A THEORETICAL CALCULATION FOR TOTAL CROSS SECTION PARAMETER OF BA ATOM

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Abstract

The work presented in this paper is focused on the theoretical study of electron-impact excitation (S-D) of Ba atom. The work addresses to the intermediate (10-200eV) incident electron energy region, where the distorted wave approximation theory is expected to work well.Results are reported in terms of total cross sectionparameter(TCS)at 35 and 65 eV.

Key Words: electron-impact excitation, Ba atom,distorted wave approximation theory, total cross section parameter(TCS)

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1-Introduction

Electron impact excitation of atoms has been the most extensively studied subject in the field of atomic collisions. Since the early days of modern physics it has greatly added to the understanding of atomic structure and the development of quantum mechanics. Such a study has numerous applications in many related fields of science and technology viz. condensed matter physics, space science, astrophysics, atmospheric physics, fusion research, laser development, gaseous discharge and plasma physics.

In the field of atomic collisions, the subject of electron-atom scattering has received the maximum attention. It is still of great interest and currently is a very rapidly expanding field in both the theoretical and experimental domains [1,2,3,4,6,7,11,12]. There has been considerable interest and progress in the recent years for both theoretically and experimentally in the study of electron impact excitation of atoms. The progress in this area can be attributed to the development in the quality of experimental technology which led several sophisticated atomic physics experiments. New type of atomic physics experiments are currently being performed in various laboratories and these are very different from the usual cross section measurements [5,8,10,13,14,16].

In this paper be we have theoretically calculated the total cross section parameter of Ba atom at 35 and 55eV with the help of both DW and RDW methods.

2-Formalism

2.1-.Distorted Wave Approximation Theory : Consider electrons having energy 'E_i' incident on an atom (with nuclear charge 'Z' and N electrons) in ground state, denoted by 'a'. As a result of collision, electrons excite the target to a higher state, denoted by 'b' and they scattered with energy 'E_b'.

Than the T-matrix for the electron-impact excitation of an atom from initial state i to final state f in distorted wave approximation can be written as.

$$T_{if}^{DW} = \left\langle \chi_f^-(1,2,\ldots..,N+1)\,|V-U_f(N+1)|\,\chi_i^+(1,2,\ldots..,N+1)\right\rangle \qquad (1)$$

where V is the target-projectile interaction given by

$$V = -\frac{Z}{r_{N+1}} + \sum_{j=1}^{N}\frac{1}{|r_j - r_{N+1}|} \qquad (2)$$

Where r_j = (j=1, 2, …. N) is the position cordinate of the target electrons and r_{n+1} is the projectile electron with respect to the nucleus of the atom.

U_f is the distertion potential which is taken to be a function of radial cordinates of the projectile electrons only.

The wave function $X_{if}^{+(-)}$ is the combined wave function of the target atomic wave function ϕ_{if} and the projectile electron distorted wave function $f_{i(f)}^{DW+(-)}$

$$\chi_{if}^{+(-)}(1,2,....., N+1) = A\Phi_{if}(1,2,....., N)\ F_{if}^{DW+(-)}(k_{i(f)}, N+1) \qquad (3)$$

$k_{i(f)}$ is the projectile electron and scattered electron wave vector after the excitation process. A is the antisymmetrization operator which takes into account the effect of electron exchange between projectile and target atom electrons.

2.2- Non-Relativistic Distorted wave Approximation Theory : In the non-relativistic distorted wave (DW) method the target is described by Hartree-Fock wave functions which is obtained by Fisher code [9] and distorted wave projectile electron wave function are obtained by solving Schrodinger wave equation.

2.3- Relativistic Distorted wave Approximation Theory : In the relativistic distorted wave (RDW) method, the target atom is represented by multi-configuration Dirac-Fock wave functions which is obtained by using Graphs 92 program of Prapia [15] and the projectile wave function are obtained by Dirac equations.

3-Calculation for TCS : The excitation of an atom from the state i having initial orbital angular momentum L_i to the final f having orbital angular momentum L_f by impact of electrons having momentum K_i can be theoretically described by scattering amplitudes is given by

$$f(L_f, M_{L_f}, k_f; L_i, M_{L_i}, k_i) = (2\pi)^2 \left(\frac{k_f}{k_i}\right)^{1/2} T_{i\to f}(L_f, M_{L_f}, k_f; L_i, M_{L_i}, k_i) \qquad (4)$$

Where, k_f is the momentum of the scattered electron.are the Z-Compared of the orbital angular momentum L_i and L_f respectively. M_{L_i}, M_{L_f}

Here the normalization of the scattering amplitude has been done according to the convention that its square modulus gives DCS

$$\sigma(L_f, M_{L_f}; L, M_{L_i}) = (f)^2 \tag{5}$$

From (4) and (5)

$$\sum \sigma = (2\pi)^4 \frac{k_f}{k_i} (T_{i\to f})^2 \tag{6}$$

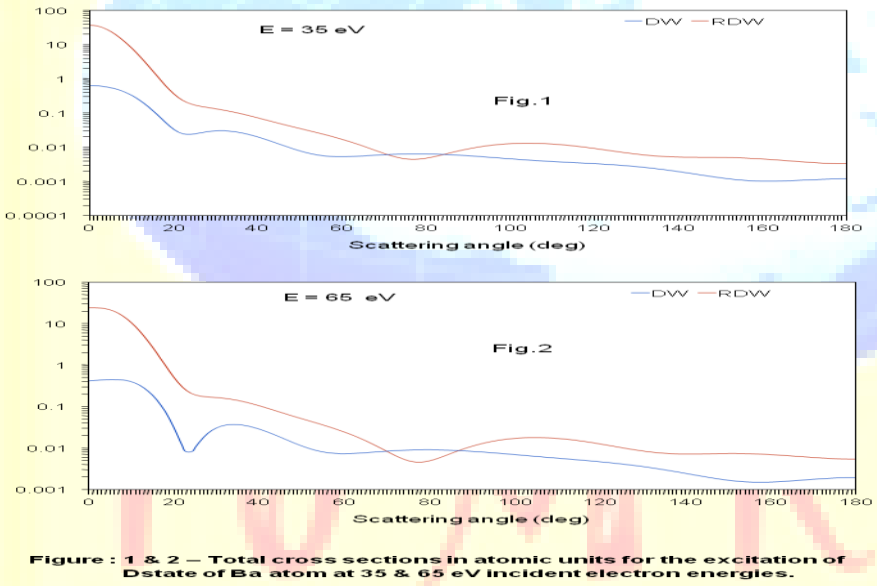

Figure : 1 & 2 – Total cross sections in atomic units for the excitation of Dstate of Ba atom at 35 & 65 eV incident electron energies.

Figure :1

4. Result and Discussion:

Here we have carried out the calculations for total cross section parameter for the excitation of Ba atom from ground state 6^1 S to the excited state 6^1 D state by the electron impact at 35 and 65eV.We do not have any other theoretical or experimental data to compare with our calculations. We therefore compare the two types of calculations using DW and RDW. We find that both DW and RDW calculations agree qualitatively andquantatively in reasonable manners at these energy level.

Conclutions: From overall work presented in the paper, we believe that our present results would be helpful in guiding the future experimental measurements and more theoretical calculations.

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