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Role of Exchange for Large Δl Excitation of Ions by Electrons

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Abstract

The role of exchange for excitation cross sections of ions by electron impact when the target electron undergoes a large change of the orbital momentum is considered. The scattering amplitudes and the cross sections are calculated in Coulomb-Born approximation with the exchange taken into account (CBE) and without it (CB). To take into account the exchange between the incident and target electrons, the orthogonalized wave-function method [1] is used. To study the influence of the channel interaction on the considered effect, the K-matrix method [2] is applied. It is shown that for the transitions with a large change of the orbital momentum, the exchange part of the cross section is larger than the direct one from several times up to an order of magnitude.

Keywords:

excitation cross section, exchange, Coulomb-Born approximation, K-matrix method

1. Introduction

Excitation cross sections of atoms and ions by electron impact decrease rapidly with an increase of Δl, where Δl is the change of the orbital angular momentum quantum number of the target electron. For example, the threshold cross sections for $1s - 4l$ transitions in He^+ ion without exchange are

l	4s	4p	4d	4f	
σ	3.1	9.9	0.94	0.02	(in units of $100\,\pi a_0^2$)

This decrease is caused by the small value of the matrix element of the $(r_</r_>)^{\kappa+1}$ operator, where κ is multipolarity.

The role of exchange increases drastically with the increase of Δl. This effect results from the fact that the direct part of the transition amplitude ($\kappa = \Delta l$) decreases more rapidly than the exchange part which includes small $\kappa'' \neq \Delta l$ (see below). For $\Delta l = 3$, the exchange amplitude becomes much larger than the direct one. In the present work the effect is considered in the first order using the Coulomb-Born approximation.

2. Coulomb-Born approximation

Excitation cross section for transition $a_0 - a_1$ in Coulomb-Born approximation are written as [1]

$$\sigma(a_0 - a_1) = \sum_{\kappa}\Big[Q'_\kappa(a_0 - a_1)\sigma'_\kappa(n_0l_0 - n_1l_1) + Q''_\kappa(a_0 - a_1)\sigma''_\kappa(n_0l_0 - n_1l_1)\Big], \quad (1)$$

where a_0 and a_1 are the sets of quantum numbers of the initial and final states, n_0l_0 and n_1l_1 are the principal and orbital quantum numbers of the target electron in the initial and final states, σ'_κ and σ''_κ are the radial parts which correspond to one-electron cross sections with multipolarity κ. σ''_κ is the exchange part and is given by

$$\sigma''_\kappa = \sum_{\lambda_0\lambda_1}\sigma''_\kappa(\lambda_0\lambda_1) = \frac{4A_0}{\varepsilon(2\kappa+1)}\sum_{\lambda_0\lambda_1}(R''_{\kappa\kappa''})^2D^{-1},$$
$$\kappa'' = |\lambda_1 - l_0| \quad (2)$$

and σ'_κ includes the direct and mixed parts:

$$\sigma'_\kappa = \sum_{\lambda_0\lambda_1}\sigma'_\kappa(\lambda_0\lambda_1) = \frac{4A_0}{\varepsilon(2\kappa+1)}\sum_{\lambda_0\lambda_1}R_\kappa{}^d(R_\kappa{}^d - R''_{\kappa\kappa''})D^{-1}, \quad (3)$$

where λ_0 and λ_1 are the orbital angular momentum of the incident and scattered electron, ε is the energy of the incident electron, $R_\kappa{}^d$ and R''_κ are the direct and exchange radial integrals, D is the normalization factor and $A_0 = 1$ for the H-like ions. Angular factors Q'_κ and Q''_κ describe the dependence on all angular quantum numbers. They are purely kinematic, i.e. they are independent of the principal quantum numbers and the real interaction of the target and incident electrons. Multipolarity κ takes on all values from $|l_1 - l_0|$ to $l_1 + l_0$. For σ'_κ all κ are of the same parity. In the present work we consider $s - l_1$ transitions for which $\kappa = l_1$.

The excitation cross sections were calculated in the Coulomb-Born approximation with account for the exchange (CBE) and without it (CB). To take into account

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the exchange the orthogonalized function method [1] was used. Partial wave functions of the incident (scattered) electron and the target ion in the initial (final) states are orthogonalized. In fact, only the waves with orbital angular momentum $\lambda_1 = l_0$ and $\lambda_0 = l_1$ are to be orthogonalized, since for $\lambda \neq l$ this condition is fulfilled automatically. In order to take into account the channel interaction the excitation cross sections were also calculated by the K-matrix method [2] with (KE) and without exchange (K).

3. Calculation results and discussion

The results of the present calculations for the transitions $1s - 4l_1$ (l_1 = s, p, d, f) in the C VI ion are presented in Fig. 1 and Fig. 2. For comparison, the data obtained by the Convergent Close-Coupling method (CCC) [3] are also plotted. The energy is in scaled units $(E - E_{01})/Z^2$ Ry and the cross section is in units of $\pi a_0{}^2/Z^4$, where E_{01} is the threshold energy and Z is the spectroscopic symbol.

The excitation cross sections for 1s – 4s and 1s – 4p transitions are shown in Fig. 1. For these transitions the direct amplitudes give the main contribution to the cross sections and the account for the exchange does not change the cross sections qualitatively. This is a standard situation.

Fig. 2 shows the cross sections of excitation with a large change of the orbital angular momentum of the target electron: $\Delta l = 2$ (1s – 4d) and $\Delta l = 3$ (1s – 4f). In this case, the account for the exchange changes the cross sections drastically. The exchange part of the cross section is larger than the direct one from several times up to an order of magnitude. This difference is caused by the different value of α in the $(r_</r_>)^{\alpha+1}$ operator: $\alpha = \kappa$, $\kappa = \Delta l$ for the direct radial integral $R_\kappa{}^d$ and $\alpha = \kappa''$, $\kappa'' = |l_1 - \lambda_0|$ for the exchange radial integral R''_κ. Good agreement with the CCC data may be explained by the fact that the channel interaction for the transitions with large Δl is less important than for the transitions 1s – 4s and 1s – 4p (Fig. 1).

The present results show that the calculation of the excitation cross sections with large Δl without taking into account the exchange will give unreasonable results.

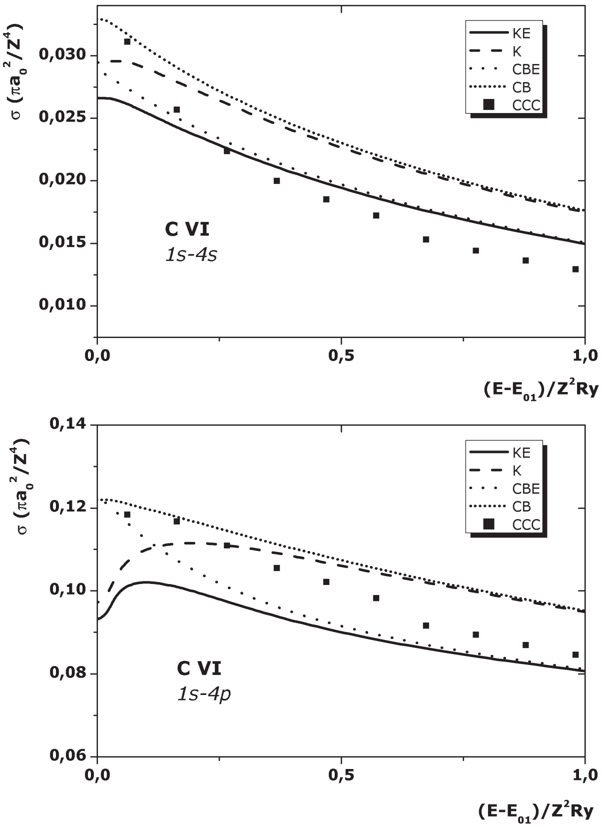

Fig. 1

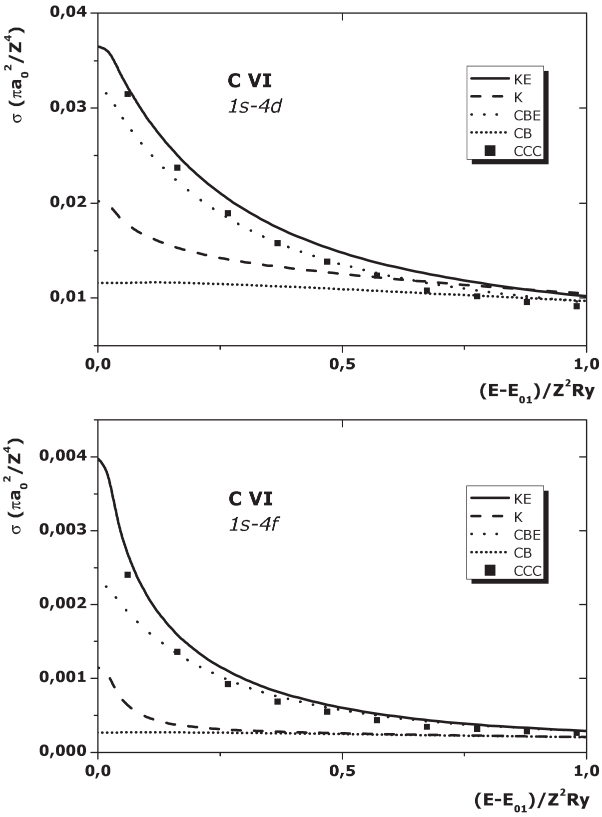

Fig. 2

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