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# Distorted-wave-method calculation of electron-impact excitation of atomic ions: He- and Be-like ions

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A distorted-wave method is applied to electron-impact excitations of He-like (Li II and O VII) and Be-like (C III) ions. In the method, the same distortion potential is assumed for both the initial and the final states, and electron exchange is taken into account only between interacting electrons. The collision strengths are calculated for the excitations of $2\,^1P$, $2\,^1S$, $2\,^3P$, and $2\,^3S$ states of the He-like ions and $2s2p\,^1P$ and $2s2p\,^3P$ states of the Be-like ion, and compared with the results of more elaborate calculations (e.g., the close-coupling-type ones). Good agreement is found in most cases if use is made of the target wave functions of the same or comparable accuracy. Also examined is the Coulomb-wave approximation, in which the distorted wave is replaced by the corresponding Coulomb wave.

## I. INTRODUCTION

Electron-impact excitations of atomic ions are fundamental processes in high-temperature plasmas in laboratory and astrophysical systems.[1] The difficulty of the measurement of the excitation cross section makes it necessary to develop a theoretical method reliably applicable to various collision systems. In the present paper an approach is proposed (a) to apply to a wide range of ionic species, transition processes, and collision energies, and (b) to clarify systematically the physical mechanisms of the excitation processes. As a test of the method, cross sections are calculated for He- and Be-like ions and compared with other theoretical results.

There are already many calculations of excitation cross section.[2,3] Many of them, however, have been carried out for the primary application to astrophysical problems and only for a lower-energy region (i.e., near threshold). When plasmas are in ionization equilibrium, the most important are the cross sections near threshold. Once a plasma becomes out of equilibrium (the situation often encountered in a fusion plasma), cross section for a wide range of collision energies are needed to analyze properties of the plasma. Furthermore, high-energy behavior of the cross section, if known, is very helpful in assessing the reliability of the low-energy part of the cross section. Needless to say, a comprehensive set of data is important in understanding the physical nature of the excitation process. The present study aims at approaching the goal of the production of a comprehensive set of the excitation cross section.

The principles of the present approach are as follows.

(1) A distorted-wave (DW) method is employed to treat collision dynamics.

(2) States of the target ion are represented by a wave function as accurately as possible.

In the case of the electron-ion collision, it has been found from experience that the accuracy of the target wave function is much more important than that of the treatment of collision dynamics. It is also of significance to avoid any ambiguity caused by the inaccuracy of the target wave function. There are elaborate methods (e.g., the close-coupling or $R$-matrix method) which may give more accurate results than the DW one for the cross-section calculation. It is, however, very laborious to apply those methods to practical problems. In principle they can be used in any collision system and at any collision energy, but in practice their applications are restricted to the excitation of lower states and at the collision energies near threshold. The DW method is much easier to apply to any problem. In this sense, the present approach is complementary to those sophisticated methods.

An advantage of the DW method is its flexibility. It can be modified in various ways depending on the problem considered. In the present paper, one of the simplest forms of the DW approximation is proposed to be applied to a wide range of excitation processes and collision energies. After its validity is examined in a number of cases, the formula could be modified to be improved, if necessary. The present method does not include resonance effects. The resonance effects are usually confined in the threshold region. The present approach, therefore, is concerned primarily with the energy range above the threshold region. In principle, the resonance effects can be taken into account in the DW method.[4,5] It will be one of the possible ways of future improvement of the present method.

In Sec. II our DW method is formulated. Some details of numerical calculation are described in Sec. III. In Secs. IV and V the cross sections calculated are presented for He-like (Li II and O VII) and Be-like (C III) ions, respectively. Comparisons are made with other calculations there. A summary of the present calculation is given in Sec. VI.

## II. DISTORTED-WAVE METHOD

The present distorted-wave method is based on the following assumptions.

 

(i) Introducing a distortion potential $U^{\mathrm{DW}}$ and regarding the difference between the true interaction and $U^{\mathrm{DW}}$ as a perturbation, we adopt the standard first-order perturbation theory to derive the transition probability. The same distortion potential is used to calculate distorted waves both for the initial and for the final states.

(ii) We assume $U^{\mathrm{DW}}$ to be a spherical average of the electrostatic potential formed by the target ion in its initial state.

(iii) An 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.

The Hamiltonian of the whole (target ion plus incident electron) system is written as (atomic units being used throughout this paper)

$$H=H_0+T+V\ , \tag{1}$$

where $H_0$ is the Hamiltonian for the target ion, $T$ is the kinetic-energy operator for the incident electron, and $V$ is the interaction between the electron and the ion. With the use of the first-order perturbation theory, the matrix element for the transition, $\alpha\rightarrow\beta$ $(\alpha\neq\beta)$ is obtained in the form

$$T_{\beta\alpha}=\langle\chi_\beta^{(-)}\,|\,(V-U^{\mathrm{DW}})\,|\,\chi_\alpha^{(+)}\rangle\ . \tag{2}$$

The (unperturbed) wave function $\chi_\alpha^{(+)}$ $(\chi_\beta^{(-)})$ is a solution of the equation

$$(H_0+T+U^{\mathrm{DW}})\chi=E\chi\ , \tag{3}$$

with the outgoing (incoming) boundary condition.

When we ignore the electron exchange, we can separate the wave function $\chi$ into the target part $\phi$ and the distorted wave $F$ for the incident electron:

$$\chi_\alpha(1,\ldots,N+1)=\phi_\alpha(1,\ldots,N)F_\alpha(N+1)\ . \tag{4}$$

Here $N$ is the number of the target electrons. The function $F$ satisfies the equation

$$(T+U^{\mathrm{DW}})F_\alpha=(E-\epsilon_\alpha)F_\alpha\ , \tag{5}$$

where $\epsilon_\alpha$ is the energy of the bound state of the ion. The interaction $V$ is expressed as

$$V=\sum_{j=1}^{N}\frac{1}{r_{j,N+1}}-\frac{Z}{r_{N+1}}\ , \tag{6}$$

where $Z$ is the nuclear charge of the ion, $\mathbf{r}_i$ denotes the coordinate of the electron $i$, and $r_{ij}=|\,\mathbf{r}_i-\mathbf{r}_j\,|$. Substituting (4) (and the corresponding form for $\chi_\beta$) and (6) into Eq. (2), we have the element of the transition matrix (direct-scattering part) in the form

$$T_{\beta\alpha}^{(\mathrm{d})}=N\left\langle\phi_\beta(1,\ldots,N)F_\beta^{(-)}(N+1)\left|\frac{1}{r_{N,N+1}}\right|\phi_\alpha(1,\ldots,N)F_\alpha^{(+)}(N+1)\right\rangle\ . \tag{7}$$

We take into account the effect of electron exchange by inserting an antisymmetrized wave function

$$\bar{\chi}_\beta^{(-)}(1,\ldots,N+1)=\sum_{p=1}^{N+1}(-1)^{N+1-p}\phi_\beta(1,\ldots,p-1,p+1,\ldots,N,N+1)F_\beta^{(-)}(p) \tag{8}$$

in the place of $\chi_\beta^{(-)}$ in Eq. (2). Then we have the exchange part of the transition-matrix element

$$T_{\beta\alpha}^{(\mathrm{ex})}=-N\left\langle\phi_\beta(1,\ldots,N-1,N+1)F_\beta^{(-)}(N)\left|\sum_{j=1}^{N}\frac{1}{r_{j,N+1}}-\left[U^{\mathrm{DW}}(N+1)+\frac{Z}{r_{N+1}}\right]\right|\phi_\alpha(1,\ldots,N)F_\alpha^{(+)}(N+1)\right\rangle\ . \tag{9}$$

The transition matrix $T_{\beta\alpha}$ is given by the sum $T_{\beta\alpha}^{(\mathrm{d})}+T_{\beta\alpha}^{(\mathrm{ex})}$. Equation (9) is the post form of the exchange part. We can also define the exchange part by antisymmetrizing the initial-state wave function (the prior form). Usually different results are obtained, depending on which form is chosen (the post-prior discrepancy).

It should be noted that the transition-matrix elements, (7) and (9), can be derived also from the application of the first-order perturbation theory to the general formula of scattering amplitude. In the present formulation, it is essential to assume the same distortion potential for the initial and final states. Otherwise the resulting nonorthogonality of the initial and the final distorted waves would introduce inconsistencies. (This point was discussed rather extensively by Fano and Inokuti.[6])

On the basis of the assumption (iii) above, we retain in Eq. (9) only the contribution from the electron exchange between the interacting electrons. Thus we have

$$T_{\beta\alpha}^{(\mathrm{ex})}=-N\left\langle\phi_\beta(1,\ldots,N-1,N+1)F_\beta^{(-)}(N)\left|\frac{1}{r_{N,N+1}}\right|\phi_\alpha(1,\ldots,N)F_\alpha^{(+)}(N+1)\right\rangle\ . \tag{10}$$

This is not only the simplest form of the exchange-matrix element but also gives the correct result when $Z\rightarrow\infty$. Furthermore, with this approximate treatment, we can avoid the post-prior discrepancy.

The differential cross section for the excitation is obtained by

$$\frac{d\sigma(\alpha\rightarrow\beta)}{d\omega}=\frac{1}{4\pi^2}\frac{k_\beta}{k_\alpha}\,|\,T_{\beta\alpha}\,|^2\ , \tag{11}$$

where $k_\alpha$ $(k_\beta)$ is the wave number of the incident (scattered) electron, and $T_{\beta\alpha}$ is the sum of the direct and exchange

parts of the transition-matrix elements as stated before.

To numerically evaluate the matrix element $T_{\beta\alpha}$, we assume that the angular momenta of the whole system are coupled according to the $L$-$S$ scheme. The cross section averaged over the initial direction of the (spin and orbital) angular momenta and summed over the final direction of them is obtained as (after the integration of the scattering angles of the electron)

$$\sigma(\alpha L^{\alpha}S^{\alpha}\rightarrow\beta L^{\beta}S^{\beta})=\frac{k_{\beta}}{k_{\alpha}}\frac{8\pi}{(2L^{\alpha}+1)(2S^{\alpha}+1)}\sum_{L}\sum_{S}\sum_{l}\sum_{l'}(2L+1)(2S+1)\,|\,\langle T^{(\mathrm{d})}\rangle_{\beta\alpha}+\langle T^{(\mathrm{ex})}\rangle_{\beta\alpha}\,|^{2} \tag{12}$$

with

$$\langle T^{(\mathrm{d})}\rangle_{\beta\alpha}=N\left\langle\psi(\Gamma_{\beta}\,|\,x_1,\ldots,x_N,\hat{x}_{N+1})u_{l'}^{(\beta)}(r_{N+1})r_{N+1}^{-1}\left|\frac{1}{r_{N,N+1}}\right|\psi(\Gamma_{\alpha}\,|\,x_1,\ldots,x_N,\hat{x}_{N+1})u_{l}^{(\alpha)}(r_{N+1})r_{N+1}^{-1}\right\rangle , \tag{13}$$

$$\langle T^{(\mathrm{ex})}\rangle_{\beta\alpha}=-N\left\langle\psi(\Gamma_{\beta}\,|\,x_1,\ldots,x_{N-1},x_{N+1},\hat{x}_{N})u_{l'}^{(\beta)}(r_{N})r_{N}^{-1}\left|\frac{1}{r_{N,N+1}}\right|\psi(\Gamma_{\alpha}\,|\,x_1,\ldots,x_N,\hat{x}_{N+1})u_{l}^{(\alpha)}(r_{N+1})r_{N+1}^{-1}\right\rangle . \tag{14}$$

Here $L^{\alpha}S^{\alpha}$ ($L^{\beta}S^{\beta}$) are the orbital and spin angular momenta of the initial (final) state of the ion, $l$ ($l'$) is the orbital angular momentum of the incident (scattered) electron, and $LS$ are the orbital and spin angular momenta of the total (electron plus ion) system ($M_L M_S$ being their $z$ components). In Eqs. (13) and (14), $\psi$ is the target wave function coupled with the angular (and spin) part of the wave function of the scattered electron, $x_i$ denotes collectively the space and spin coordinates of the $i$th electron, and $\hat{x}_i$ is the angular part of $x_i$. The function $\psi$ is specified by the channel index $\Gamma_{\alpha}=\alpha L^{\alpha}S^{\alpha}lLSM_LM_S$. The target wave function itself is a linear combination of the configuration state functions, which are properly antisymmetrized and $L$-$S$ coupled.

The radial part of the distorted-wave function, $u_l^{(\alpha)}$, is the solution of the equation

$$\left[\frac{d^2}{dr^2}+\left[k_{\alpha}^2-2U^{\mathrm{DW}}-\frac{l(l+1)}{r^2}\right]\right]u_l^{(\alpha)}(r)=0 \tag{15}$$

with the boundary condition

$$u_l^{(\alpha)}(r)\underset{r\rightarrow\infty}{\sim}k_{\alpha}^{-1}\sin[\,k_{\alpha}r+k_{\alpha}^{-1}q\ln(2k_{\alpha}r)-2^{-1}\pi l+\eta_l^{(\alpha)}]\,. \tag{16}$$

Here the distortion potential is assumed to be spherically symmetric and has an asymptotic form

$$U^{\mathrm{DW}}(r)\underset{r\rightarrow\infty}{\sim}-q/r\,. \tag{17}$$

In Eq. (16), $\eta_l^{(\alpha)}$ is the phase shift due to the potential $U^{\mathrm{DW}}$. In the actual calculation, we adopt as $U^{\mathrm{DW}}$ the spherical average of the electrostatic potential of the target ion in its initial state and, hence, $q=Z-N$. The final DW function $u_{l'}^{(\beta)}$ is the solution of Eq. (15) but with the change of $\alpha\rightarrow\beta$ and $l\rightarrow l'$. The evaluation of the angular momentum part of the matrix elements, (13) and (14), can be performed in the same way as in the general treatment of electron-atom scattering by Smith and Morgan.[7]

In the following sections, the results are expressed in the form of collision strengths defined by

$$\Omega(\alpha L^{\alpha}S^{\alpha}\rightarrow\beta L^{\beta}S^{\beta})=\pi^{-1}k_{\alpha}^{2}(2L^{\alpha}+1)(2S^{\alpha}+1)\times\sigma(\alpha L^{\alpha}S^{\alpha}\rightarrow\beta L^{\beta}S^{\beta})\,. \tag{18}$$

Before closing this section, comments are given on the comparison of the present DW method and others. The present approach of the DW method is very similar to that applied to neutral He by Madison and Shelton.[8] They also adopted the same distortion potential for both the initial and the final states. They assumed further that the continuum-state wave function be orthogonal to the bound-state single-particle wave functions. From this assumption they reached the same form of the exchange part of the transition matrix as in Eq. (10). Since the orthogonality requirement has no *a priori* justification, we do not impose that, but simply retain the exchange term between interacting electrons. The method of Madison and Shelton has not been widely applied so far.

Eissner and Seaton[9,10] have developed a DW method in which a single distortion potential (the Thomas-Fermi type) is assumed both for the initial and the final states. In their method, they use the distortion potential also to determine the bound-state single-particle wave function. Actually they adjust the distortion potential so as to produce the best bound-state wave function. In the present approach, we start our calculation under the condition that the best target wave function is already given or separately determined. It is difficult to decide which method gives more accurate results. Both the methods probably produce comparably reasonable cross sections, if the target wave functions employed are of comparable accuracy. In reality, however, a detailed comparison of the two calculations is hard to do, because it is often difficult to assess the details of the target wave function of the Eissner-Seaton method.[9,10]

The DW method of Peek and Mann[11] is somewhat more sophisticated than ours. They also use as $U^{\mathrm{DW}}$ the spherically averaged electrostatic potential of the target ion. They choose, however, different potentials for the calculation of the initial and final distorted waves. They retain in Eq. (9) the contribution from the one-electron exchange term [i.e., the term including $U^{\mathrm{DW}}(N+1)+Z/r_{N+1}$] which we ignore. Furthermore they approximately take account of the electron-exchange effect in the distortion potential. As will be shown later, however, our simpler method gives the collision strength in good agreement with theirs.

## III. NUMERICAL CALCULATION

In the present paper, the configuration interaction (CI) wave function of target ion is obtained by CIV3 code of Hibbert.[12] When a comparison is made with other calculations, the same wave functions will be used as far as possible. The distortion potential is calculated from

$$U^{\mathrm{DW}}(r_{N+1})=-\frac{Z}{r_{N+1}}+\frac{1}{4\pi}\int d\hat{r}_{N+1}\frac{1}{2L^{\alpha}+1}\sum_{M_L^{\alpha}}\left\langle\phi_{\alpha}(1,\ldots,N)\left|\sum_{j=1}^{N}\frac{1}{r_{j,N+1}}\right|\phi_{\alpha}(1,\ldots,N)\right\rangle, \tag{19}$$

where $\phi_{\alpha}$ is the target function of the initial state. In the following sections, excitations are considered only from the ground state of the He- and Be-like ions. The spherical average in Eq. (19) is not necessary there.

Once the equation (15) is solved for the radial part of the DW function, it is straightfoward to calculate the transition-matrix element $T_{\beta\alpha}$. The angular and spin part of the integral in Eqs. (13) and (14) is evaluated with the use of the respective part of the general code, NIEM,[13] for the calculation of electron-impact excitation of atoms. The convergence over the partial waves of the scattered electron is confirmed for each case. For higher partial waves ($l \geq 8$, in all the present calculations) we can use the Coulomb wave instead of the DW. Furthermore, the dipole approximation[14] (the so-called Coulomb-Bethe approximation) is applied to estimate the contribution for the higher partial waves for the dipole-allowed transition.

## IV. HE-LIKE IONS

van Wyngaarden *et al.*[15] made a (five-state) close-coupling calculation for He-like ions. We compare our results with theirs. To study the dependence on nuclear charge, calculations are carried out for Li II and O VII. The wave functions of the ions are taken to be the same as those used by van Wyngaarden *et al.* The configurations considered are as follows.

(i) $1s^2, 2s^2, 2p^2, 1s\,2s$ for $1\,^1S$ and $2\,^1S$
(ii) $1s\,2s$ for $2\,^3S$
(iii) $1s\,2p, 2s\,2p$ for $2\,^1P$ and $2\,^3P$.

The calculated values of energy difference and oscillator strength are in good agreement with experiment (see Ref. 15). Those calculated values are used in the present calculation when needed.

### A. Li II

Figures 1—4 show the collision strengths for the excitations $1\,^1S \rightarrow 2\,^1P, 2\,^1S, 2\,^3P, 2\,^3S$, respectively. The electron energy is expressed in the threshold unit, $X=E_e/\Delta E$, $\Delta E$ being the excitation energy. Each figure includes the results of our DW exchange approximation calculation (referred to as DWXA to distinguish it from other DW methods), the Coulomb-Born exchange approximation (CBXA) and the close-coupling (CC) calculation. Here the CBXA result is obtained by replacing the distorted waves, $u_l^{(\alpha)}$ 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 in the present formulation. It is a type of Coulomb-Born exchange approximation, but the exchange part of the transition matrix is assumed to have a specific form (10). For spin-allowed transitions, the result of the pure Coulomb-Born approximation (i.e., no electron exchange being included) is also plotted in the figures. It should be noted again that

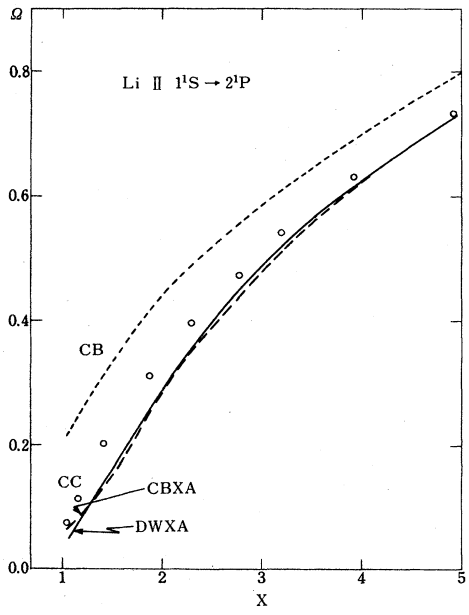


FIG. 1. Collision strengths for the $1\,^1S-2\,^1P$ transition ($\Delta E=4.5834$ Ry) in Li II as a function of electron energy, $X$, in threshold units. The present results of the distorted-wave method (DWXA, solid line) and the Coulomb-Born approximation with (CBXA, long-dashed line) and without (CB, short-dashed line) electron exchange are compared with the close-coupling (CC, circles) calculation (Ref. 15).

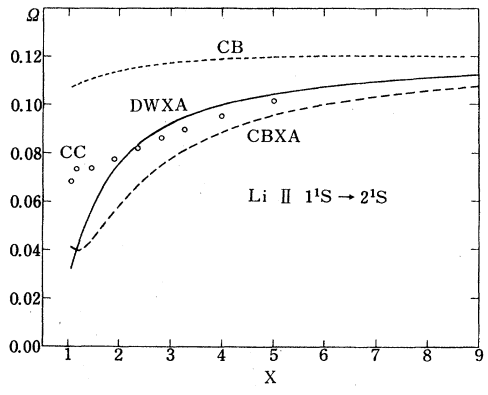


FIG. 2. Same as in Fig. 1, but for the $1\,^1S-2\,^1S$ transition ($\Delta E=4.4884$ Ry) in Li II.

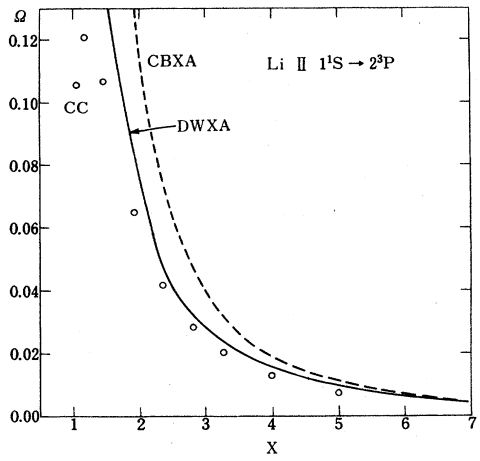


FIG. 3. Same as in Fig. 1, but for the $1\,^1S-2\,^3P$ transition ($\Delta E=4.5031$ Ry) in Li II.

all the calculations use the same wave functions of the target ion.

The DWXA results for $2\,^1P$, $2\,^1S$, and $2\,^3P$ excitations agree well with the corresponding values of the CC calculation at $X\gtrsim 2$. For $2\,^3S$ excitation, the DWXA values have an energy dependence similar to the CC ones, but the difference in magnitude is as large as 50% even around $X=2$. At $X>3$, the two calculations get closer for $1\,^1S\rightarrow 2\,^3S$. Except for the $2\,^1P$ excitation, the DWXA results near threshold ($X\sim 1$) deviate much from the CC ones. The threshold region is usually dominated by resonance effects, which are included neither in the DWXA nor in the CC calculation. We need a more elaborate calculation there.

To make a somewhat more detailed comparison, we present in Table I the partial collision strength $\Omega_L$ for each $L$ calculated at two energies. An overall agreement is good between the DWXA and CC calculations especially for the higher energy. A large disagreement arises mainly from the contribution of $s$ wave ($l=0$). Also a considerable discrepancy is seen sometimes in the very small terms of $\Omega_L$, though they are of less significance to the total collision strength. Those terms may be dominated by a higher-order effect, which is not included in the

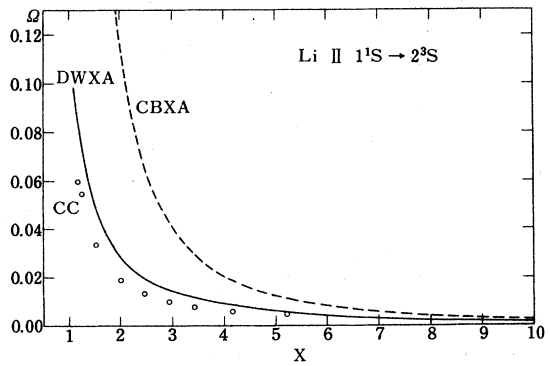


FIG. 4. Same as in Fig. 1, but for the $1\,^1S-2\,^3S$ transition ($\Delta E=4.3450$ Ry) in Li II.

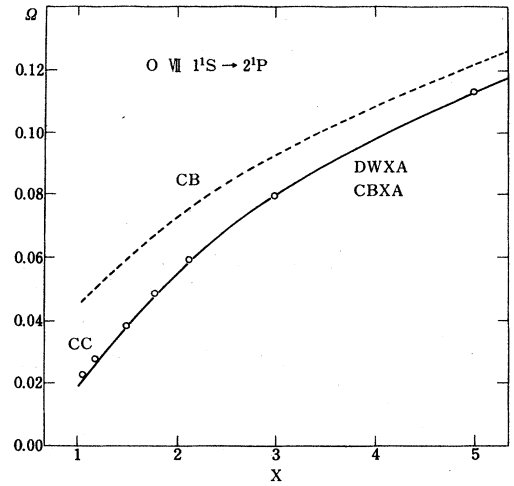


FIG. 5. Same as in Fig. 1, but for the $1\,^1S-2\,^1P$ transition ($\Delta E=42.171$ Ry) in O VII. The results of DWXA and CBXA cannot be distinguished in this scale.

first-order perturbation method like the present one.

The Coulomb-Born exchange approximation is expected to become better with increasing electron energy. As is seen from the figures, the behavior is different for different excitation processes. For a dipole-allowed transition ($2\,^1P$), the CBXA is very close to the DWXA over the entire range of $X$ considered. The Coulomb-Born exchange approximation is good at $X\gtrsim 5$ for $2\,^1S$ and $2\,^3P$ and at $X\gtrsim 7$ for $2\,^3S$. In particular, the Coulomb-Born approximation *without* electron exchange (CB) is very poor even for the dipole-allowed transition. For $2\,^1S$ excitation, it becomes good only at very high energy of electrons. This suggests the importance of electron exchange.

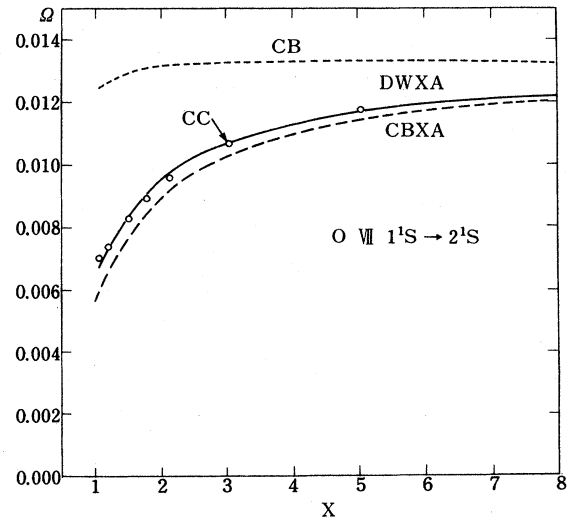


FIG. 6. Same as in Fig. 1, but for the $1\,^1S-2\,^1S$ transition ($\Delta E=42.780$ Ry) in O VII.

TABLE I. Partial collision strengths $\Omega_L$ for the excitation of Li II at the electron energies 6.54 and 12.64 Ry. The present distorted-wave (DWXA) and the Coulomb-wave (CBXA) calculations are compared with the close-coupling (CC) one (Ref. 15).

| | $2\,^3S$ | | | $2\,^1S$ | | | $2\,^3P$ | | | $2\,^1P$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $L$ | CC | DWXA | CBXA | CC | DWXA | CBXA | CC | DWXA | CBXA | CC | DWXA | CBXA |
| 6.54 Ry | | $X=1.51$ | | | $X=1.46$ | | | $X=1.45$ | | | $X=1.43$ | |
| 0 | 0.0144 | 0.0440 | 0.2272 | 0.0141 | 0.0068 | 0.0009 | 0.0080 | 0.0070 | 0.0026 | 0.0090 | 0.0052 | 0.0031 |
| 1 | 0.0041 | 0.0047 | 0.0024 | 0.0521 | 0.0383 | 0.0322 | 0.0226 | 0.0549 | 0.2217 | 0.0118 | 0.0009 | 0.0006 |
| 2 | 0.0126 | 0.0008 | 0.0008 | 0.0040 | 0.0102 | 0.0096 | 0.0685 | 0.0716 | 0.0636 | 0.0620 | 0.0423 | 0.0397 |
| 3 | 0.0022 | 0.0003 | 0.0003 | 0.0021 | 0.0012 | 0.0012 | 0.0075 | 0.0078 | 0.0075 | 0.0713 | 0.0514 | 0.0496 |
| 4 | 0.0001 | 0.0000 | 0.0000 | 0.0014 | 0.0001 | 0.0001 | 0.0003 | 0.0007 | 0.0006 | 0.0328 | 0.0270 | 0.0274 |
| 5 | | | | 0.0005 | 0.0000 | 0.0000 | | | | 0.0111 | 0.0103 | 0.0102 |
| 6 | | | | 0.0001 | | | | | | 0.0035 | 0.0032 | 0.0032 |
| $L\geq 7$ | | | | | | | | | | 0.0014 | 0.0015 | 0.0015 |
| Total | 0.0334 | 0.0498 | 0.2306 | 0.0742 | 0.0566 | 0.0440 | 0.1069 | 0.1419 | 0.2961 | 0.2029 | 0.1418 | 0.1353 |
| 12.64 Ry | | $X=2.91$ | | | $X=2.82$ | | | $X=2.81$ | | | $X=2.76$ | |
| 0 | 0.0037 | 0.0088 | 0.0395 | 0.0107 | 0.0123 | 0.0053 | 0.0026 | 0.0018 | 0.0007 | 0.0124 | 0.0093 | 0.0045 |
| 1 | 0.0045 | 0.0058 | 0.0043 | 0.0414 | 0.0401 | 0.0342 | 0.0034 | 0.0040 | 0.0203 | 0.0076 | 0.0045 | 0.0075 |
| 2 | 0.0003 | 0.0000 | 0.0000 | 0.0240 | 0.0254 | 0.0237 | 0.0134 | 0.0172 | 0.0169 | 0.0408 | 0.0410 | 0.0419 |
| 3 | 0.0009 | 0.0003 | 0.0003 | 0.0060 | 0.0091 | 0.0088 | 0.0066 | 0.0068 | 0.0066 | 0.0870 | 0.0822 | 0.0805 |
| 4 | 0.0004 | 0.0002 | 0.0002 | 0.0017 | 0.0025 | 0.0025 | 0.0018 | 0.0019 | 0.0019 | 0.0926 | 0.0858 | 0.0871 |
| 5 | 0.0001 | 0.0001 | 0.0001 | 0.0010 | 0.0006 | 0.0006 | 0.0004 | 0.0005 | 0.0005 | 0.0753 | 0.0668 | 0.0659 |
| 6 | | | | 0.0008 | 0.0001 | 0.0001 | 0.0001 | 0.0000 | 0.0001 | 0.0538 | 0.0509 | 0.0505 |
| 7 | | | | 0.0006 | 0.0000 | 0.0000 | | | | 0.0359 | 0.0370 | 0.0355 |
| $L\geq 8$ | | | | 0.0005 | | | | | | 0.0665 | 0.0685 | 0.0668 |
| Total | 0.0099 | 0.0152 | 0.0444 | 0.0867 | 0.0902 | 0.0752 | 0.0283 | 0.0323 | 0.0470 | 0.4719 | 0.4460 | 0.4402 |

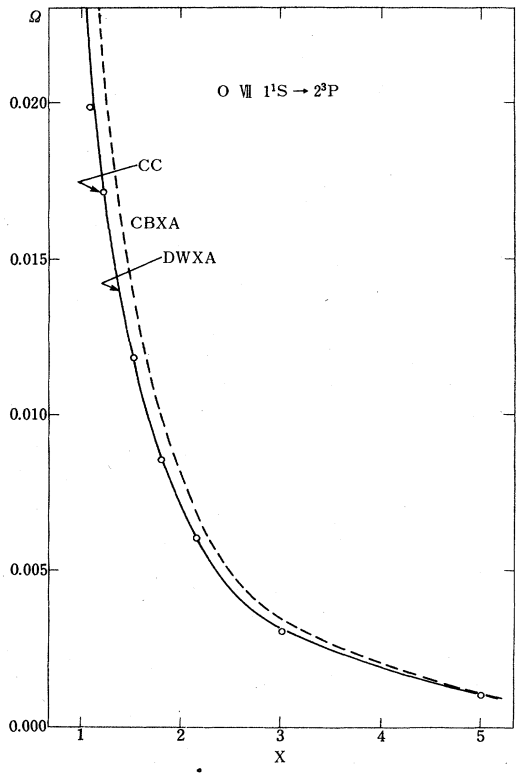


FIG. 7. Same as in Fig. 1, but for the $1\,^1S$–$2\,^3P$ transition ($\Delta E = 41.787$ Ry) in O VII.

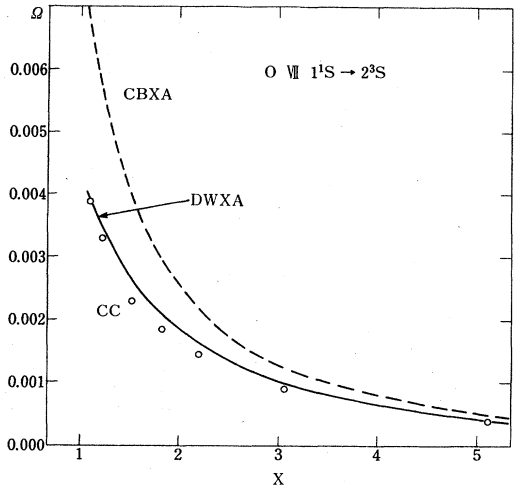


FIG. 8. Same as in Fig. 1, but for the $1\,^1S$–$2\,^3S$ transition ($\Delta E = 41.275$ Ry) in O VII.

### B. O VII

The collision strengths for the excitations of $2\,^1P, 2\,^1S, 2\,^3P, 2\,^3S$ of O VII are shown in Figs. 5–8, respectively. In this case, the agreement between the DWXA and CC is very good (within 10%) except for the $2\,^3S$ excitation. In the case of $2\,^3S$, there is a discrepancy as large as 15%. The Coulomb-Born exchange approximation (CBXA) gives almost the same results for $2\,^1P$ and $2\,^1S$ as the DWXA. While the CBXA completely agrees with the DWXA for $2\,^1P$, there remains a small difference for $2\,^1S$. The CBXA is poor at $X < 2$ for $2\,^3P$ and $X < 3$ for $2\,^3S$. It is noted that, at $X \sim 1$, the CBXA value for $2\,^3S$ is larger by a factor of 2 than the corresponding DWXA one. The CB calculation is very poor also in the case of O VII.

From the comparison with the previous case of Li II, we conclude the following in regard to the $Z$ dependence. With increasing $Z$, the present DW calculation (DWXA) becomes better as expected. In the case of O VII, the DWXA method reproduces almost completely the CC result at any electron energy. The Coulomb-Born exchange approximation also becomes better for higher $Z$. The distortion effect, however, is still of importance for a certain type of excitation at least at lower energies. The effect of electron exchange cannot be ignored at all except at a very high energy above threshold. These effects of distortion and exchange are taken into account properly by the present DW method in the case of higher $Z$.

In the case of O VII, a very accurate calculation has been made recently with the $R$-matrix method.[16] Except for the resonance effects near the threshold, the result of the $R$-matrix calculation is very similar to the CC values shown here (for details, see Ref. 16). For a comparison, the three results (the $R$ matrix, the CC, and the present DW) at $E_e = 75$ Ry are shown in Table II. A good agreement between the present DW and the $R$-matrix results indicates both the reliability of the present method and the less significance of the resonance effects at this energy. It should be noted that a part of the small discrepancy may be attributed to the slight difference in the target wave functions adopted. In fact, Tayal and Kingston[16] show some difference between their five-state calculation and the similar five-state close-coupling one by van Wyngaarden *et al.*

TABLE II. Comparison of the collision strengths of O VII, calculated at $E_e = 75$ Ry by the present DW approximation (DWXA), the 5-state close-coupling calculation (5CC, Ref. 15), and the (11-state) $R$-matrix method (RM, Ref. 16).

| | $2\,^1S$ | $2\,^1P$ | $2\,^3S$ | $2\,^3P$ |
|---|---|---|---|---|
| DWXA | 0.009 04 | 0.0466 | 0.002 12 | 0.008 78 |
| 5CC | 0.008 92 | 0.0485 | 0.001 84 | 0.008 55 |
| RM (11 state) | 0.008 3 | 0.0544 | 0.002 55 | 0.007 77 |

## V. BE-LIKE IONS

As another test of our method, collision strengths are calculated for the excitation of Be-like ion (C III). Both the Be-like and the He-like ions have the ground state of $ns^2\,{}^1S$, but, in the case of Be-like ions, a transition with $\Delta n = 0$ can occur. Here the excitations $2s^2\,{}^1S \rightarrow 2s\,2p\,{}^1P$, ${}^3P$ of C III are studied. The target states are represented by the configurations

$2s^2, 2p^2, 2s\,3s, 2p\,3p$ for $2s^2\,{}^1S$
$2s\,2p, 2s\,3p, 2p\,3d$ for $2s\,2p\,{}^1P$ and ${}^3P$.

We adopt the exponents of the orbital functions determined by Tatewaki *et al.*[17] $(1s, 2s, 2p)$ and Hibbert[18] $(3s, 3p, 3d)$. The energy difference and oscillator strength calculated with the present wave functions are in very good agreement with the results of more elaborate CI wave functions (e.g., those used in the $R$-matrix calculation described below).

Figure 9 gives the collision strengths for the excitation of $2s\,2p\,{}^1P$. The results of DWXA and CBXA are compared with the $R$-matrix calculation[19] and the distorted wave exchange (DWX) method of Peek and Mann.[11] The target wave functions used in the $R$-matrix and the DWX calculations differ from each other and slightly from the present one. All the wave functions, however, have similar quality, when judged from the resulting energy differences and oscillator strengths. All the values of collision strengths shown in Fig. 9 are in good agreement at $X \gtrsim 2$. It should be noted that the $R$-matrix calculation includes resonance effects, but they are small at $X \gtrsim 2$.

The collision strength for $2s\,2p\,{}^3P$ excitation is shown in Fig. 10. The DWXA result in this case agrees with the $R$-matrix calculation[19] (resonance effects being less significant at $X > 4$ in this case) or the DWX calculation of Mann[20] only at $X \gtrsim 6$.

The excitation energy for $2s^2\,{}^1S - 2s\,2p\,{}^3P$ of C III ($\Delta E = 0.478$ Ry) is very small compared with the other cases. The electron energy at $X = 6$ corresponds to $E_e = 3$ Ry. Considering this fact, we can understand the discrepancy shown in Fig. 10. In his DW method, Mann imposed a unitarization to his original result. We could reduce the discrepancy at lower energies by a similar procedure of unitarization. The discrepancy of the DWXA (and the DWX) from the $R$-matrix values at higher energies may be attributable to the small difference in the target wave functions. The Coulomb-Born exchange approximation (CBXA) is very poor in this case until the electron energy reaches very high values in the threshold unit ($X \sim 20$).

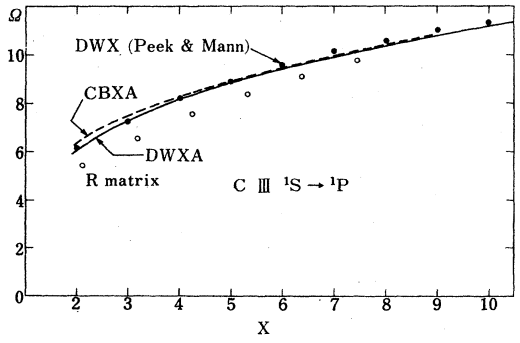


FIG. 9. Collision strengths for the $2s^2\,{}^1S - 2s\,2p\,{}^1P$ transition ($\Delta E = 0.951\,11$ Ry) in C III as a function of electron energy in threshold units. The present results of the distorted-wave method (DWXA, solid line) and the Coulomb-wave approximation (CBXA, dashed line) are compared with the results of the $R$-matrix calculation (open circles, Ref. 19) and the distorted-wave method of Peek and Mann (solid circles, Ref. 11).

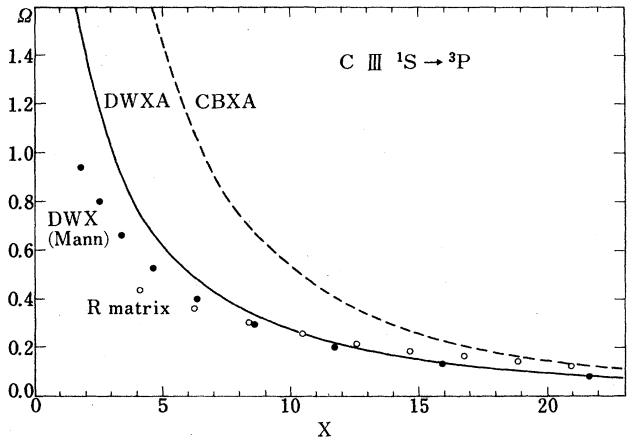


FIG. 10. Same as in Fig. 9, but for the $2s^{1}\,{}^1S - 2s2p\,{}^3P$ transition ($\Delta E = 0.477\,70$ Ry) in C III. The solid circles are the data of the DW method of Mann (Ref. 20).

## VI. CONCLUSION

We have proposed a simple DW method for the calculation of electron-impact excitation of atomic ions. In the method, the spherically-averaged electrostatic potential of the target ion in its initial state is used as the distortion potential both for the initial and for the final states. Furthermore, the electron exchange is taken into account only between interacting electrons. The method has been applied to the excitations of He-like (Li II and O VII) and Be-like (C III) ions and found very satisfactory when compared with more elaborate calculations.

The present method provides good results unless the energy of the incident or scattered electron is very low and in the energy range where resonance effects are not large. When the nuclear charge $Z$, or more precisely the effective charge $Z - N$, is large, the present DW method is quite good even near threshold. When $Z - N$ is small, the method works well at $X \gtrsim 2$–3 for large excitation energy $\Delta E$, and at $X \gtrsim 5$–10 for small $\Delta E$. As is expected, the dipole-allowed transition can be treated very well by the DW method irrespective of these conditions.

For higher electron energies, the Coulomb-wave approximation resembles the DW method more closely. Especially for dipole-allowed transitions, the Coulomb-Born exchange approximation (CBXA) gives results very close to those of the DW method even near threshold. The applicability of the Coulomb-wave approximation, in

general, is much more limited than that of the DW one.

As was stated in the Introduction, the DW method is very flexible. It is not much more difficult to modify the basic assumption imposed at the outset. There are, for instance, many different choices of the distortion potential. The treatment of electron exchange can be changed depending on the excitation process considered. After applications to more ions, we would investigate the possibilities of modification of the DW method.

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[1]M. J. Seaton, Adv. At. Mol. Phys. **11**, 83 (1975).

[2]For a bibliography on electron-ion collisions, see Y. Itikawa, K. Takayanagi, and T. Iwai, At. Data Nucl. Data Tables **31**, 215 (1984).

[3]For a review of theory, see R. J. W. Henry, Phys. Rep. **68**, 1 (1981).

[4]M. D. Hershkowitz and M. J. Seaton, J. Phys. B **6**, 1176 (1973).

[5]A. K. Pradhan, D. W. Norcross, and D. G. Hummer, Phys. Rev. A **23**, 619 (1981).

[6]U. Fano and M. Inokuti, Argonne National Laboratory Report No. ANL-76-80, 1976 (unpublished).

[7]K. Smith and L. A. Morgan, Phys. Rev. **165**, 110 (1968).

[8]D. H. Madison and W. N. Shelton, Phys. Rev. A **7**, 499 (1973).

[9]W. Eissner and M. J. Seaton, J. Phys. B **5**, 2187 (1972).

[10]W. Eissner, in *Physics of Electronic and Atomic Collisions, VII ICPEAC,* edited by T. Govers and F. J. de Heer (North-Holland, Amsterdam, 1972), p. 460.

[11]J. M. Peek and J. B. Mann, Phys. Rev. A **25**, 749 (1982).

[12]A. Hibbert, Comput. Phys. Commun. **9**, 141 (1975).

[13]R. J. W. Henry, S. P. Rountree, and E. R. Smith, Comput. Phys. Commun. **23**, 233 (1981).

[14]A. Burgess and V. B. Sheorey, J. Phys. B **7**, 2403 (1974).

[15]W. L. van Wyngaarden, K. Bhadra, and R. J. W. Henry, Phys. Rev. A **20**, 1409 (1979).

[16]S. S. Tayal and A. E. Kingston, J. Phys. B **17**, 1383 (1984); A. E. Kingston and S. S. Tayal, *ibid.* **16**, 3465 (1983).

[17]H. Tatewaki, H. Taketa, and F. Sasaki, Int. J. Quantum Chem. **5**, 335 (1971).

[18]A. Hibbert, J. Phys. B **7**, 1417 (1974).

[19]Here are plotted the results of the six-state, seven-orbital *R*-matrix calculation quoted in P. L. Dufton and A. E. Kingston, Adv. At. Mol. Phys. **17**, 355 (1981). This is an improved version of the *R*-matrix calculation by K. A. Berrington, P. G. Burke, P. L. Dufton, and A. E. Kingston, J. Phys. B **10**, 1465 (1977).

[20]J. B. Mann, as quoted in A. L. Merts, J. B. Mann, W. D. Robb, and N. H. Magee, Jr., Los Alamos Scientific Laboratory Report No. LA-8267-MS, 1980 (unpublished).