10^{-7}
	$2s^2\,2p_{3/2}$	M1	-1.15×10^{0}	-1.12×10^{0}	−2.7	3.48×10^{-1}	3.2905×10^{-1}	3.21×10^{-1}
Si X	$2s^2\,3d_{5/2}$	M2	1.13×10^{0}	1.13×10^{0}	0.33	9.65×10^{3}		
	$2s^2\,3d_{3/2}$	M2	-3.38×10^{-1}	-3.34×10^{-1}	−2.77	1.27×10^{3}		
	$2s^2\,3p_{3/2}$	E2	-1.71×10^{-1}	-1.79×10^{-1}	4.89	2.27×10^{7}		
	$2s^2\,3p_{3/2}$	M1	1.74×10^{-3}	-1.49×10^{-3}	217.08	1.06×10^{2}		
	$2s^2\,3p_{1/2}$	M1	3.80×10^{-4}	5.91×10^{-4}	57.37	7.24×10^{1}		
	$2s^2\,2p_{3/2}$	E2	-2.01×10^{-1}	-1.84×10^{-1}	−9.15	1.92×10^{-5}	1.7837×10^{-5}	1.91×10^{-5}
	$2s^2\,2p_{3/2}$	M1	-1.15×10^{0}	-1.12×10^{0}	−2.54	3.27×10^{0}	3.1475×10^{0}	3.06×10^{0}
S XII	$2s^2\,3d_{5/2}$	M2	9.67×10^{-1}	9.79×10^{-1}	1.14	3.77×10^{4}		
	$2s^2\,3d_{3/2}$	M2	-2.96×10^{-1}	-2.86×10^{-1}	−3.68	4.80×10^{3}		
	$2s^2\,3p_{3/2}$	E2	-1.24×10^{-1}	-1.30×10^{-1}	4.78	6.28×10^{7}		
	$2s^2\,3p_{3/2}$	M1	2.33×10^{-3}	-3.29×10^{-4}	808.1	1.37×10^{1}		
	$2s^2\,3p_{1/2}$	M1	5.24×10^{-4}	6.58×10^{-4}	20.4	1.10×10^{2}		
	$2s^2\,2p_{3/2}$	E2	-1.46×10^{-1}	-1.34×10^{-1}	−8.63	2.23×10^{-4}		2.29×10^{-4}
	$2s^2\,2p_{3/2}$	M1	-1.15×10^{0}	-1.13×10^{0}	−2.38	2.09×10^{1}		2.03×10^{1}

$2s^2\,3s \rightarrow 2s^2\,2p_{1/2}$ and $2s^2\,3d_{3/2} \rightarrow 2s^2\,2p_{1/2}$ transitions, from the following four terms: $\langle\Phi_f|\overline{O}|\Phi_i\rangle$, $\langle\Phi_f|\overline{O}S_i|\Phi_i\rangle$, $\langle\Phi_f|S_f^{\dagger}\overline{O}|\Phi_i\rangle$, $\langle\Phi_f|S_f^{\dagger}\overline{O}S_i|\Phi_i\rangle$ which are obtained on expanding equation (2.26) and the contributions from the normalization factor. As expected, the contribution from the term $\langle\Phi_f|\overline{O}|\Phi_i\rangle$ is large compared to the other three terms as it contains the DF term and a few core correlated terms, whereas $\langle\Phi_f|S_f^{\dagger}\overline{O}S_i|\Phi_i\rangle$ is smaller than the rest as it contains two orders in the S_v amplitude. The contribution from $\langle\Phi_f|S_f^{\dagger}\overline{O}|\Phi_i\rangle$ is larger compared to $\langle\Phi_f|\overline{O}S_i|\Phi_i\rangle$ in the $2s^2\,3s$ state, whereas it is the other way round in the case of the $2s^2\,3d_{3/2}$ state. However, the trends for all three ions are almost the same for any given transition. We have also presented the DF results in the bottom line of the table in order to emphasize the correlation contributions to the total results. The correlation effects for the electric dipole transition amplitudes are small compared to the DF values and they are negative, thereby reducing the contribution of DF values in both cases.

In table 4, we have given the DF and CCSD(T) results of the important forbidden transition amplitudes due to M1, E2 and M2 transitions, which are interesting in the astrophysical context. We have presented the percentage difference between these results (Δ) which represent the contribution due to electron correlation effects. In a recent calculation of M1 transition probabilities in B-like ions using the MRCI method with QED corrections [37], it was shown that the contribution of the inter-electronic interaction correlation is small for the transition from $2s^2\,2p_{3/2}$ to the ground state for S XII. However, we observe that the contribution from the electron correlation effects is non-negligible in many of the considered transitions. Interestingly, the M1 transition amplitude for the transition from $2s^2\,3p_{3/2} \rightarrow 2s^2\,2p_{1/2}$ has very large correlation effects which even change the sign of the CCSD(T) result from the DF result.

We have also presented, in table 4, the transition probabilities calculated using the transition amplitudes and wavelengths obtained using the CCSD(T) method. These results are compared with other calculated results available in the literature [20, 22]. As seen from table 4, our results are in good agreement with the Coulomb-gauge results of [22]. We have presented the results for a few other transitions which have not been studied earlier. One can obtain the oscillator strengths using the general formula given in equation (2.13) for these transitions using the above results.

Our results on the transition probabilities and lifetimes of the low-lying transitions in the boron iso-electronic ions may be helpful in the near future for the identification of spectral lines in the regions of extremely low-density plasma such as those present in the coronal atmospheres of the Sun and a few Sun-like stars. They also serve as bench mark results for laboratory astrophysics experiments, using eBIT.

4. Conclusion

We have calculated the weighted oscillator strengths for a few electric dipole transitions and the transition probabilities for some low-lying excited states of boron-like ions: Mg VIII, Si X, and S XII, which are abundant in the solar atmosphere, using the relativistic coupled-cluster theory. It is shown that the contributions of electron correlation effects to the transition amplitudes are non-negligible in some transitions. Our results, in general, are in good agreement with the calculated values available in the literature, thereby demonstrating the power of this theory to generate accurate and reliable atomic data for astrophysics.

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