Angular momentum transfer and polarization degree of ions with two-valence electrons by electron impact

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Abstract. We study for electron-impact excitation of ions with two valence electrons (Be\textsuperscript{2+}, C\textsuperscript{2+} and Si\textsuperscript{2+}) from the ground state to the first \textsuperscript{1}P\textsubscript{o} state using the \textit{R}-matrix method. The integral cross sections and polarization degree for this transition of each ion are obtained. The differential cross sections and angular momentum transfer are also shown at a few energies in the non-resonant region. The present angular momentum transfer for Be\textsuperscript{2+} and C\textsuperscript{2+} at small scattering angles has positive values, while it is negative for Si\textsuperscript{2+}.

1. Introduction
Excitation cross section for electron impact is important to explain spectra of astrophysical plasmas and high-temperature laboratory plasmas. The radiation emitted from ions with unbalanced magnetic sublevel population by electron impact is polarized and its detection is available as a plasma diagnostic tool [1].

For excitation process from the ground S state to the excited P state, the expectation value of angular momentum component which is perpendicular to the scattering plane is called angular momentum transfer \(L_{\perp}\). According to the propensity rule at high energies using the second-Born approximation method, the value of \(L_{\perp}\) for this transition in electron-atom collision is positive at small scattering angles [2]. Srivastava et al. [3] reported using the distorted wave calculation that the values of \(L_{\perp}\) for electron collisions with He-like ions (Z= 3, 8, \infty) are positive at small scattering angles at the incident electron energies of two and four times the excitation threshold energy. Kai et al. [4] have found a case where \(L_{\perp}\) is negative in low-energy electron scattering with Mg-like Si ion (Si\textsuperscript{2+}) using the \textit{R}-matrix method. The same method is applied to electron scatterings by doubly charged ions with one valence electron such as H-like Li (Li\textsuperscript{2+}), Li-like B (B\textsuperscript{2+}) and Na-like Al (Al\textsuperscript{2+}) [5].

Here we treat the electron-impact excitations of doubly charged ions with two-valence electrons such as He-like Be (Be\textsuperscript{2+}), Be-like C (C\textsuperscript{2+}) and Mg-like Si (Si\textsuperscript{2+}). The integral cross section (ICS), polarization degree \((P)\), the differential cross section (DCS) and \(L_{\perp}\) are presented.
2. Theory

2.1. Target wavefunctions and collision calculations

The configuration interaction method is adopted to represent atomic states. To describe scattering wavefunctions, 19, 26 and 28 target states are used for Be\(^{2+}\), C\(^{2+}\) and Si\(^{2+}\), respectively. In this work, the 1s orbital of Be\(^{2+}\) and the 1s and 2s orbitals of C\(^{2+}\) are the Hartree-Fock wave functions given by Clementi and Roettig [6] for the ground state 1s\(^2\) 1S\(^0\) and 1s\(^2\) 2s\(^2\) 1S\(^0\), respectively. The optimization of other high-lying orbitals are performed using the CIV3 atomic structure program of Hibbert [7]. The 2p, 3s, 3p, 3d, 4s, 4p, 4d and 4f orbitals of Be\(^{2+}\) are optimized on the energies of the 1s2p 1P\(^0\), 1s3s 1S\(^0\), 1s3p 1P\(^0\), 1s3d 1D\(^0\), 1s4s 1S\(^0\), 1s4p 1P\(^0\), 1s4d 1D\(^0\) and 1s4f 1P\(^0\) states, respectively. The 2p, 3s, 3p and 3d orbitals of C\(^{2+}\) are optimized on the energies of the 1s2p 1P\(^0\), 1s3s 1S\(^0\), 1s3p 1P\(^0\) and 1s3d 1D\(^0\) states, respectively. For the orbitals of Si\(^{2+}\), we adopted the orbitals optimized by Kai et al. [4]. Table 1 shows the excitation energies and oscillator strengths between the ground state and the first excited 1P\(^0\) state. The present excitation energies agree with the data of [8] within \sim 0.5\% for Be\(^{2+}\) and with those of [8, 9] within \sim 12\% for C\(^{2+}\). Our values of length and velocity oscillator strengths accord within \sim 6\% for Be\(^{2+}\) and within less than 0.1\% for C\(^{2+}\). The oscillator strengths are in fairly good agreement with the values of [9].

The \(R\)-matrix computer program of Berrington et al. [10] is used for the scattering calculation, where the experimental excitation energies [8] are adopted rather than the calculated values in Table 1.

2.2. The angular momentum transfer and polarization degree

The angular momentum transfer for 1S\(^e\) \rightarrow 1P\(^o\) transitions is given by \(L_1 = -2\sqrt{2} Im|f_1f_2^*|/\sigma\) [11], where \(\sigma\) is the DCS and \(f_M\) is the scattering amplitude for a magnetic sublevel with \(M\) of the 1P\(^0\) state. The ICS for the 1P\(^0\) state is given by \(Q = Q_0 + 2Q_1 (Q_1 = Q - 1)\). The \(Q_M\) is the ICS for the excitation into a magnetic sublevel with \(M\) of 1P\(^0\) state. The polarization degree for 1S\(^e\) \rightarrow 1P\(^o\) transitions is given by \(P = (Q_0 - Q_1)/(Q_0 + Q_1) \times 100\) [12, 13]. The quantization axis is along the incident direction. In a case of neutral atom target, \(p\) wave is dominant at the threshold, and \(Q_1\) vanishes. Hence the emission line from the 1P\(^o\) \rightarrow 1S\(^e\) transition is 100\% linearly polarized at threshold [12]. On the other hand, when the target is an ion, the \(Q_1\) does not vanish at the threshold. Other partial waves as well as \(p\) wave contribute to scattering owing to the attractive Coulomb force.

3. Results and discussion

Figure 1 shows the present results of the ICS, \(P\), DCS and \(L_\perp\) for Be\(^{2+}\) (1s\(^2\) \rightarrow 1s2p). \(P\) is about 58\% at the threshold. DCS and \(L_\perp\) at 124eV and 128eV are shown in Fig. 1 (c) and (d). With increase of energies, DCS increases at small scattering angles and decreases at large angles. The value of \(L_\perp\) is positive at small angles and the trend is similar to the result for He-like ions of
Figure 1. (a) ICS, (b) $P$, (c) DCS and (d) $L_\perp$ for the $1s^2 \, 1S^e \rightarrow 1s2p \, 1P^o$ transition of $\text{Be}^{2+}$ above the threshold.

Figure 2. The same as Fig. 1 but for the $2s^2 \, 1S^e \rightarrow 2s2p \, 1P^o$ transition of $\text{C}^{2+}$.

Srivastava et al. [3]. Figure 2 shows the present results for $\text{C}^{2+}(2s^2 \rightarrow 2s2p)$. Berrington et al. [14] have reported the collision strength for $\text{C}^{2+}$ using the $R$-matrix calculation of 6 target states constructed with many configurations. The collision strength of Berrington et al. is transformed to ICS and compared with the present one in Fig. 2(a). The agreement of the two ICS’s are reasonable, but the resonance structure in the present ICS is more pronounced than that of the 6 states calculation. $P$ at the threshold is about 25 % in Fig. 2(b). Figure 2 (c) and (d) shows DCS and $L_\perp$ at 12.8 and 15.3 eV. The DCS near backward direction decreases with energies, while it remains small at small angles. Near 12.8 eV, $L_\perp$ is positive at small angles and it takes a negative value around 70°. Figure 3 shows the results for $\text{Si}^{2+}(3s^2 \rightarrow 3s3p)$. We have reproduced the $\text{Si}^{2+}$ results of Kai et al. [4], where the data except for $P$ is already reported. $P$ is about 48 % at the threshold in Fig. 3(b). The values of $L_\perp$ at small angles are negative differently from those of $\text{Be}^{2+}$ and $\text{C}^{2+}$ in Fig. 3(d).

The excitations of doubly charged ions with two valence electrons of $\text{Be}^{2+}(1s^2 \rightarrow 1s2p)$, $\text{C}^{2+}(2s^2 \rightarrow 2s2p)$ and $\text{Si}^{2+}(3s^2 \rightarrow 3s3p)$ are analogous to those with one valence electron of $\text{Li}^{2+}(1s \rightarrow 2p)$, $\text{B}^{2+}(2s \rightarrow 2p)$ and $\text{Al}^{2+}(3s \rightarrow 3p)$, respectively. The excitations of one valence
Figure 3. The same as Fig. 1 but for the 3s 2 1S e → 3s3p 1P o transition of Si 2+.

electron such as Li 2+, B 2+ and Al 2+ are reported in [5]. It is interesting to compare the counterparts of one- and two-valence electron(s). The angular distributions of DCS are similar to each other. Similarities are also found for the sign of \( L_\perp \) at small angles, namely, they are positive for Li 2+ and Be 2+ and negative for Al 2+ and Si 2+. However, disagreement occurs for a pair of B 2+ (negative) and C 2+ (positive). Thus, comparing with analogue ions of one valence electron, the sign of \( L_\perp \) does not necessarily agree.

To summarize, the ICS, \( P \), DCS and \( L_\perp \) are calculated for electron-impact excitations of Be 2+, C 2+ and Si 2+ with two valence electrons for the transition from the ground state (1S e) to the first 1P o excited state. \( L_\perp \) at small scattering angle is positive for Be 2+ and C 2+ but negative for Si 2+. Comparing with analogous ions of one valence electron, the sign of \( L_\perp \) agrees for pairs Be 2+ – Li 2+ and Si 2+ – Al 2+, but disagrees for a pair C 2+ – B 2+. Hence the sign of \( L_\perp \) is a collision parameter sensitive to target ions. To give the physical reason is a problem to be cleared in future.

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