Calculation of Electron-Impact $2s^2 2p^4\ ^3P \rightarrow 2p^3 3s^3 S^o$ Transition in Atomic Oxygen *

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The inelastic scattering of electron from oxygen for the $2s^2 2p^4\ ^3P \rightarrow 2p^3 3s\ ^3S^o$ transition is studied using the momentum-space coupled channel optical method at 15, 17.5, 20, 22.5, 25, 27.5, 30, 50, and 100 eV. Direct ionization cross sections, i.e. differential and integral cross sections, are reported. Important continuum states are included in the coupled channel calculation via a complex equivalent-local optical potential. The present results are compared with the available experimental data and other theoretical calculation results.

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Atomic oxygen is one of the most abundant elements in the universe. Its collisions with electron become interesting in astrophysics and aeronomy. The collisions may be the reasons for producing various emission lines of atomic oxygen that are detected in Earth's airglow and aurora as well as the far ultraviolet spectra of Venus and Mars. Therefore the accurate data of cross sections are in great need to model and to interpret these observations.

Because of the experimental difficulties of generating and handling atomic oxygen for laboratory measurements, large discrepancies exist among the published data of previous experimental work on atomic oxygen. Differential cross section (DCS) and integral cross section (ICS) for excitation of various levels in the $2s^2 2p^4\ ^3P \rightarrow 2p^3 3s\ ^3S^o$ transition, which is arguably the most important resonant transition in the O I system, have been studied using energy-loss spectroscopy by Doering and co-workers,[1−3] Kanik *et al.*[4] and Johnson *et al.*[5]

There are only a few theoretical works on the electron–oxygen system. In low energies (< 15 eV), Wu and Yuan[6] have reported theoretical calculations by using the R-matrix theory. More works have been reported in the intermediate energy region 15–100 eV. Kanik *et al.*[4] reported the theoretical calculations of DCSs, using the R-matrix approach with multi-configuration interaction target wavefunctions, including 22 LS target states in the close-coupling expansion. The standard R-matrix theory cannot include the continuum states. Tayal[7] has calculated the ICSs using the R-matrix with pseudostates approach (RMPS) theory, in which the pseudostates are included to simulate the effect of continuum target states, and the results show that the continuum states for electron-impact excitation of atomic oxygen is very important. Later, Johnson *et al.*[5] used the RMPS theory to calculate the DCSs and ICSs in the energy range 15–27.5 eV, including 18 bound states, 4 autoionizing states and 19 pseudostates in the close-coupling expansion.

In this Letter, we report a detailed calculation of DSCs and ICSs for electron scattering by atomic oxygen in 15–100 eV with the coupled channel optical (CCO) method. The momentum space CCO method we used for electron–atom scattering was developed in the 1980s using an extreme screening approximation to describe the three-body breakup process.[8,9] It has given excellent ionization cross sections for electron scattering by hydrogen.[8] The CCO method for electron scattering solves coupled integral equations for discrete channels (P space) to convergence using a coupling potential that includes an ab initio polarization part describing the real and virtual excitation of the continuum of Q space. With different specific levels, the method has broad success for atoms whose structure can be described by one or two active electrons,[10−13] but applications of this method to calculate electron scattering by a complex atom have been limited. In the present work, we use a quasi-one-dimensional electron model to treat the target of oxygen. This method significantly simplifies the scattering problem, and allows us to apply the CCO method to treat the scattering of electron from the atom with an open-shell complex structure. It is a good test of how the description of target states affects the scattering cross sections.

A detailed description of the coupled-channel optical method to study electron–atom scattering processes in momentum space can be found in Ref. [9]. Here we briefly review the essential features of the CCO method.

The coupled-channel optical calculation involves the solution of the coupled integral equations[9]

$$\langle k_i i|T|jk_j\rangle = \langle k_i i|V + V^{(Q)}|jk_j\rangle$$

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$$+\sum_{l\in P}\int d^3k\langle k_i i|V+V^{(Q)}|lk\rangle \cdot\left(E^{(+)}-\varepsilon_l-\frac{1}{2}k^2\right)^{-1}\langle kl|T|jk_j\rangle, \quad (1)$$

where

$$\langle k_i i|T|jk_j\rangle=\langle k_i i|V|\Psi_j^{(+)}(k_j)\rangle, \quad (2)$$

is the T-matrix element for the transition from the $(N+1)$-electron channel state $|jk_j\rangle$ to $|ik_i\rangle$. The ket $|\Psi_j^{(+)}\rangle$ is the formally exact solution of the $(N+1)$-electron Schrödinger equation with total energy E for entrance channel j, while ε_l is the energy of the N-electron target state $|j\rangle$. The first-order electron-target potential V includes the appropriate exchange operator. The complex polarization operator $V^{(Q)}$ is written in the Feshbach formalism as

$$V^{(Q)}=PVQ\frac{1}{(E^{(+)}-QHQ)}QVP, \quad (3)$$

where the operators P and Q project the explicitly coupled channels and the remaining channels, respectively.

The optical potential matrix elements for two-electron target atoms can be written as (in the notation of Ref. [14])

$$\langle k_i i|V^{(Q)}|jk_j\rangle=\int d^3k\sum_{l\in Q}(a_S+b_S P_r)\langle k_i i|V|\Psi_l^{(-)}(k)\rangle \cdot\left(E^{(+)}-\varepsilon_l-\frac{1}{2}k^2\right)^{-1}\langle\Psi_l^{(-)}(k)|V|jk_j\rangle. \quad (4)$$

Here $\Psi_l^{(-)}(k)$ is the three-body wavefunction for a final target state l with the appropriate boundary conditions, and P_r is the space-exchange operator. The spin coefficients a_s and b_s which depend on the total spin S are explicitly detailed in Ref. [14]. For the continuum target states l the summation is replaced by momentum integration.

In the present work, the considered Q-space only includes the continuum channels. Using the screening approximation[8] we can write the continuum polarization potential as

$$\langle k_i i|V^{(Q)}|jk_j\rangle=\int d^3k'\int d^3k\sum_{l\in Q}(a_S+b_S P_r) \cdot\langle k_i i|V|\Psi_l^{(-)}(k_<)k_>\rangle \cdot\left[E^{(+)}-\frac{1}{2}(k^2+k'^2)\right]^{-1} \cdot\langle k_>\Psi_l^{(-)}(k_<)|V|jk_j\rangle, \quad (5)$$

where $\Psi_l^{(-)}(k_<)$ is the Coulomb wave (orthogonalized to the bound state from which the electron was excited) which represents the slower electron. For computational tractability, an angular momentum projection is used to approximate the non-local optical potential and k_j is taken to be on the energy shell.[8]

The angular momentum projection of the optical potential matrix element is

$$V_{l''l'l}(K)=\sum_{m''m'}C^{l''l'l}_{m''m'm}\int d\hat{K}\langle k_i i|V^{(Q)} \cdot|jk_j\rangle i^{-l''}Y^*_{l''m''}(\hat{K}), \quad (6)$$

where $K=k_j-k_i$, the orbital angular momentum quantum numbers l', m' and l, m belong to the target states i and j respectively, and $C^{l''l'l}_{m''m'm}$ denotes the Clebsch–Gordan coefficients. For the optical potential calculation the target states are represented by the appropriate Hartree–Fock configuration. Here we assume that the spin projection of electron in excited states is $-1/2$. The set of coupled integral equations (1) is solved by following the numerical techniques as detailed by McCarthy and Stelbovics.[9]

In the present calculation, seven discrete states of oxygen are included in P space. They are $2p^4\ ^3P$, $2p^3 3s\ ^3S$, $2p^3 3p\ ^3P$, $2p^3 4s\ ^3S^o$, $2p^3 3d\ ^3D^o$, $2p^3 4p\ ^3P$, $2p^3 5s\ ^3S^o$. The optical potentials in Q space that describe the target continuum are in the couplings $2p-2p$, $2p-3s$, $2p-4p$, $2p-5s$, $2p-4s$, $3p-3p$, $3p-4s$, $3s-3s$, $4p-4p$, $4s-4s$, $2p-3p$, and $5s-5s$. In the present calculation the single configuration Hartree–Fock approximation is used to describe the target states. The orbitals of target are represented by the Slater-type orbital wavefunction.

The ionization cross section results of the present CCO method and the binary-encounter Bethe (BEB) model[15] are displayed in Fig. 1. It shows that the present result is lower than the result of BEB at energies >50 eV. The results of BEB model are total ionization cross sections containing the autoionized state, which is an important state connecting the discrete states with the continuum states, and the CCO results are direct ionization cross sections without the auto-ionized state. That may be the main source of the differences between both the methods.

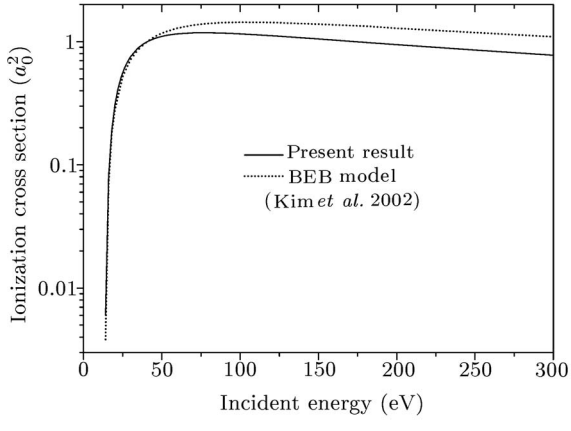


Fig. 1. Ionization cross sections for electron scattering by oxygen.

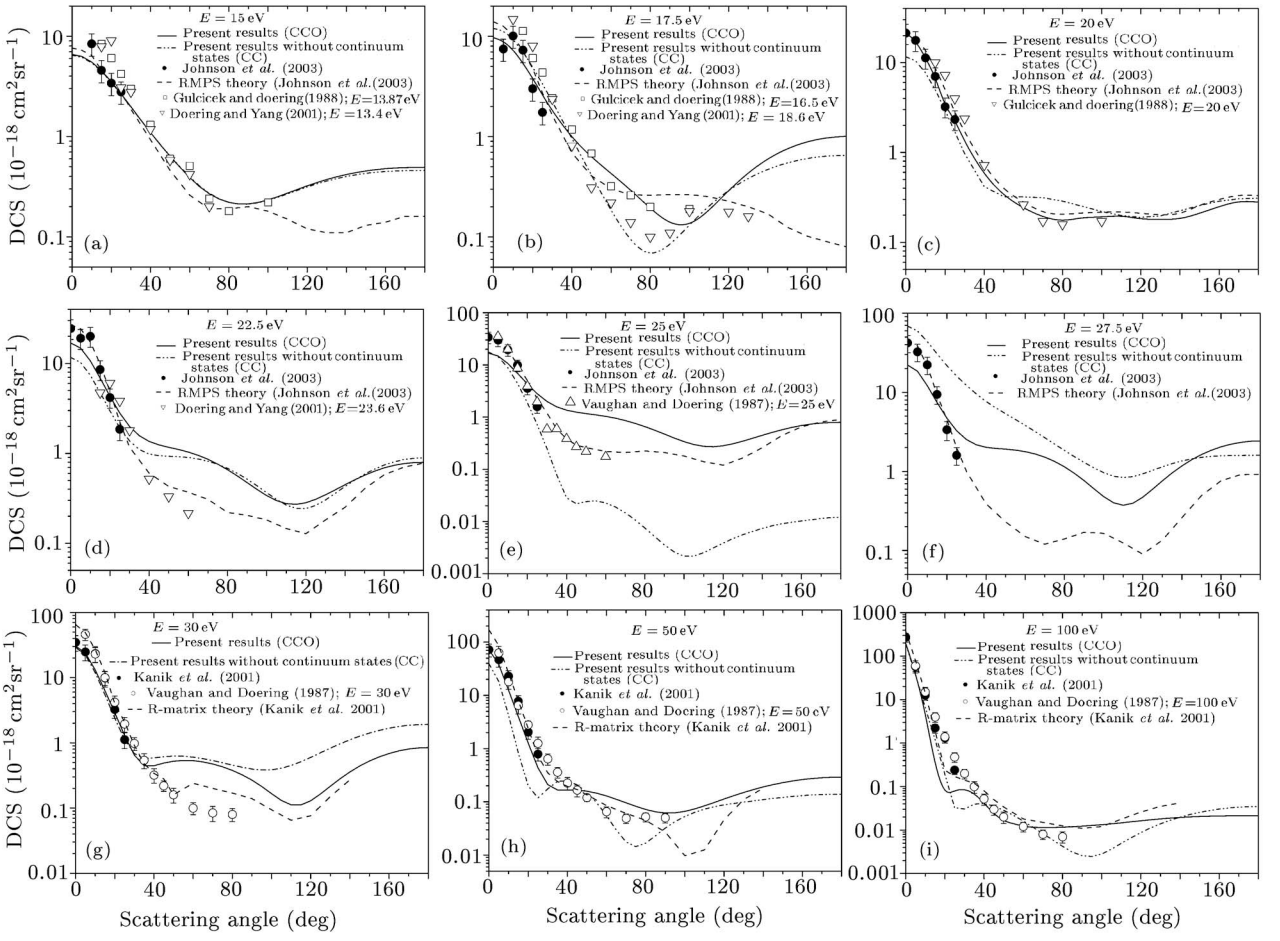


Fig. 2. DCS for electron scattering by oxygen at different energies.

The DCS calculations of $2s^2 2p^4\ ^3P \rightarrow 2p^3 3s\ ^3S^o$ transition are depicted in Figs. 2(a)–2(i) that correspond to impact energies in 15–100 eV, respectively. There are the present CCO and CC (without continuum states) results, along with the R-matrix and RMPS calculation results of Refs. [4,5], and the experimental data from Kanik and co-workers,[4,5] Doering and co-workers[1−3] in these figures. The ICS results are shown in Fig. 3, compared with the experimental data of Refs. [1–5] and the RMPS calculation results.[4,5]

It is clear from Fig. 2(a) that there is good agreement in shape between the present results and the experimental data at 15 eV impact energies. The present results agree better than the RMPS theory at scattering angles $\geq 15°$, though at small angles the present results are slightly lower than the RMPS theory. Moreover, the same trend to the experimental data is observed at middle angles (60°–120°). At this energy the CCO curve coincides with the CC curve. This indicates that the continuum states may not play a great role in the low–intermediate energy region.

In Fig. 2(b), different theoretical calculations have different results, and so do the different experimental data. The CCO results agree with the experimental data of Gulcicek and Doering[2] well at angles 40°–80°, while there is good agreement in shape between the CC results and experimental data of Doering and Yang[3] at angles 40°–100°. The RMPS curve shows similar trend with the experimental data of Doering and Yang[3] at larger angles ($> 100°$). However, it seems that more experimental data are needed at this energy because the data of Doering and coworkers[2,3] were not exactly at 17.5 eV.

Figure 2(c) shows that the CCO and RMPS curves are similar at 20 eV. Furthermore, at scattering angles larger than 5°, the RMPS results are slightly higher than the present CCO results and the experimental data. Compared to the CC curve, the CCO curve improves significantly at angles smaller than 110°.

The CCO results differ in shape from the experimental data at 22.5 eV in Fig. 2(d), while the RMPS results agree with the experimental data better. Nonetheless, they present a similar trend. The CCO results improve greatly, compared with the CC results. Then the similar situations appear at 25, 27.5, and 30 eV in Figs. 2(e), 2(f), and 2(g). In this energy region, the present CCO results are higher than both

the experimental data and the RMPS results at scattering angles larger than 20° (at angles larger than 30° in Fig. 2(g)). This may be due to the fact that the effect of discrete states is large in this energy region and only seven discrete channels in P space are not enough for describing the electron–oxygen interaction system, and the influence of autoionized states seems to be important in this energy region.

At 50 and 100 eV in Figs. 2(h) and 2(i), the present CCO results are lower than the experimental data at angles larger than 40°. However, compared with CC, the CCO results improve significantly. Furthermore, the CCO curves show a similar trend with the experimental data. They are better than the RMPS curves.

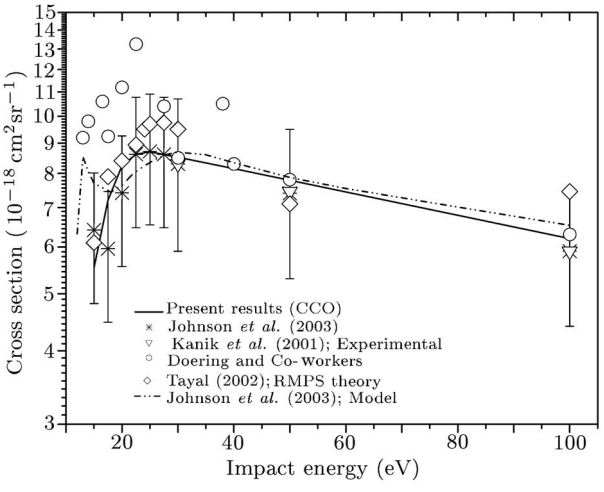


Fig. 3. ICS for electron scattering by oxygen.

As is expected, the present results with optical potentials are obviously in better agreement than the results without continuum states, which can be observed in Figs. 2(c)–2(i). This implies that the continuum states play a significant role in intermediate energies. At large scattering angles, the experimental data are scarce and we can only compare our results with the theoretical calculations.

Figure 3 shows that the present ICS results are similar to the model of Johnson *et al.*[4] at energies $\geq$ 30 eV. While in the low–intermediate energies, they present opposite outlines, and the CCO results are closer to the experimental data. Tayal's RMPS results[7] show the same trend with the present results at energies smaller than 25 eV. It seems that the present ICS results show excellent agreement.

The calculation results show that the CCO method can reproduce data that agree well with the experimental data. It is evident that the CCO method has the ability to treat electron–atom system which has an open-shell complicated structure.

The present results prove that the single configuration Hartree–Fock approximation represents the target wave state properly, which means that the configuration interact (CI) wavefunction could not play a large part in describing the electron–oxygen interaction system.

In the present calculation, the optical potential plays a significant role in intermediate energies. It is indicated that the continuum states give a great effect on the electron scattering by atomic oxygen. In low–intermediate energies the discrete channels may have a great effect. In the present calculation, autoionized states, which are proven to have an important effect in energies 22.5 to 30 eV, have been omitted. This may be the main source of differences with RMPS results.

In future work, we plan to develop a complete method that can take all channels, including autoionized states, into account.

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