Differential Cross Sections Parmeters of D States of Ca & Sr Atoms

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Abstract
The present paper carries out Relativistic Distorted Wave (RDW) and Non-Relativistic Distorted wave (DW) calculations for electron impact excitation of n ^{1}D state of calcium (n=4) and strontium (n=5) from ground n^{1}S state. Differential Cross Section (DCS) results are presented at incident electron energies 17.5 eV and 37.5 eV respectively. Good agreement is found comparison of both relativistic and non-relativistic distorted wave methods with each other and the importance of relativistic effects is also explored.

Keywords: Relativistic Distorted Wave, Non-Relativistic Distorted Wave, Differential Cross Section, Relativistic Effects.

1. Introduction

Most of the earlier studies on electron impact excitation of atoms have been confined to S-S and S-P transitions [1-5]. The excitation of the D states of atoms is of increasing interest. The study of D state excitation is confined to simpler form like helium [6, 7]. The DCS of relativistic and non-relativistic calculations of S-D excitation of Ca and Sr atoms give good results at incident energies of 17.5 eV and 37.5 eV respectively and behavior of the curve shows a good result for the same incident energies. The present study considers these excitations which show good calculation for the DCS. The comparison thus provides the importance of relativistic effects.

2. Theoretical Considerations

2.1. T-matrix in DW Approximation

Alkaline earth atoms (viz. Ca and Sr) are treated as two electron systems and the effect of core electrons is incorporated in the form of a core potential. The transition matrix for the electron impact excitation of alkaline earth atoms from its initial state i to a final magnetic sub-state f_M in the non-Relativistic Distorted Wave approximation (DW) can be written as:

$$T_{if_M} = \left\langle \chi^-_{f_M} \left| V - U_f \right| A\chi^+_i \right\rangle \quad (1)$$

Where A is the anti-symmetrization operator which takes into account the electron exchange effect between projectile and target electrons, V is the total interaction potential between the target alkaline earth atom and the projectile electron is expressed by (atomic units are used throughout)

$$V = -\frac{2}{r_3} + \frac{1}{|\mathbf{r_2} - \mathbf{r_3}|} + \frac{1}{|\mathbf{r_1} - \mathbf{r_3}|} + V^{core}(r_3) \tag{2}$$

Here $\mathbf{r_1}$, $\mathbf{r_2}$ and $\mathbf{r_3}$ are respectively, the position co-ordinates of the target valence electrons and the projectile electron with respect to the target nucleus. Further, the core potential, V^{core}, of the alkaline earth atom is given by

$$V^{core} = \sum_{n=1}^{j} N_{nl} \int \frac{|R_{nl}(r)|^2 r^2 dr}{r_>} \tag{3}$$

Where j = 3 and 4 respectively for Ca and Sr atoms, N_{nl} represents the occupation number of the electrons in different orbital's referred to by n and l quantum numbers and R_{nl} is the corresponding radial wave functions.

$\chi_i^+ (\chi_{f_M}^-)$ is the combined wave function of the distorted wave projectile electron and target state of alkaline atoms in the initial (final) channel. It is defined as

$$\chi_{i(f_M)}^{+(-)} = F^{+(-)}(\mathbf{k}_{i(f)}, \mathbf{r_3}) \Psi_{i(f_M)}(\mathbf{r_1}, \mathbf{r_2}) S_{i(f)}(1,2,3) \tag{4}$$

Where $\psi_{i(f_M)}$ is the initial (final) state wave function of the target alkaline atom and $S_{i(f)}(1, 2, 3)$ is the initial (final) state spin function for the composite system consisting of the incident projectile and the target. $F_{i(f)}^{+(-)}$ represents the initial (final) channel projectile distorted wave with the wave vector $\mathbf{k_i}(\mathbf{k_f})$ and the associated superscript +(-) indicates the usual outgoing (incoming) wave boundary condition. The distorted waves are the solution of

$$[\nabla_3^2 + \mathbf{k}_{\mathbf{i(f)}}^2 - 2U_{i(f)}(\mathbf{r_3})] F^{+(-)}(\mathbf{k_{i(f)}}, \mathbf{r_3}) = 0 \tag{5}$$

Here $U_{i(f)}$ [8, 9] is the distorted potential in the initial (final) channel.

Further, on substituting the expressions for χ_i^+ and $\chi_{f_M}^-$ from above equations into the expression of the T-matrix, we get

$$\begin{aligned} T_{if_M} = &\left\langle F^-(\mathbf{k_f}, \mathbf{r_3}) \psi_{f_M}(\mathbf{r_1}, \mathbf{r_2}) S_f(1,2;3) \middle| V - U_f \middle| F^+(\mathbf{k_i}, \mathbf{r_3}) \psi_i(\mathbf{r_1}, \mathbf{r_2}) S_i(1,2;3) \right\rangle \\ &- \left\langle F^-(\mathbf{k_f}, \mathbf{r_3}) \psi_{f_M}(\mathbf{r_1}, \mathbf{r_2}) S_f(1,2;3) \middle| V - U_f \middle| F^+(\mathbf{k_i}, \mathbf{r_1}) \psi_i(\mathbf{r_3}, \mathbf{r_2}) S_i(3,2;1) \right\rangle \end{aligned} \tag{6}$$

Further, the scattering amplitude a_M in the 'collision reference frame' for the electron impact excitation of the atom from an initial state i to a final magnetic sub state f_M is related to the DWA transition matrix element T_{if_M} by

$$a_M = -\left(\frac{1}{2\pi}\right) T_{if_M} \tag{7}$$

The expression for the T-matrix equation can be simplified further for a specific transition by carrying out the integration over the spin co-ordinates. DCS can be calculated. The excitation is to the ground n ^{1}S state to excited n$'$ ^{1}D, i.e., singlet to singlet (SS) transition in Ca (n=4, n$'$=4, 5) and Sr (n=5, n$'$=5, 6).

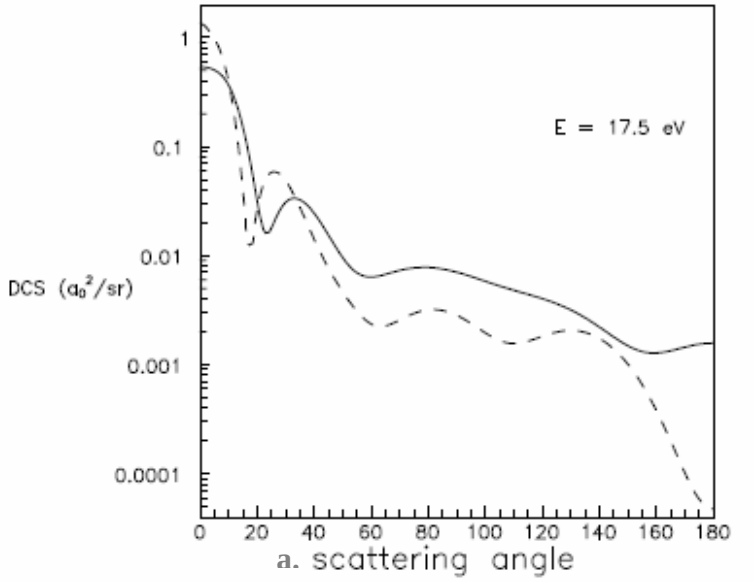
2.2. T-matrix in RDW Approximation

Similarly, in order to evaluate the relativistic T-matrix, we require the wave function for target atom in its initial and final states. The Dirac Wave Function has been used to represent bound states of the atoms. The details of these calculations for atoms having two valence electrons are given [10]. DCS can be calculated.

3. Results and Discussion

The comparison of the two types of calculations- Distorted and Non-Relativistic Calculations shows the results of the differential cross-sections of DW and RDW of S- D excitations of Ca and Sr atoms at 17.5 and 37.5 eV in Figures 1 and 2 and provides the importance of relativistic effects.

Figure 1 Differential Cross Section in atomic units for the excitation of the 4^{1}D State of Calcium atom by electron impact at 17.5 and 37.5 eV. ___ DW; ----- RDW.



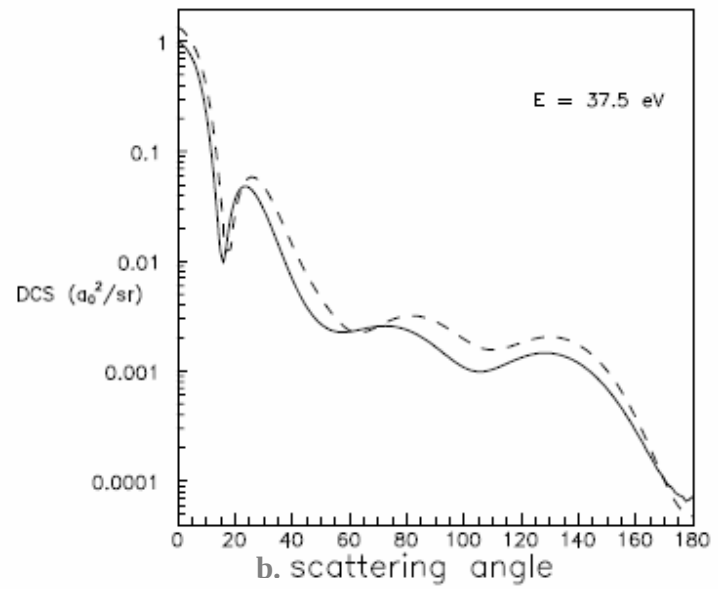
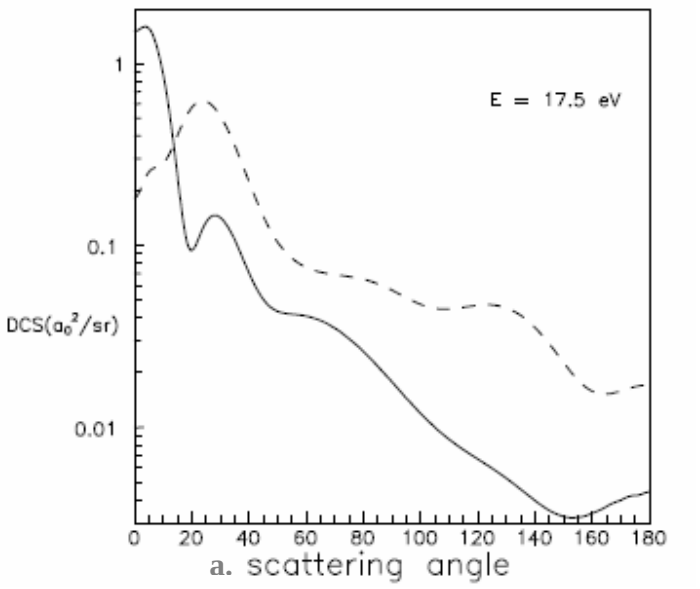
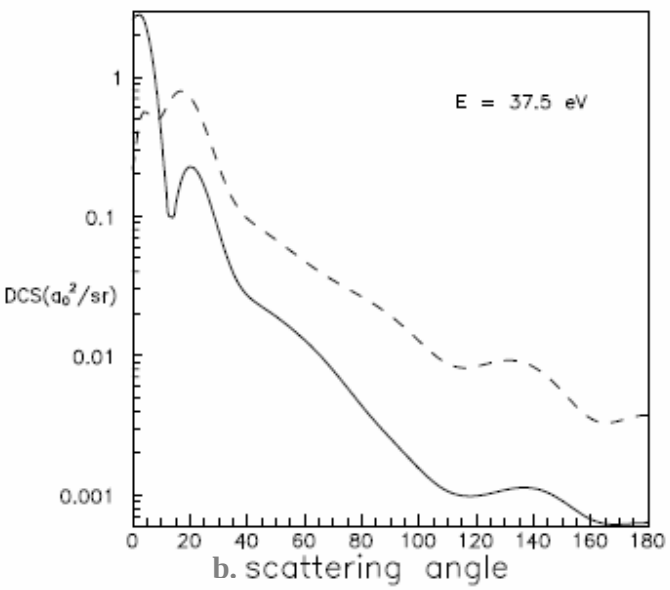


Figure 2 Differential Cross Section in atomic units for the excitation of the 5^1D state of strontium atom by electron impact at 17.5 and 37.5 eV . ___ DW; ----- RDW.





4. Conclusions

This paper has presented the DW and RDW calculations of the DCS parameter of S-D excitation for the alkaline atoms (Ca and Sr atoms). The nature of the curve show good behavior at different incident energies. The result of the DW and RDW calculations for the DCS suggests the importance of relativistic effect. It would be interesting to have the experimental confirmation of these results.

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