

Elastic Scattering of Electron by a Calcium Atom using Distorted Wave Method at High Impact Energies

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Abstract

Distorted wave method has been employed in the calculation of the differential and integral cross sections for elastic scattering of electron by calcium atom at impact energies between 60 and 200 eV. The results obtained were compared with experimental and theoretical results available. The present results for the differential cross-sections are in good agreement with both theoretical and experimental literature results while the integral cross-sections shows that present results are compare well with the available experimental results.

Key words: *Cross-sections, distortion potential, distorted wave, static potential and spherical harmonics*

Introduction

Cross sections for electron scattering from atoms and molecules play an important role in the understanding of electron interaction with the targets and in the determination of dynamics of the collision processes. The cross sections for inelastic scattering are applied in laser development as well as in plasma physics. Elastic scattering cross sections are useful in X-ray photoelectron spectroscopy and Auger-electron spectroscopy. A study for the elastic scattering of electron by calcium atom at low impact energies (10, 15, 20, and 40 eV) has been reported in Kinyanjui *et al* 2020. In this study the distorted wave method was applied in calculation of the differential and integral cross sections for elastic scattering of electron by calcium atom at electron impact energies between 60 and 200 eV. Being an elastic scattering both the initial and final distortion potential were taken as the static potential of a calcium atom in the initial state. The distorted waves have been determined by partial wave expansion method by expanding them in terms of spherical harmonics while the radial equation corresponding to distorted waves have been evaluated using Numerov method. A computer program DWBA1 developed for electron-hydrogen scattering is here modified to perform the numerical calculations for electron-calcium scattering. The calculated results for differential and integral cross sections are then compared

with the available experimental and theoretical literature data. The comparison of the present calculation with other theoretical and experimental results show that present DWBA1 results are in good qualitative and quantitative agreement with the experimental data.

Previously, Milisavljevic *et al.* (2005) used a crossed electron-atom beam experimental technique to measure differential and integral cross sections for elastic scattering of electron by calcium atom at electron-impact energies of 10, 20, 40, 60 and 100 eV and for a range of scattering angles (θ) from 10° up to 150° . Raj *et al.* (2007) used complex optical-potential method to calculate differential cross-sections (DCS) and integral cross-sections (ICS) for elastic scattering of electrons by calcium atom at electron impact energies of 10 to 500 eV. In 2010, Pandya *et al.* used a complex optical potential to calculate DCSs for elastic electron scattering by calcium atom at electron impact energies 10, 60 and 100 eV. The two theoretical approaches results when compared with experimental results do not agree well. The observed discrepancy has motivated the study of differential and integral cross sections for elastic electron-calcium scattering using the distorted wave method in the energy range of 60 – 200 eV.

Theoretical framework

In the distorted wave method, the total Hamiltonian H , for electron-calcium elastic collision is given as (Singh, 2004; Madison and Bartschat, 1996)

$$H = H_a + T + V \quad (1)$$

where H_a is the Hamiltonian for the isolated atom, T is the kinetic energy operator for the projectile electron and V is the interaction between the projectile electron and the atom. The initial state full scattering wave function Ψ_i^+ is a solution of Schroedinger equation

$$(H - E)\Psi_i^+ = 0. \quad (2)$$

The T-matrix for the electron-target collision in the two potential approach as given by Madison and Bartschat (1996) is

$$T_{if} = (N+1) \langle \chi_f^-(0) \psi_f(1, \dots, N) | V - U_f | A \Psi_i^+(0, \dots, N) \rangle \\ + \langle \chi_f^-(0) \psi_i(1, \dots, N) | U_f | \psi_i(1, \dots, N) \beta_i \rangle \quad (3)$$

where

$$\beta_i = \exp(i\mathbf{k} \cdot \mathbf{r}_0) \quad (4)$$

and ψ_i and ψ_f are the initial and final wave functions of the calcium atom respectively. A is the antisymmetrization operator for the electron-atom system, generally given as

$$A = \frac{1}{N+1} \left(1 - \sum_{i=1}^N P_{i0} \right) \quad (5)$$

where P_{i0} is the operator that exchanges the i^{th} atomic electron with the incident electron (labeled 0). χ_f^- is a solution of the wave equation

$$(\nabla_0^2 - U_f + k_f^2) \chi_f^- = 0. \quad (6)$$

The Born series expansion is done for Ψ_i^+ and considering the first term of it only, then we get

$$T_{if} = (N+1) \langle \chi_f^-(0) \psi_f(1, 2, \dots, N) | V - U_f | A \psi_i^+(1, 2, \dots, N) \chi_i^+(0) \rangle \\ + \langle \chi_f^-(0) \psi_f(1, 2, \dots, N) | U_f | \psi_i(1, 2, \dots, N) \beta_i(0) \rangle. \quad (7)$$

When the target is one electron atom or quasi one electron atom (when we consider only one electron of the atom in the collision process) and elastic collision is being considered, then the direct and exchange transition matrices corresponding to the above T_{if} can be separated as follows.

$$T^d = \langle \chi_f^-(0) \psi_i(1) | V | \psi_i(1) \chi_i^+(0) \rangle + \langle \chi_f^-(0) | U_i(0) | \beta_i(0) - \chi_i^+(0) \rangle \quad (8)$$

and

$$T^{ex} = \langle \chi_f^-(0) \psi_i(1) | V | \psi_i(0) \chi_i^+(1) \rangle - \langle \chi_f^-(0) | U_i(0) | \psi_i(0) \rangle \langle \psi_i(1) \chi_i^+(1) \rangle \quad (9)$$

since $\psi_i = \psi_f$ (for elastic collision processes) and $U_i = U_f$. Here, χ_i^+ is the distorted wavefunction representing the projectile electron in the initial channel and is a solution to the wave equation

$$(\nabla_0^2 - U_i + k_i^2) \chi_i^+ = 0. \quad (10)$$

Here, U_i is an arbitrarily chosen potential for the distortion of the initial state projectile electron and k_i is the initial wave vector of the projectile electron. In this study $U_i = U_f$ and has been taken as the initial state static potential of calcium atom.

For the elastic scattering the terms in T^d having distorted waves (both $\chi_f^-(0)$ and $\chi_i^+(0)$) will vanish and direct matrix T^d takes the form

$$T^d = \langle \chi_f^-(0) | V_{ii} | \beta_i(0) - \chi_i^+ \rangle \quad (11)$$

where $V_{ii} = U_i$. The second term on the right hand side of equation (9) contains the overlap integral between the bound and distorted waves. The oscillatory nature of the distorted wave will tend to cause this integral to vanish, particularly when the distorted wave oscillates significantly more rapidly than the bound state wave function which is the case for intermediate to high projectile energies. As a consequence, this overlap term is ignored and exchange matrix is approximated as follows.

$$T^{ex} = \langle \chi_f^-(0) \psi_i(1) | V | \psi_i(0) \chi_i^+(1) \rangle \quad (12)$$

The distorted waves χ_i^+ and χ_f^- for the projectile in the initial and final states are expanded in terms of partial waves (Singh, 2005) as

$$|\chi_i^+\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_i r} \sum_{l, m_i} i^l \chi_{li}(k_i, r) Y_{li, m_i}(\hat{r}) Y_{li, m_i}^*(\hat{r} k_i) \quad (13)$$

and

$$|\chi_f^-\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_f r} \sum_{l_f m_f} i^{l_f} \chi_{l_f}^*(k_f, r) Y_{l_f m_f}(\hat{r}) Y_{l_f m_f}^*(\hat{k}_f) \quad (14)$$

where Y_{lm} are spherical harmonics. Substituting equations (11) and (12) into equations (10) and (6) respectively, the radial distorted waves become the solution of the following equation.

$$\left(\frac{d^2}{dr^2} - \frac{l_s(l_s + 1)}{r^2} - U_s(r) + k_s^2 \right) \chi_{l_s}(r) = 0 \quad (15)$$

with $s = i$ for the initial state and $s = f$ for the final state distorted waves. In the asymptotic region, they will satisfy the boundary condition

$$\lim_{r \rightarrow \infty} \chi_{l_s}(k_s, r) = j_{l_s} + B_{l_s}(\eta_{l_s} + i j_{l_s}) \quad (16)$$

where j_l and n_l are the regular and irregular Ricatti-Bessel functions and B_l is given as

$$B_l = \exp(i\delta_l) \sin \delta_l \quad (17)$$

with δ_l being the elastic scattering phase shift.

Since elastic scattering was considered, both the initial and final distortion potentials were taken as the static potential of a calcium atom in the initial state that is

$$U_i = U_f = \langle \psi_i | V | \psi_i \rangle \quad (18)$$

where U_i and U_f are initial and final distortion potentials respectively. The mathematical formulation of static potentials is generally expressed as

$$U_s = \langle \psi_s | V | \psi_s \rangle \quad (19)$$

where ψ_s is the target wave function.

The radial distorted wave equations (13) for initial and final states is solved using Numerov method and the differential cross sections calculated using the relation

$$\frac{d\sigma}{d\Omega} = 4\pi^4 \frac{k_f}{k_i} \left(\frac{1}{4} |T^d + T^{ex}|^2 + \frac{3}{4} |T^d - T^{ex}|^2 \right) \quad (20)$$

This is integrated to obtain the expression for total cross section

$$\begin{aligned} \sigma &= \int \frac{d\sigma}{d\Omega} d\Omega \\ \sigma &= 2\pi \int_0^\pi \frac{d\sigma}{d\Omega} \sin \Theta d\Theta \end{aligned} \quad (21)$$

Results and discussions

The newly calculated DWBA results have been compared to some of the available theoretical calculations as well as the measured results of Milisavljevic *et al.* (2005). At impact energy of 60 eV the

picture on the left side of figure 1, shows that the present results are in better qualitative and quantitative agreement with experimental results of Milisavljevic *et al.* (2005) compared to the calculated optical potential results of Khare *et al.* (1985), Raj and Kumar (2007) and Pandya *et al.* (2010). The present result replicates the two minima observed in measured results of Milisavljevic *et al.* (2005) and calculated optical potential results of Khare *et al.* (1985), Raj and Kumar (2007) and those calculated by Pandya *et al.* (2010). This shows that the DWBA method is equally accurate in the calculation of the cross-sections. The minimum of the present results is slightly shifted to the right at 145° in comparison with the experimental results of Milisavljevic *et al.* (2005).

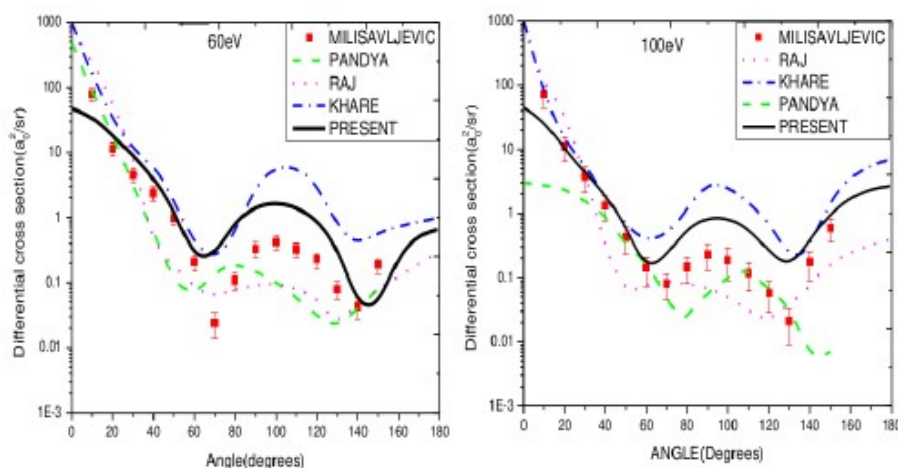


Figure 1: Differential cross sections for elastic scattering of electrons by calcium atom at 60 and 100 eV incident energy respectively

The same comparison is observed in the case of 100 eV right hand side of figure 1 where the calculated results of Khare *et al.* (1985) overestimates the present DWBA calculation while those calculated Raj and Kumar (2007) and by Pandya *et al.* (2010) underestimates the DWBA results. The positions of the two minimas in the present results coincide with those of the measured results of Milisavljevic *et al.* (2005). It is worth noting that the present result have their minimas higher as compared to the mentioned experimental data. In comparison of the calculated results at impact energies of 60, 100 and 200 eV, shown in figures 1 and left side of figure 2, the minimas appear to shift to the left as the impact energy increases. For the case of 200 eV, the present result is intermediate between the optical potential results of Raj and Kumar (2007) and the complex optical potential results of Khare *et al.* (1985).

A study of the integral cross-sections (ICS) for elastic scattering of electrons by calcium atom was conducted as shown on the right hand-side of figure 2. This study was performed for the impact energies between 40 eV and 200 eV. The present DWBA results for this range falls within the error bars of the experimental results of Milisavljevic *et al.* (2005). This is another reason to show that distorted wave Born-approximation method can accurately be used to calculate both differential and integral cross-sections for this system.

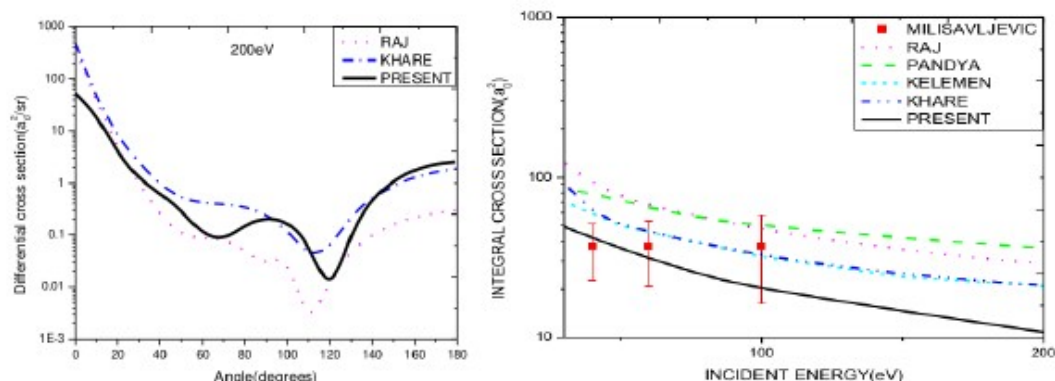


Figure 2: Differential cross sections for elastic scattering of electrons by a calcium atom at 200 eV incident energy and the total cross sections respectively

Conclusion

The DWBA method has been successfully employed in the calculation of both the differential and total cross-sections of elastic scattering of electrons by calcium atom. The present results have shown better qualitative and quantitative convergence to the experimental results as compared to the mentioned optical potential and complex optical potential methods. In the outlook, the DWBA method can be extended to investigate the cross-sections for elastic scattering of positron by calcium atom as well as other atomic systems.

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