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

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Abstract. We carry out the R-matrix calculations for electron-impact excitations of ions with one valence electron. The integral cross sections and polarization degree are obtained for the excitation process from the ground state to the first 2P^o state of Li^{2+}, B^{2+} and Al^{2+} as functions of electron incident energy. The differential cross sections and angular momentum transfer are also shown at non-resonant low-energy points. As for the angular momentum transfer (L_\perp) at small scattering angles, they are negative for B^{2+} and Al^{2+}, while it is positive for Li^{2+}. Thus L_\perp of doubly charged ions with one-valence electron is not simple.

1. Introduction

Excitation cross sections for positive ions by electron impact are required in order to interpret spectra of astrophysical plasmas and high-temperature laboratory plasmas. The cross sections from the ground S state to the lowest P state are of fundamental importance.

When velocity distribution of electrons in plasma is anisotropy, ions in excited states have unequal distribution for magnetic sublevels owing to collisions with such electrons. Radiation emitted from ions with unbalanced sublevel population is polarized. The detection of polarization degree is available for a plasma diagnostic [1].

In magnetic sublevels of final P state of atoms and ions formed in an electron-impact excitation from an initial S state, the expectation value of component of perpendicular to the scattering plane in angular momentum is called angular momentum transfer L_\perp. We pay attention to L_\perp at small scattering angles. In electron-atom scattering, the value of L_\perp near forward direction is positive for S → P transition [2]. It hold without exception in reported works. Srivastava et al.[3] have shown using the distorted wave calculation that L_\perp is also positive for electron collisions with H-like ions (Z=2, 6, \infty) at X=2 and 4, where X is the incident electron energy in threshold unit. Kai et al.[4] have found a case where L_\perp was negative in low-energy electron scattering with Mg-like Si ion using the R-matrix method.

In order to obtain acquaintances about L_\perp in electron-impact excitation of doubly charged ions, we have applied the R-matrix calculation in electron scattering for ions with one valence electron such as H-like Li (Li^{2+}), Li-like B (B^{2+}) and Na-like Al (Al^{2+}). For the excitation processes of Li^{2+}(1s → 2p), B^{2+}(2s → 2p) and Al^{2+}(3s → 3p), the integral cross section (ICS) and polarization degree (P) are calculated, and the differential cross section (DCS) and L_\perp are presented at selected energies in non-resonant region.
Table 1. Target states in the present R-matrix calculations.

| Symmetry | Li$^{2+}$ (RM13) | B$^{2+}$ (RM11) | Al$^{2+}$ (RM11) |
|----------|------------------|------------------|------------------|
| $2S^e$   | 1s, 2s, 3s, 4s, 5s | 2s, 3s, 4s, 5s, 5s | 3s, 4s, 5s       |
| $2P^o$   | 2p, 3p, 4p, 5p    | 2p, 3p, 4p, 5p, 5p | 3p, 4p, 5p       |
| $2D^e$   | 3d, 4d, 5d        | 3d, 4d, 5d, 5d    | 3d, 4d, 5d       |
| $2F^o$   | 4f               | 4f               | 4f, 5f           |

Table 2. Excitation energies (eV) and oscillator strengths for Li$^{2+}$, B$^{2+}$ and Al$^{2+}$.

| Target  | State | Present | Other | Oscillator strength | Present | Other |
|---------|-------|---------|-------|---------------------|---------|-------|
|         |       | Length  | Velocity | Length | Velocity |
| Li$^{2+}$ | 2p $2P^o$ | 91.839  | 91.841$^a$ | 0.4162 | 0.4162 |
| B$^{2+}$  | 2p $2P^o$ | 6.0508  | 5.9984$^a$ | 0.3745 | 0.4089 | 0.36327$^b$ | 0.36325$^b$ |
| Al$^{2+}$ | 3p $2P^o$ | 6.6089  | 6.6751$^a$ | 0.889  | 0.844  | 0.890$^c$    | 0.847$^c$ |
|         |       | 6.6124  |         |         |         |       |

$a$ NIST [8]. $b$ Godefroid et al. [9]. $c$ Dufton and Kingston [10].

2. Theory

2.1. Target wavefunctions and collision calculations

Target states used in the present R-matrix calculations are listed in Table 1. The target wave functions of Li$^{2+}$ are exact. The target states of B$^{2+}$ and Al$^{2+}$ are constructed in terms of configuration interaction expansions. The number after the letter "RM" in Table 1 indicates the number of coupled target states in the calculations. The 1s and 2s orbitals of the B$^{2+}$ are the Hartree-Fock wave functions given by Clementi and Roetti [5] for the ground state $1s^22s^22s^2$. The 2p, 3s, 3p, 3d, 4s, 4p, 4d and 4f orbitals of B$^{2+}$ are optimized on the energies of the $2p^22P^o$, $3s^22S^e$, $3p^22P^o$, $3d^22D^e$, $4s^22S^e$, $4p^22P^o$, $4d^22D^e$ and $4f^22F^o$ states, respectively, using the CIV3 atomic structure program of Hibbert [6]. The 5s and 5p pseudo-orbitals of the B$^{2+}$ are also determined by optimizing on the energy of the $2s^22S^e$ and $2p^22P^o$, respectively. For the orbitals of Al$^{2+}$, we adopt the orbitals used by Kimura et al. [7]. Table 2 shows excitation energies and oscillator strengths between the ground state and the first excited state in $2P^o$ symmetry of Li$^{2+}$, B$^{2+}$ and Al$^{2+}$. Present excitation energies are in good agreement with those in [8, 9, 10]. There is a difference between length and velocity forms of our results. Our length forms compare reasonably well with the values reported by Godefroid et al. [9] and Dufton and Kingston [10]. Our wavefunctions of B$^{2+}$ are less accurate compared with those of Godefroid et al., since much more configurations are used in their multiconfiguration Hartree-Fock method. We perform scattering calculations for target Li$^{2+}$, B$^{2+}$ and Al$^{2+}$ using the R-matrix computer program of Berrington et al. [11].

2.2. The angular momentum transfer and polarization degree

For electron-impact excitation $2S^e \rightarrow 2P^o$ in the present case, the angular momentum transfer $L_\perp$ at a given scattering angle is given by $L_\perp = -Im[f_M^0 f_0^o + 3 f_1^1 f_1^1]/(\sqrt{2} \sigma)$ [12], where $f_M^S$ is the scattering amplitude for a magnetic sublevel with $M$ of the $2P^o$ state and for the total spin $S$, and $\sigma$ is the DCS for the $2P^o$ state. The ICS for the $2P^o$ state is given by $Q = Q_0 + 2Q_1$. The $Q_M$ is the ICS for the excitation into a magnetic sublevel with $M$ of the $2P^o$ state. The
Figure 1. (a) ICS, (b) $P$, (c) DCS and (d) $L_\perp$ for the $1s^2S^e \rightarrow 2p^2P^o$ transition of Li$^{2+}$ above the threshold.

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

Figure 3. The same as Fig. 1 but for the $3s^2S^e \rightarrow 3p^2P^o$ transition of Al$^{2+}$. 
polarization degree for the $^2S^e \rightarrow ^2P^o$ transition is given by $P = 3(Q_0 - Q_1)/(7Q_0 + 11Q_1) \times 100$ [13]. The quantization axis is along the incident direction. In the case of neutral atom target, the emission line from the $^2P^o \rightarrow ^2S^e$ transition is linearly polarized and $P$ is about 43 % at threshold [13], which is derived by setting $Q_1 = 0$ in the above expression. When the target is an ion, $Q_1$ does not vanish at the threshold and $P$ deviates from 43 %.

3. Results and discussion

Figure 1(a) and (b) show present results for ICS and $P$ of Li$^{2+}$. The $P$ is about 23 % at the threshold. The DCS and $L_{\perp}$ at incident energies 92 and 96 eV are shown in Fig. 1(c) and (d). As the incident energy increases, the DCS’s increases at small angles and decreases at large angles. $L_{\perp}$’s are positive at small angles, which is consistent with the result of Srivastava et al. for hydrogenic ions [3].

The results of B$^{2+}$ are shown in Figure 2. Fig. 2(a) includes the ICS calculated by Marchalant et al. [14] using the $R$-matrix method with pseudo-states (RMPS), which used nine physical states and sixteen pseudo states. Though the calculation of Marchalant et al is more elaborate than the present one, the agreement of the two ICS’s is good. The $P$ is about 13 % at the threshold (Fig. 2(b)) and monotonic up to 11.5 eV. We show the DCS’s at energies around 7 – 11 eV in Fig. 2(c). The DCS near backward direction decreases with energies, while it remains small near forward angle. $L_{\perp}$ in Fig. 2(d) is negative at small angles.

The results for Al$^{2+}$ are shown in Figure 3. Mitroy and Norcross [15] have reported the ICS in a close-coupling calculation with nine states (9CC) of five atomic state and four pseudo states. In Fig. 3(a), the present ICS is larger than that of Mitroy and Norcross. This is due to difference of states adopted in the calculations. The $P$ is about 17 % at the threshold and shows a rapid increase due to a resonance just above the threshold in Fig. 3(b). We show the DCS’s at energies around 7 – 11 eV in Fig. 2(c). The DCS near backward direction decreases with energies, while it remains small near forward angle. $L_{\perp}$ is negative at small angles like the $L_{\perp}$ of B$^{2+}$ case.

To summarize, the ICS, $P$, DCS and $L_{\perp}$ for Li$^{2+}$, B$^{2+}$ and Al$^{2+}$ are calculated using $R$-matrix method. The DCS and $L_{\perp}$ are calculated at selected energies in non-resonant region. The $L_{\perp}$ at small angles are positive for Li$^{2+}$ and negative for B$^{2+}$ and Al$^{2+}$, and $L_{\perp}$ of doubly charged ions with one-valence electron is not simple. Further studies are required to understand the physical mechanism.

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