Distorted-wave-method calculation of electron-impact inner-shell excitation of Li-like ions

Yukikazu Itikawa and Kazuhiro Sakimoto
Institute of Space and Astronautical Science, Komaba, Meguroku, Tokyo 153, Japan

Shinobu Nakazaki
Department of Applied Physics, Faculty of Engineering, Miyazaki University, Miyazaki 889-21, Japan
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Cross sections are calculated for the electron-impact excitation of $1s^22s^11s2s2l$ in Li-like ions (C$^{3+}$ and O$^{5+}$). The results obtained by the distorted-wave method of Itikawa and Sakimoto [Phys. Rev. A 31, 1319 (1985)] are compared with those of a six-state close-coupling calculation for the electron energies $E/\Delta E = 1-5$ ($\Delta E$ being the energy of the respective threshold). When the same target wave functions are used, the distorted-wave method gives cross sections very close to those obtained by the close-coupling calculation.

I. INTRODUCTION

In the electron-impact ionization of atomic ions, an inner-shell excitation followed by autoionization often has a large contribution. To estimate the contribution, cross sections for the inner-shell excitation have been calculated for a number of ions. For the sake of simplicity, many of the calculations reported so far are based on the distorted-wave method (DWM). Though the DWM is generally reliable in the calculation of outer-shell excitation of ions, its validity for inner-shell excitations has not been thoroughly tested.

In the case of Na-like ions (Mg$^+$, Al$^2+$, and Si$^3+$), Henry and Msezane calculated the inner-shell cross section by the close-coupling (CC) method. When comparing their result with those of DWM, they conclude that the DWM gives a much larger cross section than the CC method. A similar conclusion has been reached recently for Mg-like ions (S$^{4+}$, C$^{6+}$, and Ar$^{8+}$), for which the R-matrix method was applied by Tayal and Henry to compare with the DWM calculation. For inner-shell excitations of O$^{5+}$ (Li-like), Bely-Dubau et al. compared their DWM calculation with the result of the CC method of Henry. They found a rather large discrepancy between the two methods of calculation.

It should be noted here that, in the comparison of the different calculations mentioned above, different wave functions were employed for the same target ion. In the calculation of electron-ion collisions, the resulting cross section is often much more sensitive to the target wave function than to the scattering approximation used. It is most desirable to compare different calculations under the condition of the same target wave functions. In the present paper, we calculate inner-shell cross sections for Li-like ions with the distorted-wave method proposed recently by Itikawa and Sakimoto and compare the result with a CC calculation using the NIEL code. The same [configuration-interaction-]CD type target wave-functions are used in the DWM and the CC calculations.

For Li-like ions, Henry applied the NIEL code to obtain the CC result for the inner-shell cross section. To enable a detailed comparison to our DWM result, we repeated the CC calculation and extended that to higher energies. We could completely reproduce the cross sections of C$^{3+}$ obtained previously by Henry, but could not those of O$^{5+}$. From the detailed comparison of the DWM and the CC results along the isoelectronic sequence of ions, Henry's cross section for O$^{5+}$ is most likely in error.

II. METHODS OF CALCULATION

The details of the present distorted-wave method [called distorted-wave exchange approximation (DWXA)] are shown in previous papers. 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. The same distortion potential is used to calculate the distorted wave both for the initial and for the final states.

3. In the actual calculation, $U^{DW}$ is taken to be a spherical average of the electrostatic potential formed by the target ion in its initial state.

4. Electron exchange is taken into account only between the interacting two electrons and the possibility of the ejection of the third one is ignored.

5. Use is made of the wave functions of Cl type for the target ion, which are given independently at the outset of the calculation.

The method has been successfully applied to the calculation of the (outer-shell) excitations of He$^+$, Be$^+$, and C$^+$ ions.

The close-coupling calculation is carried out here using the noniterative integral equation method. The actual calculation was performed with the use of the computer code NIEL.

The target states of the ion considered are $1s^22s^11s2s2l$, $1s^22p$, $1s2s^2$, $1s2s2p^4P^0$, $1s2s^2(1S)2p^2P^0$, $1s2s^2(3S)2p^2P^0$. In the present calculation, the LS scheme is adopted for the an-
gular momentum coupling. The transitions to the last four states from the ground one are of interest here, but all the six states are taken coupled in the close-coupling calculation (designated hereafter by 6CC). With the CIV3 code of Hibbert, we construct CI wave functions for the target states. The excited energies obtained in the CI calculation are used in the cross-section calculation. The details of the CI coefficients and the energies obtained are given in Henry's paper.

III. RESULTS AND DISCUSSIONS

The cross sections for the inner-shell excitations
\[ 1s^2 2s^2 2S - 1s2s^2 2p^2 4P, 1s2s ({}^1S_2p) ^2P, 1s2s ({}^1S_2p) ^2P^* \]
are calculated for two Li-like ions, C^{3+} and O^{5+}. Figures 1 and 2 show the collision strengths for those transitions as a function of electron energy. The collision strength \( \Omega \) is related to the cross section \( \sigma \) (in units of \( \pi a_0^2 \))

\[ \Omega = g_i E(Ry) \sigma (\pi a_0^2) , \]

where \( g_i (= 2 \) in the present case) is the statistical weight of the initial state and \( E \) is the energy of the incident electron in rydbergs. The abscissa of the figures indicates the electron energy in the threshold units (i.e., \( X = E/\Delta E \), \( \Delta E \) being the excitation energy).

Each figure compares the results of the DWM calculation (DWXA) with those of the CC one. In all the cases shown, the DWXA gives the cross section in close agree-

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**FIG. 1.** Collision strengths for the inner-shell excitation of C^{3+}, plotted against the electron energy. The electron energy is expressed in the threshold unit \( X = E/\Delta E \), \( \Delta E \) being the excitation energy. The distorted-wave method calculation (DWXA, solid lines) is compared with the six-state close-coupling one (CC, circles). The initial state is 1s^2 2s^2 2S and the final states are (a) 1s2s ({}^1S_2p) ^2P^* (\( \Delta E = 22.55 \) Ry), (b) 1s2s ({}^1S_2p) ^2P^* (\( \Delta E = 22.18 \) Ry), (c) 1s2s2p ^2P^* (\( \Delta E = 21.82 \) Ry), and (d) 1s2s ^3S (\( \Delta E = 21.58 \) Ry).
ment with the CC value. The agreement is fairly good even near threshold.

The most interesting case is the spin-forbidden transition $1s^22s^2S^* - 1s2s2p^6P^*$. For both the ions, the difference in the collision strengths obtained by the DWXA and the 6CC calculations is less than a few percent for the transition. To make a more detailed comparison, Fig. 3 shows the partial collision strengths $\Omega_{LS}$ for the transition in $\text{O}^{1+}$. Here $L$ and $S$ denote the total orbital and spin angular momenta of the system, respectively. (Note that for the spin-forbidden transition only the term with $S = 1$ appears.) At the collision energy of 25 Ry (Fig. 3), $\Omega_{LS}(\text{DWXA})$ with $L = 1, S = 1$ is by about 40% larger than the corresponding CC value. The discrepancy, however, is canceled with that of other partial collision strengths, so that the total collision strengths show the closer agreement. At larger energies, a better agreement is seen in each partial collision strength. We have the same trend in the case of $\text{O}^{2+}$. Thus the agreement between the collision strengths of the two calculations for

FIG. 2. Collision strengths for the inner-shell excitation of $\text{O}^{1+}$. Three theoretical calculations are compared: the present distorted-wave method (DWXA, solid lines), the six-state close-coupling calculation (CC, circles), and the distorted-wave method calculation done by Bely-Dubau et al. (DWUCL, dashed lines) (Ref. 6). The initial state is $1s^22s^2S^*$ and the final states are (a) $1s2s^2(1S)2p^6P^*$ ($\Delta E = 41.96$ Ry), (b) $1s2s^2(1S)2p^6P^*$ ($\Delta E = 41.50$ Ry), (c) $1s2s2p^6P^*$ ($\Delta E = 40.90$ Ry), and (d) $1s2s^2S^*$ ($\Delta E = 40.60$ Ry).
FIG. 3. Partial collision strengths for each total orbital \( L \) and spin \( S \) angular momenta for the excitation \( 1s^22s^22S \rightarrow 1s2s2p^2P \) of \( C^{+} \) at the collision energy of 25 Ry. The distorted-wave method calculation (DWXA, solid lines) is compared with the six-state close-coupling one (CC, dashed lines). In this transition, only the term with \( S=1 \) appears.

The spin-forbidden transition is rather fortuitous near threshold, but we get real agreement between them as the collision energy increases.

For the analysis of satellite spectra of oxygen ions, Bely-Dubau et al.\(^5\) calculated the inner-shell cross sections for \( O^{+4} \) with the use of a DWM. They employed the computer code developed at the University College, London (called hereafter DWUCL).\(^1\) Their result is compared in Fig. 2 with the present DWM (DWXA) and the CC calculations. As is seen in the figures, the result of DWUCL is much more deviated from that of the CC calculation than the DWXA. Actually in their paper, Bely-Dubau et al. concluded that the DWM generally results in a large difference from the CC method. The DWUCL is not much different from the DWXA in the method of cross-section calculation (for the detailed comparison of various DWM, see a recent review by Iitikawa\(^1\)). Most part of the discrepancy between the DWUCL and the CC (and the DWXA) results, therefore, comes from the difference in the target wave functions employed. Usually the target wave function in the DWUCL calculation is generated with the same distortion potential as used for the continuum electrons. On the other hand, the DWXA assumes that the best wave function is given independently and can incorporate any type of CI wave function into the cross-section calculation. The wave function of Bely-Dubau et al. gives the oscillator strengths for the transitions \( 1s^22s^22S \rightarrow 1s2s2p^2P \) and \( 1s^22s^22S \rightarrow 1s2s (^1S) 2p^2P \) to be 0.681 and 0.0415, respectively. The wave function used in the present paper gives the corresponding values of 0.532 and 0.0649. These differences in the oscillator strengths can easily explain the difference in the energy dependence of the collision strengths at larger energies of the two dipole-allowed transitions [see Figs. 2(a) and 2(b)].

As was mentioned in the previous sections, we took in our CC calculation exactly the same procedure as Henry did.\(^7\) For \( C^{+} \), the collision strength of our CC calculation completely agrees with Henry’s corresponding value. For \( O^{+4} \), we have different result. Table I compares the two CC calculations (and the DWXA for reference). We see quite a large (up to 30%) discrepancy between the two CC values for the transition \( 1s^22s^22S \rightarrow 1s2s2p^2P \) at all the energies considered and \( 1s^22s^22S \rightarrow 1s2s2p^2P \) at lower energies. If we compare the DWXA result for \( 1s^22s^22S \rightarrow 1s2s2p^2P \) to Henry’s value, we have a large difference between the DWM and the CC calculations for \( O^{+4} \). A preliminary calculation for \( N^{+4} \), however, shows a close agreement of the DWXA and the CC (Henry’s) collision strengths for the spin-forbidden transition, very similarly to the case of \( C^{+} \). From this and other trends along the isoelectronic sequence, we conclude that Henry’s calculation for \( O^{+4} \) has some numerical errors. The sum of the four inner-shell cross sections [denoted by \( \Sigma \sigma(1s2s2l) \)] obtained by the present CC calculation, however, is not much different from that of Henry (see Table I). Very recently Crandall et al.\(^1\) remeasured the electron-impact ionization cross section of \( O^{+4} \) and deduced therefrom the inner-shell cross section. Comparing their result with the \( \Sigma \sigma(1s2s2l) \) of Henry’s CC calculation, they concluded that the CC theory is in agreement with the deduced experimental excitation cross section. Their conclusion does not need to be changed when Henry’s calculation is revised by the present CC calculation. Actually the present calculation shows even better agreement with the experiment [i.e., the values of \( \Sigma \sigma(1s2s2l) \) at 45 Ry obtained by Henry, the present CC calculation, and the experiment being, respectively, \( 7.47 \times 10^{-20}, 7.70 \times 10^{-20}, \) and \( 8.0 \times 10^{-20} \) cm\(^2\)].

IV. CONCLUSION

When a comparison is made with the close-coupling calculation, it has been found that the distorted-wave method can produce well the cross section for the inner-shell excitation of Li-like ions, provided that an accurate wave function is used for the target state. This remarkable success of the perturbation theory (DWM) in this case is probably due to the smallness of the transition probability. It is of interest to see how this conclusion can be extended to other isoelectronic sequence.
TABLE I. Collision strengths for the inner-shell excitations of O$^{+}$. The present six-state close-coupling calculation is compared with the same calculation done by Henry (Ref. 7). The result of the distorted-wave method calculation (DWXA) is also shown for comparison. The last column indicates the sum of the collision strengths for the four excitation processes.

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<tr>
<th>Energy (Ry)</th>
<th>Excited states</th>
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<tr>
<td></td>
<td>1s2s$^{2}$ 2S</td>
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<tr>
<td>45.0</td>
<td>6CC</td>
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<td></td>
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<td></td>
<td>DWXA</td>
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<tr>
<td>50.0</td>
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<td>100.0</td>
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<td>6CC (Henry)</td>
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<td></td>
<td>DWXA</td>
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Another conclusion drawn from the present study is that the electron-impact excitation cross section is very sensitive to the target wave function. Any comparison of different calculations should be made on the basis of the same target wave function.

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