Differential cross sections for the electron-impact excitation of He-like ions: $2\,^1S$ and $2\,^1P$ states

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Differential cross sections for the electron-impact excitation of ions are calculated and compared along the He-like isoelectronic sequence. A distorted-wave method is used to obtain the cross sections for the transitions $1\,^1S \rightarrow 2\,^1S$ or $2\,^1P$ in Li^+, O^{6+}, and Si^{12+}. To complete the systematic study, a comparison is also made to the cross sections for neutral He and in the limit $Z \rightarrow \infty$ (Z being the nuclear charge). Dependence on the collision energy and comparisons to the cross sections obtained by other methods are discussed in detail. For the $2\,^1P$ excitation, an apparent generalized oscillator strength is derived for the ions using the present differential cross section. Their behavior is very different from the corresponding values of He.

I. INTRODUCTION

In order to get insight into the physical mechanism of any collision process, it is very helpful to see differential cross sections (DCS). Furthermore, a difference in various theoretical approximations can be seen when a comparison is made of the DCS. The number of works on DCS in electron-ion collisions, however, has been limited so far. Recently the present authors have started to calculate DCS for the electron-ion collision to study the general feature of them.[1,2]

In a previous paper,[1] the excitation of $2\,^3S$ and $2\,^3P$ in He-like ions was studied. A similar study of the excitation of $2\,^1S$ and $2\,^1P$ states is made in the present paper. In the present case, many more partial waves contribute to the DCS than in the previous case, because a long-range interaction dominates here. The convergence over the partial-wave expansion should be confirmed carefully. As in the previous study,[1] the DCS are calculated using the distorted-wave exchange approximation (DWXA) developed by Itikawa and Sakimoto.[3] This method is rather simple and has been successfully applied to the calculation of integrated cross sections for the excitations in He-, Be-, and C-like ions.[3,4]

In the present paper, DCS are calculated for several He-like ions. They are compared with each other to see a systematic trend along the isoelectronic sequence. The comparison includes two extreme cases: neutral He and the limit $Z \rightarrow \infty$. In the case of the $2\,^1S$ excitation, a comparison is also made to the DCS obtained by other methods to see the difference in the theoretical approximations.

II. METHOD OF CALCULATION

Details of the present method of calculation (DWXA) are given in the previous paper.[3] The method is based on the following assumptions.

(1) Introducing a distortion potential U^{DW} and regarding the difference between the true interaction and U^{DW} as a perturbation, we adopt the standard theory of first-order perturbation to derive the transition probability.

(2) We take as U^{DW} a spherical average of the electrostatic potential formed by the target ion in its initial state.

(3) The distortion potential is used to calculate the distorted wave for both the initial and the final states.

(4) Electron exchange is taken into account only between the two interacting electrons.

(5) The LS scheme is taken for the angular momentum coupling. Thus no relativistic effects are considered.

The differential cross section for the transition $\alpha \rightarrow \beta$ is given by

$$\frac{d\sigma(\alpha \rightarrow \beta)}{d\omega} = \frac{1}{4\pi^2}\frac{k_\beta}{k_\alpha}|T_{\beta\alpha}|^2 , \tag{1}$$

where k_α (k_β) is the wave number of the incident (scattered) electron and $T_{\beta\alpha}$ is the respective element of the transition matrix. Atomic untis are used throughout the present paper. A more detailed form of the DCS and the method of the numerical calculation are shown in the previous paper.[1] In comparison to the excitation of the triplet state, the convergence of the partial-wave expansion is much slower for the transition to the singlet state. For the higher partial waves in the dipole-allowed transition, use is made of the dipole-approximation formula described in the paper by Burgess *et al.*[5] For the excitation of $2\,^1S$ state, the analytical method of Nakazaki[6] is employed to evaluate the matrix element for the higher partial waves.

As in the previous study, the target state is represented by a configuration-interaction- (CI) type wave function produced with the computer code (CIV3) developed by Hibbert.[7]

III. RESULTS

Calculations are carried out for the three He-like ions: Li^+, O^{6+}, and Si^{12+}. The limiting value at $Z \rightarrow \infty$ is also

evaluated on the basis of the method by Sampson[8] (the details of the method being shown in the Appendix of the previous paper[1]). To compare the DCS for the ions with different nuclear charge Z, it is convenient to plot the scaled DCS, $Z^4 d\sigma/d\omega$ against scattering angles θ at the same electron energy in threshold units, X ($=E/\Delta E$, ΔE being the threshold energy).

A. $2\,^1S$

Figure 1 shows the DCS calculated for the ions with $Z=3,8,14,\infty$ at $X=1.8$. In this case only the partial waves with $L=0-10$ are needed to obtain the convergence over L. Here L is the total orbital angular momentum of the system and, in the present case, equals to the orbital angular momentum of the incident electron. When a multipole expansion is made for the electron-ion interaction, only the monopole moment contributes to the transition $1\,^1S\rightarrow 2\,^1S$. In Fig. 1 also shown are the DCS for He calculated by Thomas *et al.*[9] at $X=1.95$. Their method is basically the same as the present DWXA. As was found in the previous work,[1] the present scaling of the DCS appears very satisfactory in presenting DCS for different ions. The scaled DCS for O^{6+} and Si^{12+} almost coincide with each other. Furthermore both the cross sections are very close to the limiting value for $Z\rightarrow\infty$. The angular dependence for Li^+ is rather similar to that for He. They have a minimum at around 60°. This structure in the angular dependence is smeared out as Z increases so that the DCS for the ions with large Z look different from that for the neutral atom.

Bhatia and Temkin[10] and Srivastava and Katiyar[11] also calculated the DCS for the excitation of $2\,^1S$ in O^{6+}. Their results are compared to ours in Fig. 2. Bhatia and Temkin used a distorted-wave method based on the "one sided" approximation. They took into account the distortion due to the electrostatic potential only in the initial channel, while the pure Coulomb wave is employed for the scattered electron. Furthermore their target wave function is very simple when compared to the present one. As is noted in the previous paper,[1] the DCS for the excitation of $2\,^3S$ state of Li^+ are completely different from those calculated in the DWXA. In the case of the $2\,^1S$ excitation of O^{6+}, however, the DCS of Bhatia and Temkin are close to those obtained by the DWXA (see

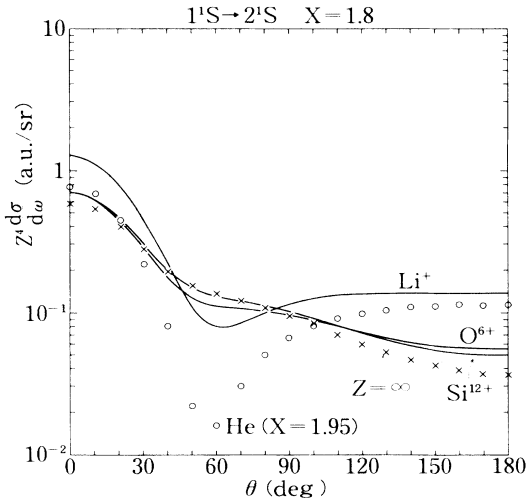

FIG. 1. The scaled differential cross section $Z^4 d\sigma/d\omega$ (in a.u./sr), calculated for the excitation $1\,^1S\rightarrow 2\,^1S$ of the He-like ions Li^+, O^{6+}, and Si^{12+}. The values in the limit $Z\rightarrow\infty$ are also shown. All the DCS for the ions were calculated at the electron energy $X=1.8$ ($X=E/\Delta E$, ΔE being the excitation energy). A comparison is made to the DCS for He [calculated by Thomas *et al.* (Ref. 9) at $X=1.95$].

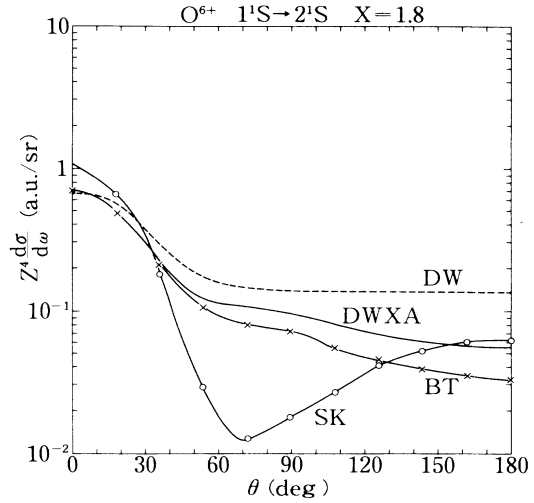

FIG. 2. Comparison of the scaled DCS for $1\,^1S\rightarrow 2\,^1S$ of O^{6+} calculated at $X=1.8$ by different methods: DWXA, the present calculation; DW, the present calculation without electron exchange; BT, Bhatia and Temkin (Ref. 10); SK, Srivastava and Katiyar (Ref. 11).

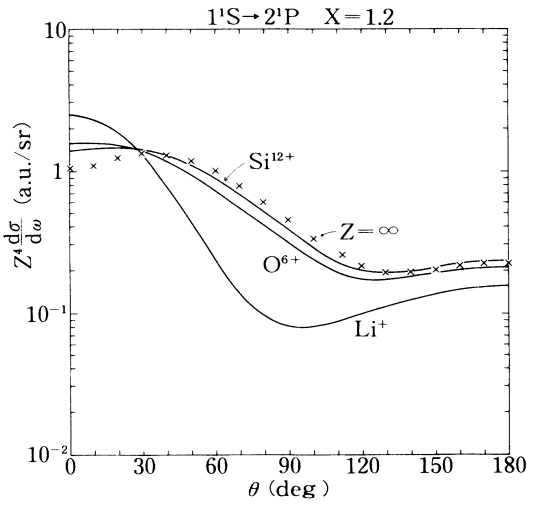

FIG. 3. The scaled DCS calculated for the excitation $1\,^1S\rightarrow 2\,^1P$ of the He-like ions with $Z=3,8,14,\infty$ at $X=1.2$.

Fig. 2). This is probably because the difference between our approximations and those of Bhatia and Temkin becomes less important as the nuclear charge increases.

Srivastava and Katiyar employed a distorted-wave method very similar to the present one. They adopted, however, the Bonham-Ochkur approximation to calculate the exchange part of the transition matrix. They calculated cross sections with various target wave functions, but reported only the DCS with the Hartree-Fock-type wave function. In contrast to our DCS and that of Bhatia and Temkin, the DCS of Srivastava and Katiyar have a rather deep minimum at around 70°. Srivastava and Katiyar indicated that their Hartree-Fock-type wave function is similar to the one adopted by Bhatia and Temkin. Thus the large dip of the DCS of Srivastava and Katiyar is ascribed primarily to the difference in the treatment of the exchange term. The Bonham-Ochkur approximation is not good at such a low collision energy as twice the threshold.

In Fig. 2 we also compare the calculation of DCS with (DWXA) and without (DW) the exchange interaction. The electron exchange considerably affects the DCS at large angles ($>50°$). It is important, therefore, to know how the exchange term is treated in the DCS calculation.

B. $2\,^1P$

In this case, the maximum numbers of the partial waves considered is about 50. For higher partial waves, use is made of the dipole approximation. The convergence over the partial-wave expansion is confirmed by comparing to the calculation with a fairly large L (say $L=90$).

Figures 3–5 show the DCS at $X=1.2$, 2.0, and 2.5, respectively. The DCS in the limit $Z\to\infty$ is also shown. In Fig. 4 the DCS for He (calculated at $X=2.36$) is compared to those for ions. The He cross section was obtained by Madison with a distorted-wave method similar to ours. (The numerical values of the DCS for He shown in Fig. 4 are unpublished, but the principle of the calculation has been described by Madison and Winters.[12]) The overall features of the scaled DCS along the isoelectronic sequence and their dependence on the collision energy are very similar to those for other transitions presented before.

In Fig. 5 we see a weak undulation in the DCS for Li^+. This is not the artifact due to the unconvergence of the partial-wave expansion. It has been confirmed, for example, that the same structure appears in the calculations with the maximum angular momentum of 60 and 90. The structure is not changed when we raise the angular momentum above which the dipole approximation is used to estimate the partial-wave contribution. A similar undulation was noted by Pangantiwar and Srivastava[13] when they calculated the DCS for the excitation of Mg^+, Zn^+, and Cd^+.

Figure 6 shows the DCS calculated in the Coulomb-Born exchange approximation (CBXA).[3,4] In this approximation, the distorted wave is replaced by the corresponding Coulomb wave. From a comparison between Figs. 4 and 6, we can see that there is not much difference between the two calculations (i.e., DWXA and CBXA) in this case, except in the large-angle scattering in $e+Li^+$. In the previous case of $2\,^3S$ excitation of Li^+,[1] the CBXA gave a completely different angular dependence from that obtained by the DWXA. Because of the dominance of higher partial waves in the dipole-allowed transition, the CBXA gives reasonably good results for the excitation of $2\,^1P$ state even for the lower charged ion.

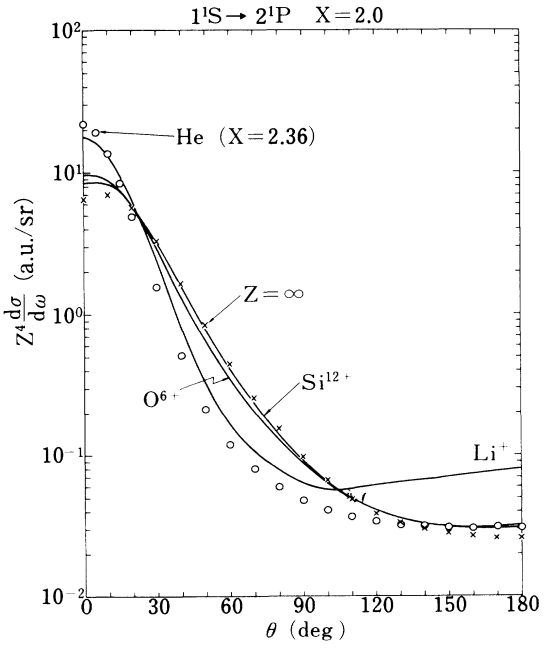

FIG. 4. Same as Fig. 3, but for $X=2.0$. The DCS for He (calculated by Madison at $X=2.36$) are also shown.

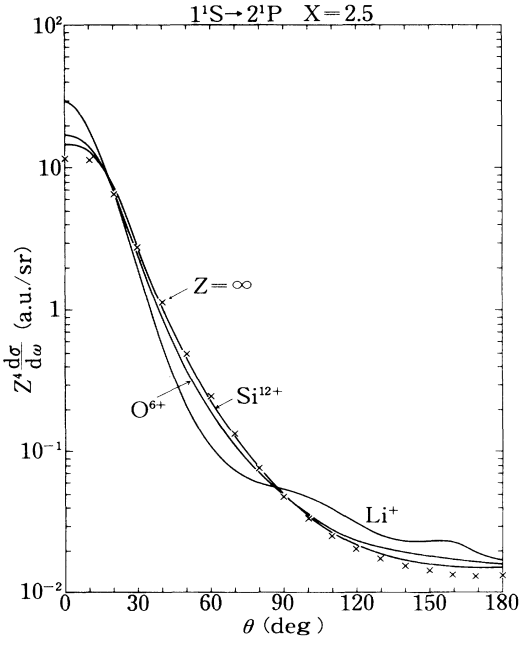

FIG. 5. Same as Fig. 3, but for $X=2.5$.

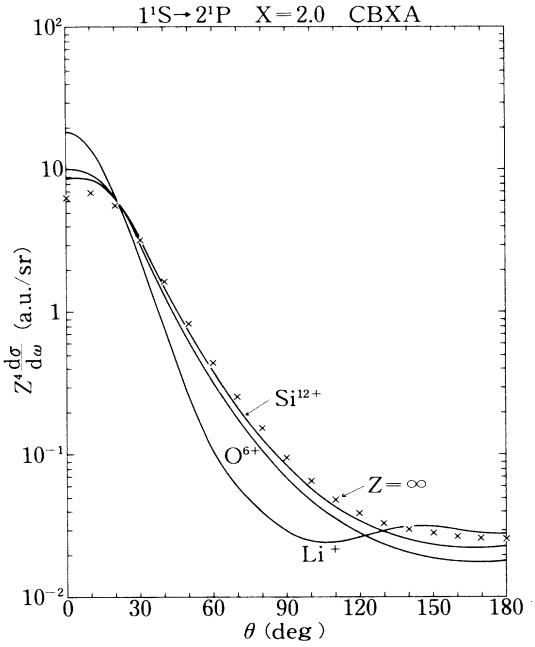

FIG. 6. Same as Fig. 3, but calculated by the Coulomb-Born exchange approximation (CBXA) at $X=2.0$.

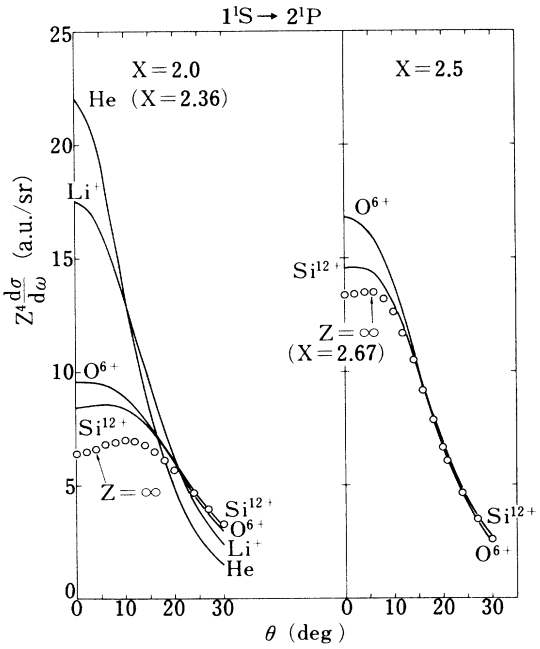

FIG. 7. The scaled DCS at small scattering angles, calculated for $1\,^1S\rightarrow 2\,^1P$ in He and He-like ions. The left panel shows the DCS at the collision energy $X=2.0$, except for He (for which the values at $X=2.36$ are plotted). The right panel gives the DCS at $X=2.5$, except for $Z=\infty$ (for which the calculation is done at $X=2.67$).

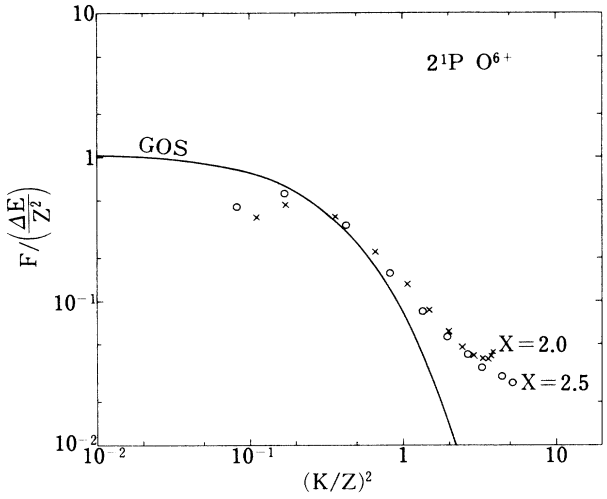

FIG. 8. Apparent generalized oscillator strengths (reduced by $\Delta E/Z^2$) for the $1\,^1S\rightarrow 2\,^1P$ transition in O^{6+}, derived with the DCS shown in Figs. 4 and 5. Dependence on the collision energy (X) is shown. The abscissa indicates the momentum-transfer squared (scaled by Z^2). Solid line is the corresponding generalized oscillator strength.

A noticeable feature is seen in the small-angle region of the DCS shown in Figs. 4 and 5. That is, the peak at $\theta=0$ becomes flattened and moves toward a larger angle with increasing Z. This is shown more clearly in Fig. 7, where the small-angle region is enlarged. To show this in another way, we introduce an apparent generalized oscillator strength[14] (GOS)

$$F(K,E)=\frac{1}{4}\frac{k_\alpha}{k_\beta}K^2[\Delta E(\mathrm{Ry})]\frac{d\sigma}{d\omega}\left[\frac{\text{a.u.}}{\text{sr}}\right], \tag{2}$$

where K is the momentum transferred during the collision. When the right-hand side of Eq. (2) is calculated

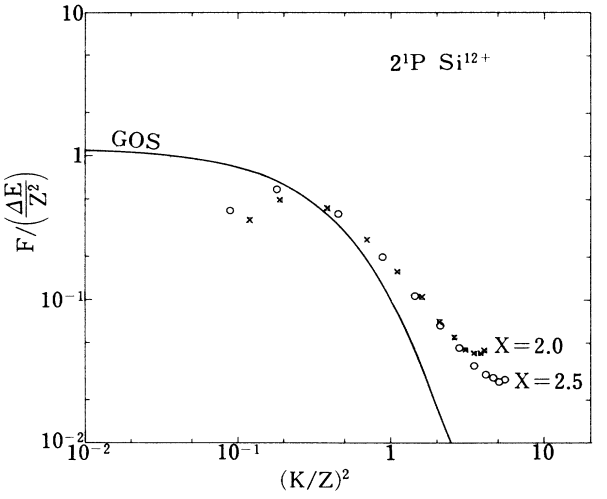

FIG. 9. Same as Fig. 8, but for Si^{12+}.

in the plane-wave Born approximation, the quantity F is equal to the GOS itself and becomes independent of the incident energy E. Figure 8 shows a reduced quantity $F/(\Delta E/Z^2)$ as a function of $(K/Z)^2$, calculated for O^{6+} with the DCS obtained in the DWXA. Figure 9 presents the values for Si^{12+}. In both figures, the GOS for the respective ions is plotted as a reference. The GOS was calculated using the same target wave function as in the DWXA calculation.

In the region of small K, the apparent GOS decreases as K decreases and deviates much from the corresponding value of GOS. This simply reflects the flattening of the DCS near $\theta=0°$. The deviation from the GOS is more apparent for the ions with larger Z. This peculiar behavior of the small-angle scattering in the electron-ion collision has been already noticed by Mitroy[15,16] for Be^+ and Mg^+ and by Nakazaki and Itikawa[2] for H-like ions.

IV. SUMMARY

The differential cross sections (DCS) for the excitation $1\,^1S \rightarrow 2\,^1S$, $2\,^1P$ in He-like ions have been studied systematically. The distorted-wave method developed by the present authors has been used to calculate the DCS for the ions. In the case of $2\,^1S$ excitation, a detailed comparison has been made with the results of two other calculations. For the $2\,^1P$ excitation, a peculiar feature has been found in the small-angle scattering. To see the feature from a different view point, an apparent generalized oscillator strength was also calculated.

Together with the previous study[1] of the excitations of $2\,^3S$ and $2\,^3P$ states, the present calculation of the $2\,^1S$ and $2\,^1P$ excitations constitutes the first systematic study of the DCS for the $n=2$ excitation of He-like ions. It would be of interest to extend this work to other isoelectronic sequences.

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