Distorted-wave-method calculation of electron-impact excitation of atomic ions. II. C-like ions

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Electron-impact excitations of C-like ions (O III, Ne V, Si IX, and Ca XV) are studied theoretically by a distorted-wave (DW) method previously proposed [Y. Itikawa and K. Sakimoto, Phys. Rev. A 31, 1319 (1985)]. When compared with the calculations of the close-coupling method and R-matrix theory, the DW method is confirmed to give reasonably good results. By supplementing the R-matrix calculation, the present DW method thus extends the availability of reliable cross-section data to higher energies. A comparison is also made with the calculation by Mason, Bhatia, and coworkers using the DW-method computer package developed at the University College, London, to examine the reliability of the calculation.

I. INTRODUCTION

In a previous paper (hereafter referred to as paper I),[1] a relatively simple method of distorted-wave (DW) approximation has been proposed to calculate cross sections for electron-impact excitation of atomic ions. The method was applied to the excitations of He-like (Li II and O VII) and Be-like (C III) ions. When compared with more elaborate calculations (i.e., close-coupling or R-matrix type), the DW method has been found to give generally good results. In the present paper, the calculation is extended to C-like ions.

C-like ions are not only of significance in applications (e.g., in laboratory and astrophysical plasmas) but also of interest in atomic physics. They have a typical open-shell structure; their ground state has the symmetry of ^3P (not the simple one of ^1S). Actually, a number of theoretical papers have been published on the excitation of C-like ions.[2] In particular, Aggarwal[3-11] performed a comprehensive calculation using the R-matrix method for several ions. Those calculations will be used later to delineate the accuracy of the present DW method. Another systematic study of C-like ions has been made by Bhatia, Mason, and others by using the DW method developed at the University College, London (called hereafter DWUCL).[12-16] The results of DWUCL are in general accord with those of the R-matrix calculation. In some cases, however, there is a large discrepancy between the two calculations. One of the aims of the present paper is to clarify the discrepancy.

For dipole-allowed transitions, the present DW method [called the distorted-wave exchange approximation (DWXA)] is expected to give good results for any ions over a wide energy range, as any other perturbation approach does. This will be confirmed by the calculation of the cross section for O III and Ne V. As for the spin forbidden transitions, a rather systematic study along the isoelectronic sequence (i.e., O III, Ne V, Si IX, Ca XV) will be made for two representative processes (with low and high excitation energies). A discrepancy of a factor of 3 has been reported for some forbidden transitions in Ca XV between the results of the DWUCL and the R-matrix methods. It is of practical interest, therefore, to compare our results for Ca XV with those two calculations.

Though the close-coupling or R-matrix method is believed to provide accurate cross sections, it is hard to apply that to a wide range of collision systems and energies. Because of its ease of application and the flexibility, a DW method is suitable for a systematic study of excitation mechanisms. The paucity of experimental data makes it difficult to determine the accuracy of theoretical cross sections, and complicated computer codes are often vulnerable to computational errors. Calculations of different types would be helpful in assessing the resulting cross section. The present method will serve also as a tool for such studies.

It should be noted that the present method does not include resonance effects. Though it is possible to take into account resonance effects in a DW method, the present formulation ignores the effects for simplicity. Our primary concerns, therefore, are the energy region somewhat above the threshold (i.e., above about twice the excitation energy) where resonance effects are less significant.

II. DISTORTED-WAVE METHOD

The present DW 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 waves 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 in such a way that the incident electron is allowed to interchange only with the bound electron interacting directly with it.

Another important ingredient of the present approach of cross-section calculation is that the target ion is represented by as accurate a wave function as possible. Use is assumed of wave functions of configuration-mixing type for the target state. Details of the formulation were given in paper I. Only its outline is described below.

The collision strength for the excitation from the state $\alpha L^{\alpha}S^{\alpha}$ to $\beta L^{\beta}S^{\beta}$ is given by (atomic units being used)

$$\Omega(\alpha L^{\alpha}S^{\alpha}\rightarrow\beta L^{\beta}S^{\beta})=8k_{\alpha}k_{\beta}\sum_{L}\sum_{S}\sum_{l}\sum_{l'}(2L+1)(2S+1)\,|\,\langle T^{(\mathrm{d})}\rangle_{\beta\alpha}+\langle T^{(\mathrm{ex})}\rangle_{\beta\alpha}\,|^{2}\,, \tag{1}$$

with the transition matrix elements

$$\langle T^{(\mathrm{d})}\rangle_{\beta\alpha}=N\left\langle\psi(\Gamma_{\beta}\,|\,x_1,\ldots,x_N,\hat{x}_{N+1})u_{l'}^{(\beta)}(r_{N+1})r_{N}^{-1}\left|\frac{1}{r_{N,N+1}}\right|\psi(\Gamma_{\alpha}\,|\,x_1,\ldots,x_N,\hat{x}_{N+1})u_{l}^{(\alpha)}(r_{N+1})r_{N}^{-1}\right\rangle\,, \tag{2}$$

$$\langle T^{(\mathrm{ex})}\rangle_{\beta\alpha}=-N\left\langle\psi(\Gamma_{\beta}\,|\,x_1,\ldots,x_{N-1},x_{N+1},\hat{x}_{N})u_{l'}^{(\beta)}(r_{N})r_{N}^{-1}\left|\frac{1}{r_{N,N+1}}\right|\psi(\Gamma_{\alpha}\,|\,x_1,\ldots,x_N,\hat{x}_{N+1})u_{l}^{(\alpha)}(r_{N+1})r_{N}^{-1}\right\rangle\,. \tag{3}$$

In the present calculation, we assume the L-S coupling scheme for the angular momenta of the whole system: $L^{\alpha}S^{\alpha}$ ($L^{\beta}S^{\beta}$) are the orbital and spin angular momenta of the initial (final) state of the ion, l (l') the orbital angular momentum of the incident (scattered) electron, LS the orbital and spin angular momenta of the total (target ion plus electron) system, $M_L M_S$ the z components of LS. The function $\psi(\Gamma_{\alpha})$ [$\psi(\Gamma_{\beta})$] is the target wave function coupled with the spin and angular part of the incident (scattered) electron wave function, and specified by the channel index $\Gamma_{\alpha}=\alpha L^{\alpha}S^{\alpha}lLSM_LM_S$ ($\Gamma_{\beta}=\beta L^{\beta}S^{\beta}l'LSM_LM_S$). The target wave function itself is a linear combination of the configuration state functions, which are properly antisymmetrized and L-S coupled. All the wave functions used throughout the present paper are the configuration-interaction (CI) wave functions produced with CIV3 code of Hibbert.[17] The radial part of the wave function of the incident (scattered) electron is given by $u_l^{(\alpha)}$ ($u_{l'}^{(\beta)}$) and depends on the wave number of the electron k_{α} (k_{β}). The whole system has $N+1$ electrons, whose space and spin coordinates are denoted by $x_1,x_2,\ldots,x_{N+1}$ ($\mathbf{r}_i$ being the space part of x_i and $\hat{x}_i$ being the spin and angular part of x_i). The transition matrix elements $\langle T^{(\mathrm{d})}\rangle_{\beta\alpha}$ and $\langle T^{(\mathrm{ex})}\rangle_{\beta\alpha}$ arise from the direct and exchange interactions, respectively. The kernel r_{ij}^{-1} means $|\,\mathbf{r}_i-\mathbf{r}_j\,|^{-1}$.

The wave function of the incident electron is determined by the distortion potential. That is, the function $u_l^{(\alpha)}$ (the initial distorted wave) is the solution of the equation

$$\left[\frac{d^2}{dr^2}+\left[k_{\alpha}^2-2U^{\mathrm{DW}}-\frac{l(l+1)}{r^2}\right]\right]u_l^{(\alpha)}(r)=0\,, \tag{4}$$

with the asymptotic condition

$$u_l^{(\alpha)}\sim k_{\alpha}^{-1}\sin[k_{\alpha}r+k_{\alpha}^{-1}q\,\ln(2k_{\alpha}r)-2^{-1}\pi l+\eta_l^{(\alpha)}]\,,\quad r\rightarrow\infty\,. \tag{5}$$

Here the U^{DW} is assumed to have an asymptotic form

$$U^{\mathrm{DW}}(r)\sim -q/r,\quad r\rightarrow\infty \tag{6}$$

and $\eta_l^{(\alpha)}$ is the phase shift due to the potential U^{DW}. The distorted wave for the final state $u_{l'}^{(\beta)}$ is the solution of Eq. (4) but with the change $\alpha\rightarrow\beta$ and $l\rightarrow l'$. Details of the methods of evaluation of U^{DW} and calculation of the transition matrix elements, Eqs. (2) and (3), are given in paper I.

In the following sections, the calculated values of the collision strength are graphically shown as a function of electron energy. The electron energy (denoted by X) is expressed in the threshold units with the excitation energy ΔE indicated in the caption of each figure. Use is made of the excitation energies calculated with the target wave functions employed.

III. DIPOLE-ALLOWED TRANSITIONS

To illustrate the level structure of C-like ions, Fig. 1 shows that of O III. We ignore the fine structure of the levels for simplicity. For Ca XV, an inversion occurs between the levels $2s\,2p^3\,{}^1D^0$ and ${}^3S^0$.

As the first example, collision strengths have been calculated for two transitions in O III: $2s^2 2p^2\,{}^3P\rightarrow 2s\,2p^3\,{}^3D^0,{}^3S^0$. Figures 2 and 3 show the results and compare them with other calculations. There are two elaborate calculations for this system: the R-matrix (RM) of Aggarwal[10] and the two-state close coupling (2CC) of Ho and Henry.[18] The figures show also two representative results of other DW methods: the DWUCL of Bhatia *et al.*[15] and Mann's method.[19]

The present calculation gives the collision strengths very close to those obtained by the two sophisticated methods (RM and 2CC), especially RM. A small discrepancy between the results of DWXA (and RM) and 2CC probably arises from the slight difference in the target wave functions used. Both the DWXA and the RM use the same wave functions, the details of which are given in Ref. 20. The two DW results, DWUCL and Mann's, are much higher than the DWXA for the ${}^3D^0$ excitation, and in large disagreement with the elaborate calculations (RM and 2CC). This may reflect the inaccuracy of the target wave function used in those DW calculations, as stated by Ho and Henry.

As in paper I, the Coulomb-wave exchange approximation (called CBXA) is used to examine the effect of wave distortion. The CBXA result is obtained by replacing the

distorted waves (i.e., $u_l^{(\alpha)}$ and $u_l^{(\beta)}$) with the corresponding Coulomb waves, or equivalently by using the Coulomb potential $-(Z-N)/r_{N+1}$ as the distortion potential. Figures 2 and 3 show that the CBXA results are larger than the DWXA ones, indicating the importance of the distortion in this case. In the previous cases of He- and Be-like ions (paper I), the effect of distortion is very small for dipole-allowed transitions. The large effect of distortion in the C-like ions may be attributed to the larger electron cloud and their open-shell structure.

As another example, Fig. 4 presents the collision strength for the transition $2s^2 2p^2\,{}^3P \rightarrow 2s\,2p^3\,{}^3D^0$ in Ne V. The situation is very similar to the case of O III. The target wave function has also been adopted from the work using the R-matrix calculation.[6,21] In this case we can make a more detailed comparison between the methods of DWXA and RM. Figure 5 illustrates the partial collision strength for each symmetry LS_π (π being the parity of the total system), calculated at an electron energy of 10 Ry. An overall agreement can be seen between the results of DWXA and RM. Furthermore, Fig. 5 shows a few representative values of the 2CC calculation with the NIEM code.[22] It should be noticed that all three calculations here employ the same target wave function. The DWXA agrees slightly better with the 2CC than with the RM method. The small difference between the results of the 2CC and RM methods may be caused by the coupling of the states $2s^2 2p^2\,{}^3P$ and $2s\,2p^3\,{}^3D^0$ with other states. In fact, the collision strength for the transition from $2s\,2p^3\,{}^3D^0$ to $2p^4\,{}^3P$ is shown to be rather large by the R-matrix calculation.[11]

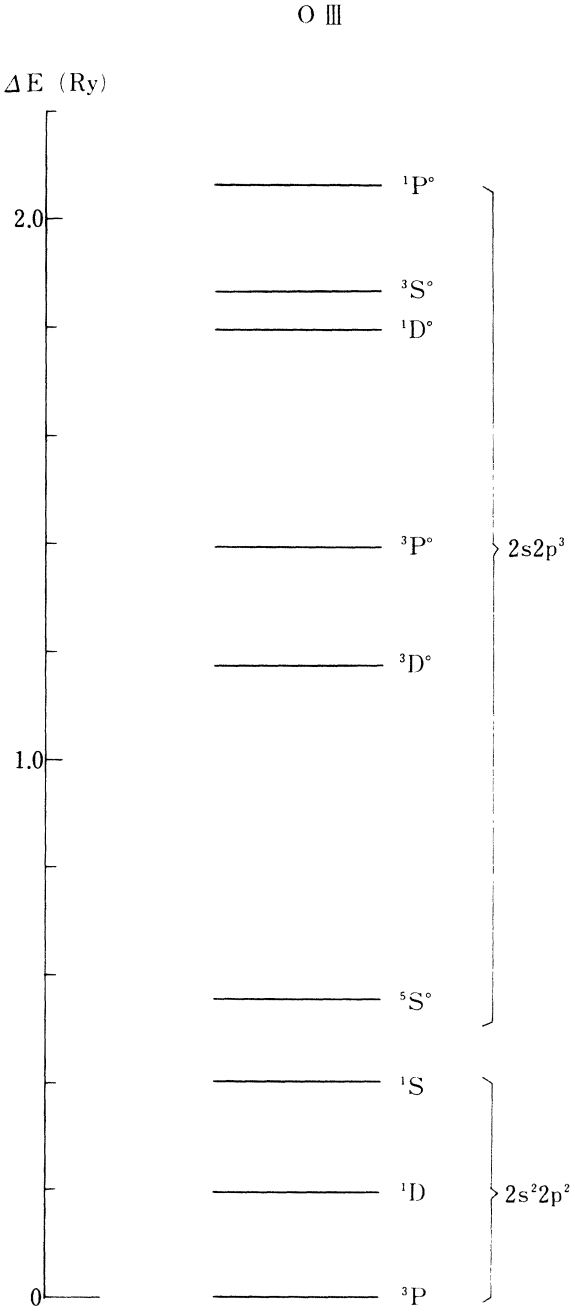

FIG. 1. Energy levels of O III. The level spacings are based on the CI calculation of Baluja *et al.* (Ref. 20).

IV. FORBIDDEN TRANSITIONS

Collision strengths are calculated for two spin-forbidden transitions, $2s^2 2p^2\,{}^3P \rightarrow 2s^2 2p^2\,{}^1S$ and

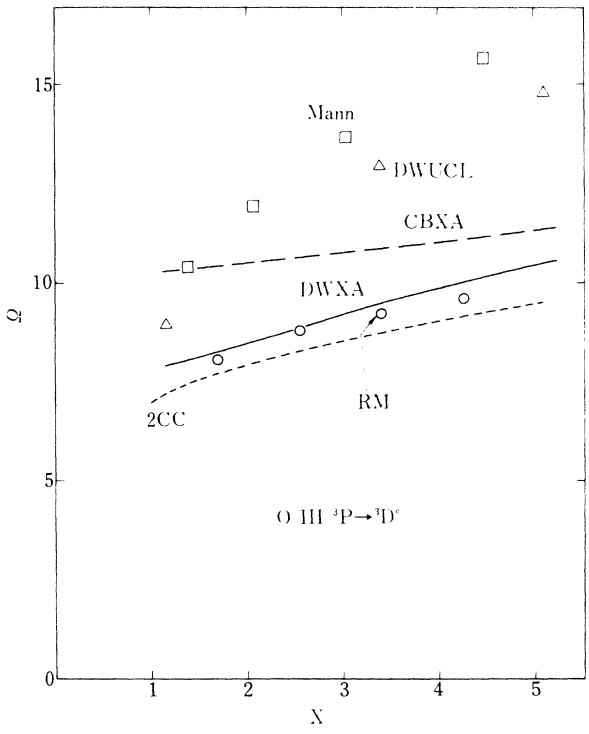

FIG. 2. Collision strengths for the $2s^2 2p^2\,{}^3P$-$2s\,2p^3\,{}^3D^0$ transition ($\Delta E = 1.175$ Ry) in O III as a function of electron energy, X, in threshold units. The present results of the distorted-wave method (DWXA, solid line) and the Coulomb-wave approximation (CBXA, dashed line) are compared with the results of the R-matrix method (Ref. 10) (RM, circles), the two-state close-coupling calculation (Ref. 18) (2CC, dotted line), and the two other distorted-wave calculations [DWUCL (Ref. 15), triangles, and Mann's (Ref. 19), squares].

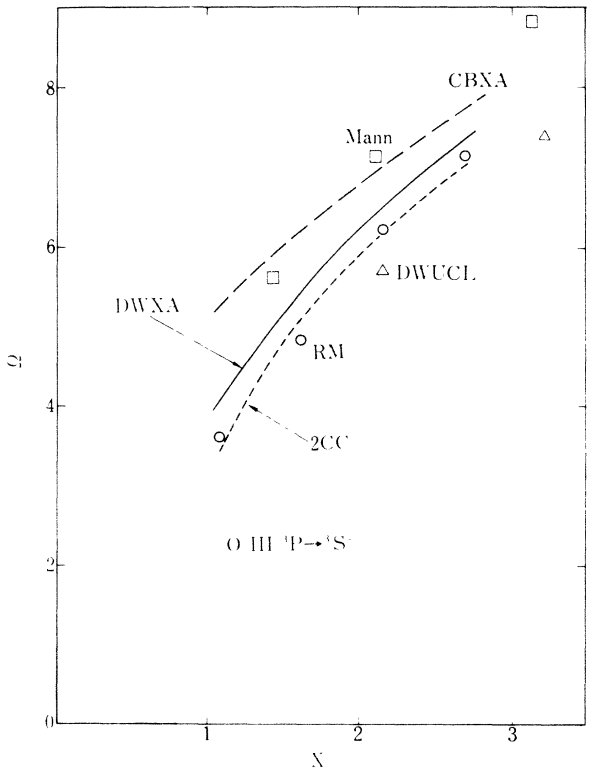

FIG. 3. Same as in Fig. 2, but for the $2s^2 2p^{2\,3}P$-$2s\,2p^{3\,3}S^0$ transition ($\Delta E = 1.868$ Ry) in O III.

$2s\,2p^{3\,1}P^0$, in O III, Ne V, Si IX, and Ca XV. The results are shown in Figs. 6–13. In each figure the present results of DWXA and CBXA calculations are compared with the corresponding results of the R-matrix and the DWUCL methods. The wave functions have been taken to be the same as those used in the R-matrix calculations (for details, see Ref. 20 for O III, Refs. 6 and 21 for Ne V, Ref. 4

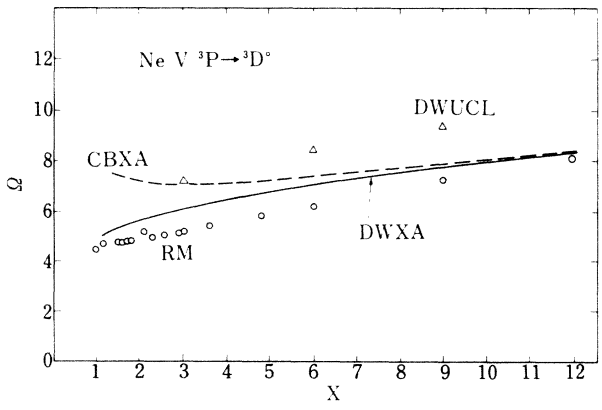

FIG. 4. Collision strengths for the $2s^2 2p^{2\,3}P$-$2s\,2p^{3\,3}D^0$ transition ($\Delta E = 1.677$ Ry) in Ne V. The present results of the distorted-wave method (DWXA, solid line) and the Coulomb-wave approximation (CBXA, dashed line) are compared with the results of the R-matrix method (Ref. 11) (RM, circles) and the other distorted-wave calculation by Bhatia (Ref. 16) (DWUCL, triangles).

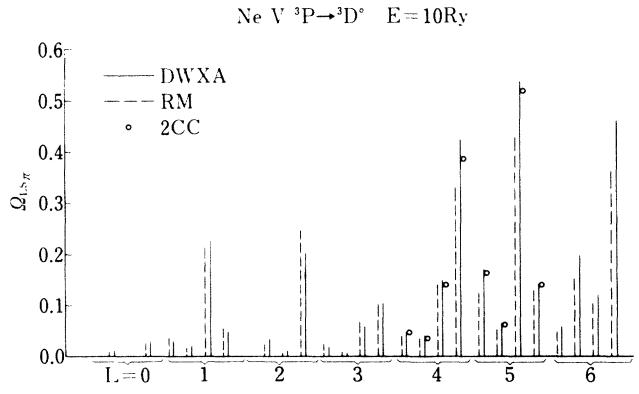

FIG. 5. Comparison of the partial collision strengths Ω_{LS_π} for the $2s^2 2p^{2\,3}P$-$2s\,2p^{3\,3}D^0$ transition in Ne V, calculated by the present distorted-wave method (DWXA, solid lines), the R-matrix method (Ref. 11) (RM, dashed lines), and the two-state close-coupling approximation (2CC, circles). The electron energy is 10 Ry (i.e., $X = 5.96$). For each L, there are four sets of Ω_{LS_π} shown, with, from left to right, ($S = \frac{1}{2}, \pi =$ even), ($S = \frac{1}{2}, \pi =$ odd), ($S = \frac{3}{2}, \pi =$ even), and ($S = \frac{3}{2}, \pi =$ odd). For $L = 0$, only odd parity is allowed. The values for ($L = 2$, $S = \frac{1}{2}$, $\pi =$ even) are too small to be plotted.

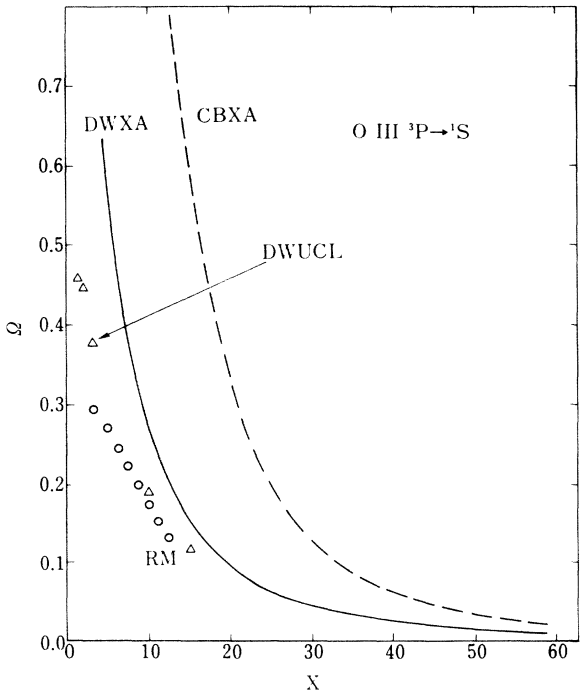

FIG. 6. Collision strengths for the $2s^2 2p^{2\,3}P$-$2s^2 2p^{2\,1}S$ transition ($\Delta E = 0.4076$ Ry) in O III. The present results of the distorted-wave method (DWXA, solid line) and the Coulomb-wave approximation (CBXA, dashed line) are compared with the values obtained by the R-matrix method (Refs. 7 and 24) (RM, circles) and the other DW method by Bhatia *et al.* (Ref. 15) (DWUCL, triangles).

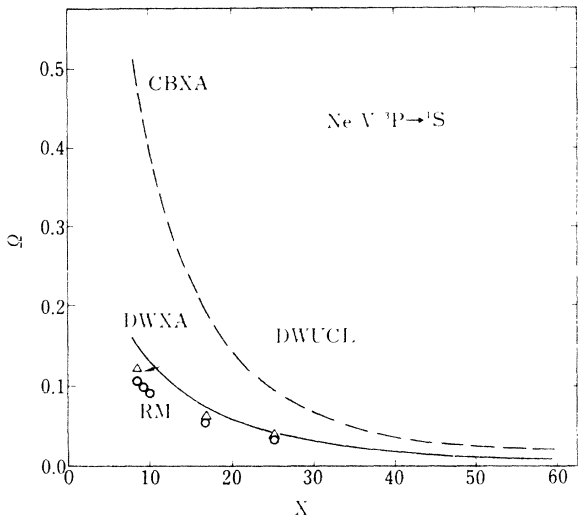

FIG. 7. Same as in Fig. 6, but for Ne V ($\Delta E = 0.5914$ Ry). The values of RM and DWUCL are taken from Refs. 8, 21, and 16.

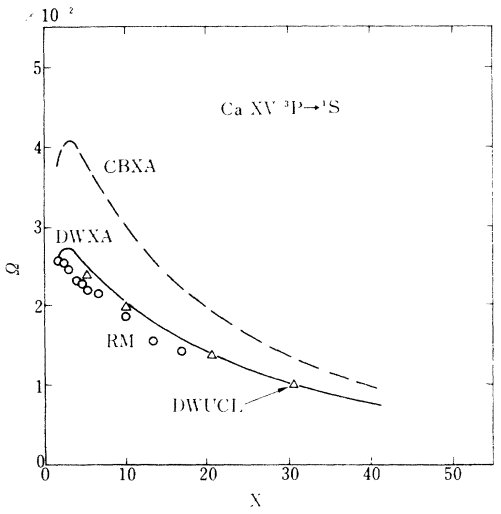

FIG. 9. Same as in Fig. 6, but for Ca XV ($\Delta E = 1.482$ Ry). The values of RM and DWUCL are taken from Refs. 5, 12, and 14.

for Si IX, and Ref. 5 for Ca XV). All the collision strengths reported for the relevant processes are plotted in the figures for RM and DWUCL. Though an extensive calculation has been done, the result of the RM method is available mostly in the form of rate coefficients. Here, a comparison in the form of collision strengths is preferred to show the calculations' details.

From Figs. 6–13 we can see the general trend in which the agreement between DWXA and RM is getting better with increasing nuclear charge and/or incident energy. For Ca XV the agreement is within 20%, except in the very vicinity of the threshold. We could expect a similar good agreement for Si IX, but unfortunately the RM data are available only at one energy for Si IX. It should be noted that the threshold region is dominated by resonance effects, which are not included in the DW calculation.

The results of CBXA differ considerably from those of DWXA even for highly charged ions. This can be reasonably understood from the fact that only a few lowest partial waves dominate in the spin-forbidden transitions and

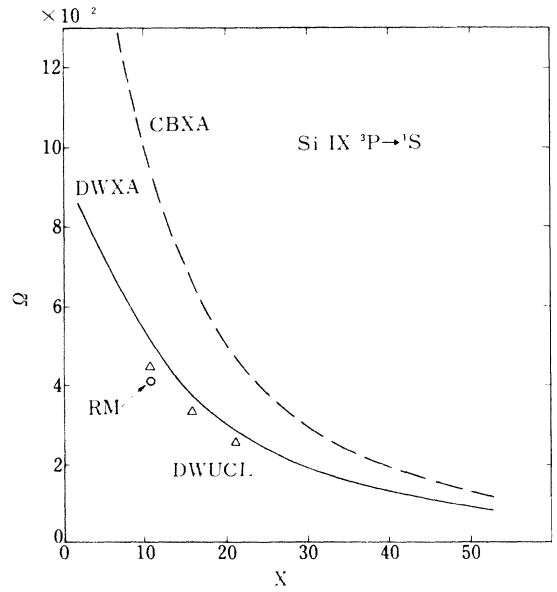

FIG. 8. Same as in Fig. 6, but for Si IX ($\Delta E = 0.9504$ Ry). The values of RM and DWUCL are taken, respectively, from Refs. 4 and 13.

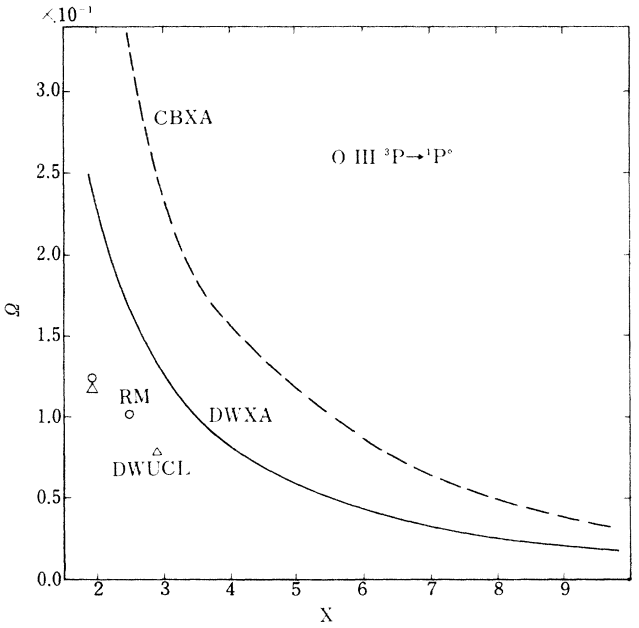

FIG. 10. Collision strengths for the transition $2s^2 2p^2\,{}^3P$-$2s2p^3\,{}^1P^0$ ($\Delta E = 2.066$ Ry) in O III. The present results of the distorted-wave method (DWXA, solid line) and the Coulomb-wave approximation (CBXA, dashed line) are compared with the values obtained by the R-matrix method (Ref. 7) (RM, circles) and the other DW method by Bhatia *et al.* (Ref. 15) (DWUCL, triangles).

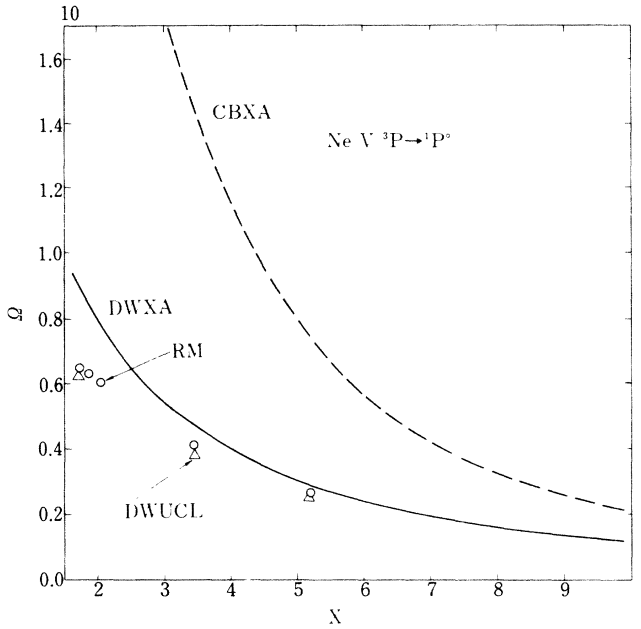

FIG. 11. Same as in Fig. 10, but for Ne V (ΔE=2.904 Ry). The values of RM and DWUCL are taken from Refs. 8, 21, and 16.

the distortion is quite effective for those partial waves. It is worth noting that the distortion is larger for the C-like ions than for the He-like ones, which were studied in paper I. The CBXA, therefore, gives poorer results for the former than the latter.

When compared with the RM method, the DWUCL method seems better than the DWXA. This is partly due to the unitarization procedure incorporated in the DWUCL computer package. In some cases, however, the

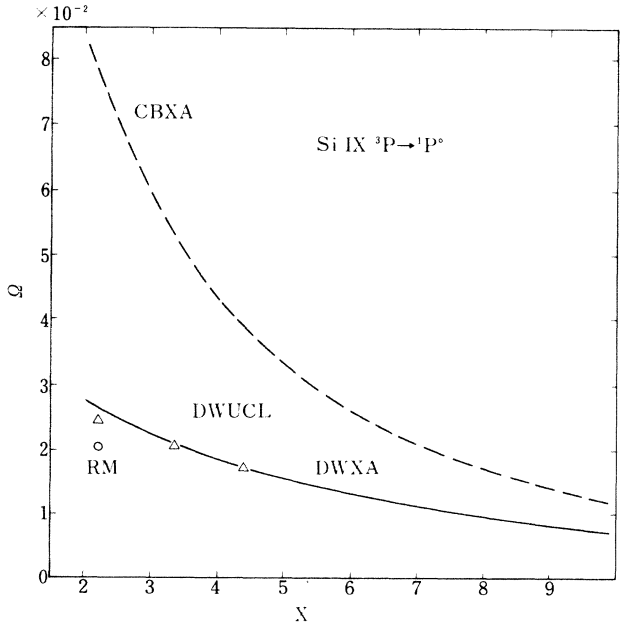

FIG. 12. Same as in Fig. 10, but for Si IX (ΔE=4.541 Ry). The values of RM and DWUCL are taken, respectively, from Refs. 4 and 13.

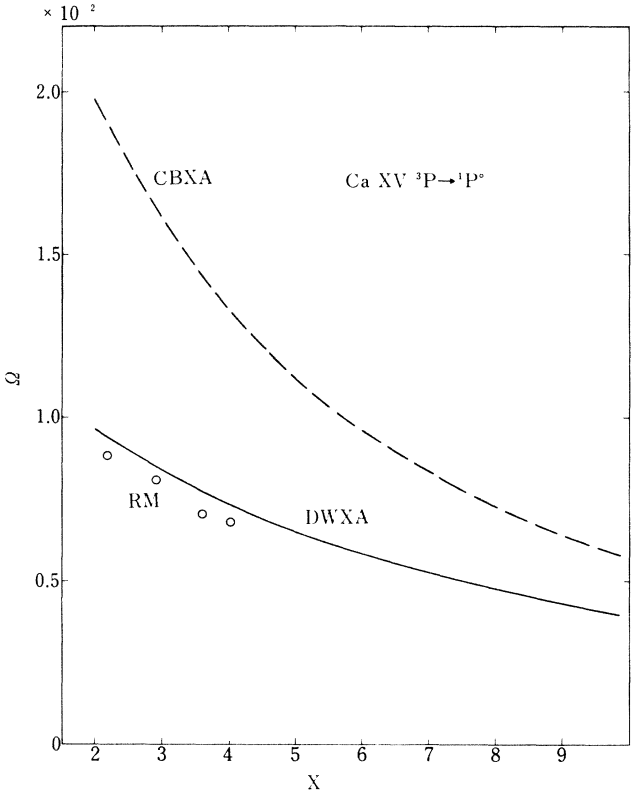

FIG. 13. Same as in Fig. 10, but for Ca XV (ΔE=6.972 Ry). The values of RM are taken from Ref. 5.

DWUCL results disagree very much with the RM results. Two examples are $2s^2 2p^2\,{}^3P \rightarrow 2s\,2p^3\,{}^1P^0$ and $2s^2 2p^2\,{}^3P \rightarrow 2s\,2p^3\,{}^1D^0$ in Ca XV. In both cases, the discrepancy reaches up to a factor of 3.[5] The present DW calculation (DWXA) produces values very close to those of the RM method (see Figs. 13 and 14). The difference

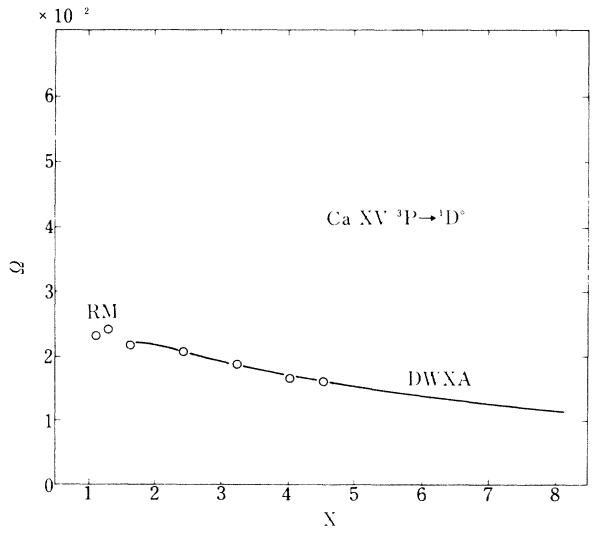

FIG. 14. Collision strengths for the $2s^2 2p^2\,{}^3P$-$2s\,2p^3\,{}^1D^0$ transition (ΔE=6.197 Ry) in Ca XV. The results of the present DW method (DWXA, solid line) are compared with the values obtained by the R-matrix method (Ref. 5) (RM, circles).

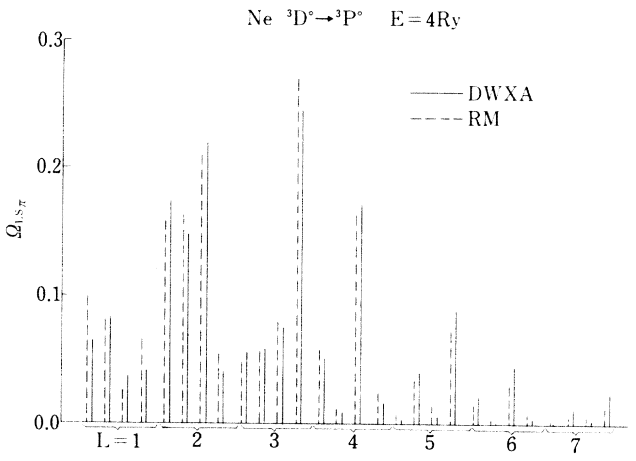

FIG. 15. Comparison of the partial collision strengths Ω_{LS_π} for the $2s2p^3\,^3D^0$-$2s2p^3\,^3P^0$ transition (ΔE=0.3080 Ry) in Ne V, calculated at 4 Ry by the present DW method (DWXA, solid lines) and the R-matrix one (Ref. 8) (RM, dashed lines). For each L, there are four sets of Ω_{LS_π} shown, with, from left to right, ($S=\frac{1}{2},\pi$=even), ($S=\frac{1}{2},\pi$=odd), ($S=\frac{3}{2},\pi$=even), and ($S=\frac{3}{2},\pi$=odd).

between the DWUCL results and the DWXA (and RM) ones may partly come from the difference in the target wave functions used. It should be noted here that the DWUCL calculation was carried out in the intermediate-coupling scheme and thus included some relativistic effects. On the other hand, both the present calculation (DWXA) and the R-matrix calculation are based on the LS-coupling scheme. The relativistic effects may be so strong for Ca that a simple comparison cannot be made between the calculations of different coupling scheme.

Nothing has been published for the partial collision strengths for the spin-forbidden transitions calculated in the R-matrix method. Aggarwal[8] published partial collision strengths for $2s2p^3\,^3D^0 \rightarrow 2s2p^3\,^3P^0$ in Ne V and Si IX. In Fig. 15, a comparison is made for the partial collision strengths for Ne V calculated with the RM and DWXA methods at 4 Ry of electron energy. We can see a good general agreement between the two results. This figure further indicates that the present approach is satisfactorily applicable also to the transition between excited states.

V. SUMMARY AND CONCLUDING REMARKS

The distorted-wave-method approach proposed in paper I is applied to the excitation of C-like ions. The validity of the present approach (DWXA) has been examined by comparing it with the R-matrix and the two-state close-coupling calculations. For dipole-allowed transitions, the DWXA result is very good except near the threshold. For forbidden transitions, the DWXA result for O III is rather poor and becomes good only at higher energies. With increasing nuclear charge, however, the reliability of the DWXA increases rapidly for forbidden processes. For Ca XV, for instance, the DWXA agrees with the RM method within 20% at any energy but near threshold. It should be noted that the Coulomb-Born-type calculation (even with electron exchange) is valid only at higher energies (say, $X > 10$) for the forbidden transitions in Ca XV.

Another systematic comparison has been made with the DWUCL method (the distorted-wave computer package developed at the University College, London). In some cases a difference is caused by the method of representation of the target ion. In the calculation of DWUCL, target wave functions are generated with the same distortion potential as used for the production of the distorted waves for continuum electrons. The present approach (DWXA) assumes that the best target wave function is given independently. In the latter approach, the systematics of the collision dynamics can better be studied without being bothered by any ambiguity in the target wave function. Also in the latter approach, the present method can reliably supplement the R-matrix calculation to extend the availability of the cross-section data. Actually, the present calculation has been used in determining best values of the rate coefficients for the excitation of C-like ions,[23] together with the result of the R-matrix method. Another discrepancy between the present DW method and the DWUCL can arise if the relativistic effects are not properly taken into account in the latter. The effects may be significant for heavier ions, for which we should more carefully compare the theoretical results.

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