Vol 16 No 1, January 2007
1009-1963/2007/16(01)/0072-05
Chinese Physics
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Elastic cross sections for electron–carbon scattering*

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(Received 28 April 2006; revised manuscript received 27 July 2006)

We used the close-coupling optical (CCO) approach to investigate the open-shell carbon atom. The elastic cross sections have been presented at the energies below 90eV, and the present CCO results have been compared with other theoretical results. We found that polarization and the continuum states have significant contributions to the elastic cross sections. The present calculations show that the CCO method is capable of calculating electron scattering from open-shell atoms.

Keywords: close-coupling optical-model method, electron–atom scattering, carbon, cross-section
PACC: 3480, 3480D

1. Introduction

The cross sections for electron-impact atomic carbon are widely used in astrophysics, atmospheric science, x-ray lasers, magnetic fusion, radiation physics, and semiconductor fabrication etc. The elastic scattering is a crucial process in the electron–carbon scattering problem. So it is not surprising that many theoretical studies of low-energy electron collisions with atomic carbon have been carried out during the past 40 years, but calculations of cross sections remain theoretical challenges. All previous elastic cross-section calculations are limited in low energies, and there are no experimental data on electron–carbon elastic scattering. The theoretical difficulties are likely due to the character of atomic carbon as an open-shell system, in which both short-range correlation and polarization effects are expected to be very important. Furthermore, about 75% of the ground-state polarizability arises from its coupling with the continuum.[1]

In 1962, Cooper and Martin[2] have computed the elastic cross sections for electron scattering from carbon in the energy range $0-15$ eV using the modified Klein–Brueckner (KB) model. Five years later, Robinson and Geltman[3] used the modified Hartree–Fock–Slater (HFS) model to calculate elastic cross section in the energy range from 0.005–0.9 Ry, then Smith, Henry and Burke[4] used the continuum Hartree–Fock (CHF) equations to calculate the elastic cross sections at the impact energy between 0 and 4 Ry. In 1970's, the polarized orbital method[5] and earlier close–coupling model (CC)[6] have been applied by Henry *et al* to calculate the differential cross-sections of the $2s^22p^2$ electronic configuration by electron impact and the elastic cross sections at low energies, and Thomas *et al* calculated the elastic cross sections using the matrix variational method in single configuration (SC) approximation and near-degenerate configuration interaction (CI) approximation.[7,8] However, all the above calculations of elastic cross sections were limited in low-energy impact region.

In the low-energy impact region, the velocity of the incident electrons is of the same order of or less than the velocity of the electrons in the target, which take an active part in the collision. The intermediate-energy region from the ionization threshold extends up to the energy where the velocity of the incident electron is typically about four times the velocity of the active target electrons, which is the region most difficult to treat theoretically since an infinite number of target states can be excited and ionizing collisions are possible. Studies of electron–atom scattering at intermediate energies need developments in the methods for investigation.

To date, only the coupled-channel optical method (CCO) of McCarthy *et al*[9−11] the intermediate- energy R-matrix (IERM) method of Scott *et al*[12] the B-spline R-matrix method of Zatsarinny *et al.*[13] and the convergence of the close–coupling (CCC) method of Bray and Stelbovics[14] could treat the continuum

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states. However, the improved R-matrix methods and the CCC method can treat the effect of continuum channels by using pseudo-states in the close–coupling expansion. The purpose of pseudo-states is to mimic the effects of continuum channels, but it has some limitations. For example, the results of the pseudo-state method have to depend on the number and angular momentum of pseudo-states, and pseudo-resonances can exist.

The CCO method[9] treated the continuum states via an *ab initio* complex-polarization potential, in which P space consists of a finite set of discrete physical channels, and Q space consists of the remaining channels including continuum. It has broad success for a number of atoms whose structure can be described by one or two active electrons, for example hydrogen, alkali-metal atoms, helium, and magnesium etc.[15−18] In this paper, we extend this method to calculate the elastic cross sections of electron scattering by atomic carbon, and compare the present results with other theoretical and experimental results. We hope that the present theoretical investigation will encourage new experimental and theoretical work.

2. Theoretical details

The momentum space CCO method is an *ab initio* approach to electron–atom scattering, which can be found in Refs.[9]–[11] for details. Here we briefly review the essential features of the CCO method.

The coupled-channels optical calculation involves the solution of the CCO equations:

$$\langle \boldsymbol{k}_r, \phi_i | T | \phi_j, \boldsymbol{k}_j \rangle = \langle \boldsymbol{k}_r, \phi_i | v_1 + v_3' + V^{(Q)} | \phi_j, \boldsymbol{k}_j \rangle + \sum_{l \in P} \int \mathrm{d}^3 k_{r'} \langle \boldsymbol{k}_r, \phi_i | v_1 + v_3' + V^{(Q)} | \phi_l, \boldsymbol{k}_{r'} \rangle \times \frac{1}{E^+ - \varepsilon_l - \frac{1}{2} k_{r'}^2} \langle \boldsymbol{k}_{r'}, \phi_l | T | \phi_j, \boldsymbol{k}_j \rangle, \tag{1}$$

$$\langle \boldsymbol{k}_r, \phi_i | T | \phi_j, \boldsymbol{k}_j \rangle = \langle \boldsymbol{k}_r, \phi_i | V | \phi_j, \mu_j^+(\boldsymbol{k}_j) \rangle. \tag{2}$$

Here the space of target states has been divided into two parts. The P space consists of all the discrete states $|i\rangle$, including the ground state $|0\rangle$. The Q space is the continuum. Sufficient states in P-space are included for convergence in the total cross section.

The differential cross section for scattering from channel j to channel i at an angle θ is

$$\frac{\mathrm{d}\sigma_{ij}}{\mathrm{d}\Omega} = (2\pi)^4 \frac{k_i}{k_j} \frac{\hat{S}^2}{\boldsymbol{l}^2} \sum_{m,m'} |\langle \boldsymbol{k}_i; n', l', m' | T | n, l, m; \boldsymbol{k}_j \rangle|^2 ,$$

$$\langle \boldsymbol{k}_i; n', l', m' | T | n, l, m; \boldsymbol{k}_j \rangle = \sum_{L, L', J} (4\pi)^{-1} \hat{L}' \hat{L} \left[\frac{(L' - |M'|)!}{(L' + |M'|)!} \right]^{1/2} \Theta(M') C_{L' l' J}^{M' m' m} C_{LlJ}^{0mm} T_{nLl}^{n' L' l' (J)} P_L^{|M'|}(x),$$

$$\Theta(M') = 1, M' < 0, \qquad \Theta(M') = (-1)^{M'}, \quad M' \geq 0 . \tag{3}$$

The corresponding total cross section is

$$\sigma_{ij} = (2\pi)^4 \frac{k_i}{k_j} \frac{\hat{S}^2}{\hat{l}^2} \frac{1}{4\pi} \sum_{LL'J} (2J+1) |T_{nLl}^{n' L' l' (J)}|^2 . \tag{4}$$

The complex polarization operator $V^{(Q)}$ is written in the Feshbach formalism as

$$V^{(Q)} = PVQ \frac{1}{(E^+ - QHQ)} QVP, \tag{5}$$

$$\langle \boldsymbol{k}_r, \phi_i | V^{(Q)} | \phi_j, \boldsymbol{k}_j \rangle = \int \mathrm{d}^3 k_{r'} \sum_{l \in Q} (a_s + b_s P_r) \langle \boldsymbol{k}_r, \phi_i | v_1 + v_3' | \phi_l, \boldsymbol{k}_{r'} \rangle \frac{1}{E^+ - \varepsilon_l - \frac{1}{2} k_{r'}^2} \langle \boldsymbol{k}_{r'}, \phi_l | v_1 + v_3' | \phi_j, \boldsymbol{k}_j \rangle, \tag{6a}$$

$$a_S = \frac{1}{2} [(1+s')(1+s)]^{1/2} \sum_{N' N n' n n_\alpha n_\beta} \begin{bmatrix} \frac{1}{2} & s' & S(5) \\ N' & n' & N_s \end{bmatrix} \begin{bmatrix} \frac{1}{2} & s & S \\ N' & n & N_s \end{bmatrix} \langle n_\alpha | n_\beta \rangle \langle N' | N \rangle, \tag{6b}$$

$$b_s = \frac{1}{2}[(1+s')(1+s)]^{1/2} \sum_{N'Nn'nn_\alpha n_\beta} \begin{bmatrix} \frac{1}{2} & s' & S \\ N' & n' & N_s \end{bmatrix} \begin{bmatrix} \frac{1}{2} & s & S \\ N' & n & N_s \end{bmatrix} \langle n_\alpha|N\rangle\langle N'|Nn_\beta\rangle. \tag{6c}$$

Here a_s and b_s which depend on the total spin S were explicitly given in Ref.[9].

$$\langle \boldsymbol{k}_r, \phi_i|V^{(Q)}|\phi_j, \boldsymbol{k}_j\rangle = \int \mathrm{d}^3k_{r'} \int \mathrm{d}^3k_{r''} \sum_{l\in Q} (a_s + b_s P_r)\langle \boldsymbol{k}_r, \phi_i|v_1 + v_3'|\chi^{(-)}(\boldsymbol{k}_<)\boldsymbol{k}_>\rangle$$
$$\times \frac{1}{E^+ - \frac{1}{2}(k_{r'}^2 + k_{r''}^2)} \langle \boldsymbol{k}_>\chi^{(-)}(\boldsymbol{k}_<)|v_1 + v_3'|\phi_j, \boldsymbol{k}_j\rangle. \tag{7}$$

$\chi^{(-)}(\boldsymbol{k}_<)$ is a time-reversed Coulomb wave which is orthogonal to ϕ_i; $\boldsymbol{k}_>$ and $\boldsymbol{k}_<$ are the greater and lesser absolute momenta of the outgoing particles.

3. Results and discussions

In this paper, twelve states of atomic carbon are included in P space. They are $(2s^22p^2)^3P_0$, $(2p3s)^3P_1$, $(2p3p)^3D$, $(2p3d)^1D$, $(2p4s)^1P$, $(2p4p)^3D$, $(2p4d)^1D$, $(2p5s)^1P$, $(2p5p)^1P$, $(2p5d)^1D$, $(2p6s)^1P$ and $(2p7s)^1P$. These states are described by the single configuration Hartree–Fock approximation. The orbitals of the target are presented by the Slater-type orbital wavefunctions. For finding out the effect of continuum on elastic cross sections, we calculate with CC12 and CCO12 methods. In the CC12 model, no continuum optical potentials are included in the calculation. The CCO12 model has its continuum optical potentials in Q space, which describe the target continuum in the $^3P_0$—$^3P_0$, $^3P_0$—$^3P_1$ and $^3P_1$—$^3P_1$ couplings.

A preliminary check of the validity of the method for a particular target is to test the ability of the continuum optical potential in reproducing the ionization cross sections. Thus, we calculate the ionization cross sections in the energy region from threshold up to 200 eV, and compare them with other theoretical and experimental results.[19−21] (see Fig.1)

In Fig.1, the present results are lower than the results obtained by using the binary encounter Bethe (BEB) model in which the autoionization contributions were included and also were lower than the experimental results; and they are much lower than those obtained by using the distorted-wave model at intermediate and high energy regions, but higher than those at lower energy region. Because the experimental results include the autoionization contributions, the distorted-wave results would include the ionization from inner-shell. The present results are closer to the direct ionization cross sections obtained by using the BEB model. Therefore, these disagreements emerge because the present calculations have omitted the ionization from metastable and inner-shell, as well as the excitation–autoionization states.

When the energy increases above 180 eV, the present result becomes closer to the experimental and other theoretical results. From the comparisons, we can conclude that the effects of excitation–autoionization become weak as the impact energy increases.

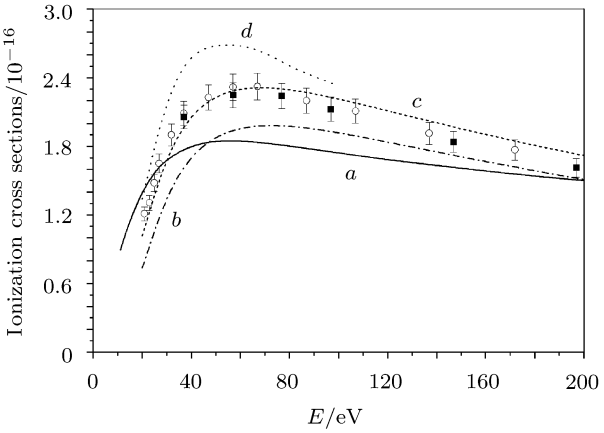


Fig.1. Ionization cross sections of the carbon atom as functions of incident electron energy E. Solid curve a: present CCO12 calculations. Dot-dashed curve b and short dashed curve c: Kim and Deschaun.[19] Dotted curve d: Pindzola *et al.*[20] Open circles and solid squares: experimental data by Brook *et al.*[21]

The difference still exists between present results and the direct results of BEB model. It is probably due to the weak–coupling and equivalent-local approximations used in the present calculations, which are the main error sources of the CCO12 method. It is shown that the optical potential is capable of cal-

culating the continuum states for open-shell carbon atoms.

The present results obtained by using the CCO12 method and CC12 method are presented in Fig.2, along with other theoretical results, at collision energies ranging from 4 to 90 eV.

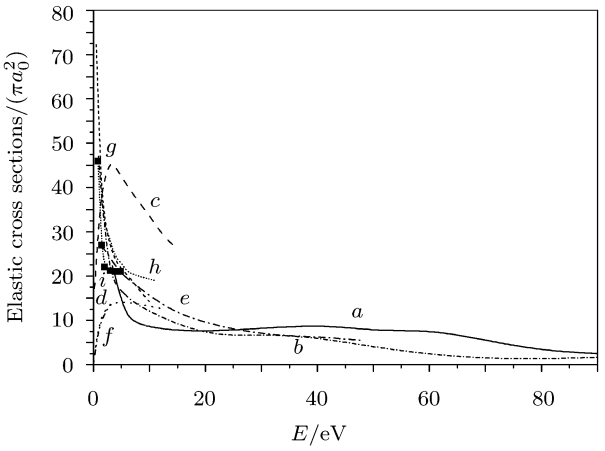


Fig.2. Elastic cross sections of the carbon atom as functions of the incident electron energy E. Solid curve a: present result (CCO12). Short dash-dotted curve b: present result (CC12). Dashed curve c: the KB results from Ref.[2]. Dotted curve d: the results obtained by HFS model from Ref.[3]. Dot-dashed curve e: the results obtained by continuum HF equations from Ref.[4]. Dash-double-dotted curve f: the results obtained by polarized-orbital model from Ref.[5]. Short Dashed curve g: the early CC results from Ref.[6]. Chain curve h and solid square-Dotted curve i: the results obtained by matrix variational method in SC and CI approximations from Ref.[7].

From Fig.2, we find that all results agree well in shape except the results obtained by KB and polarized-orbital models; however the discrepancies in magnitude exist among all these calculations. The value of the elastic cross section obtained by the CCO12 method is only half of the value obtained by the calculations of the KB model, and about 20% lower than the results of polarized-orbital calculations at energies below 6 eV. The main discrepancies of the calculated cross sections reflect the different descriptions in the target continuum in different theoretical models. No continuum states are included in all other methods, while the CCO12 method includes the continuum state via optical potential in the calculations. The optical potential includes two parts, the real potential describing virtual excitations of discrete and ionized states, and the imaginary part describing real excitations of these states.

The matrix variational method in the CI approximation includes only partially the effect of polarization at the level of Bethe–Goldstone continuum equations, and the matrix variational method in the SC approximation neglects the important polarization. Comparing the matrix variational calculations, we could find that full inclusion of polarization effects would move the curves downward in the low-energy region significantly.

The present results of CC12 method are closer to the results of the CHF method and the matrix variational method in the CI approximation, and all these methods have not included the continuum states and polarization effects. Comparing the results of CC12 and CCO12 methods, we find that the transitions of continuum made significant contributions to the polarizability of the target, and the effect of polarization reduces the elastic cross section at low energies significantly. As the impact energy increases above the ionization threshold, the result of CCO12 calculation becomes higher than the result of CC12 calculation and other theoretical calculation results. This shows that the continuum contributions will enhance the elastic cross sections at impact energies above ionization threshold.

4. Conclusions

In this paper, the elastic cross sections for electron–carbon collision have been calculated at energies below 90 eV, and we find that polarization and continuum states have significant contributions to elastic cross sections.

In summary, the present results show that the CCO method is a valid method for calculating elastic cross sections of electron scattering from open-shell atoms. Furthermore, it is highly desired to carry out experimental and additional theoretical studies in order to establish reliable electron scattering data for atomic carbon.

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