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Electron impact elastic scattering by a calcium atom using the first order distorted wave method with a complex potential

Waswa, V. E.[1*], Jobunga, E. O.[2], Kariuki, P. K.[1]

[1*1]Department of Physics, Kenyatta University; P.O. Box 43844 – 0100, Nairobi, Kenya
[2]Department of Mathematics and Physics, Technical University of Mombasa;
P. O. Box 90420 – 80100, Mombasa, Kenya

[1*]Corresponding Author's Email: waswavincent@gmail.com

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ABSTRACT

Electron-atom scattering data is required in diverse fields of physics. In particular, inelastic collision cross sections data are needed in photonics and radiation physics. Elastic collision data, on the other hand, are useful in material science for surface analysis. There is a lack of accuracy and completeness of atomic data obtained using theoretical methods relative to experimental techniques. Furthermore, the distorted wave Born approximation method with a complex potential is yet to be applied in calculating cross sections. Differential and total cross sections have been calculated for electron-calcium scattering in the impact energy range 10 – 100 eV. There is good shape resonance between the present results with a complex potential and experimental values as well as other theoretical results.

Keywords: Electron, Distorted wave, Complex potential, Cross section, Scattering.

INTRODUCTION

Scattering theory is a framework for studying and understanding the dynamics of collisions of particles. Thorough analysis of experimental findings together with scattering theory yields more knowledge about the atomic structure of interacting particles. The accuracy and completeness of the atomic data is crucial in various modeling applications. For instance, accurate atomic data is needed in the modeling of modern X-ray spectra that are used to study and analyze the physical sources that power astrophysical charge-exchange plasmas (Gu *et al.*, 2022).

The electron-calcium elastic scattering has been studied widely, employing both experimental and theoretical techniques. The experimental results of Milisavljevic *et al.* (2005) are considered in this work because our calculations were done within the same energy range as the experimental work. They employed crossed beam of electrons to measure Differential Cross Section (DCS) and integral cross section values at intermediate energies. However, their measurements have uncertainties of 0.1 eV and 1.5°. Further, they did not measure cross sections below 10° because of direct beam contributions.

Most of the theoretical studies applied the optical potential model and focused on elastic scattering and excitation (Zatsarinny *et al.*, 2019). Unfortunately, they employed approximations even if the wave function is exact and complete like that of the hydrogen atom (Schiff, 1968). Gregory and Fink (1974) conducted their study utilizing a static potential only and neglected the effects of electron exchange, polarization, and absorption interactions. Khare *et al.* (1985) adopted the optical potential method. They only considered the real part of the optical potential and excluded the effects of absorption interactions. Kelemen *et al.* (1995) adopted a complex optical potential, however, they used the Staszewska *et al.* (1983) absorption potential, which yields unreliable results at large scattering angles and high impact energies. Raj and Kumar (2007) investigated the impact of absorption effects, adopting an optical potential realism. However, their model overestimates the flux loss from elastic scattering. Pandya *et al.* (2010) reported cross section results at intermediate energy employing a complex optical potential. Their calculations are in agreement with the experiment for scattering angles

up to 30° but, thereafter, they deviate. Also, their model is suitable for symmetric targets only. Hasan *et al.* (2013) applied a complex potential to evaluate cross sections. Their calculations fit the experimental values reasonably in the entire energy region except for 10 eV at high scattering angles, where they differ considerably. This disparity may be attributed to the inclusion of indirect processes that are significant for low energies. Zatsarinny *et al.* (2019) applied the R-matrix technique, producing results that are in good accord with the measured data for high energies. However, their calculations underestimate the experimental values for low energies. In this study, the Distorted Wave Born Approximation (DWBA) method with a complex potential was applied.

THEORY

In the DWBA method, there are three potentials that specify the type of distorted waves to be calculated (Madison and Bartschat, 1996). Two potentials affect the first order term while the third potential affects the higher order terms. The T-matrix element is evaluated by approximations since the wave function and electron-electron interaction potential are not exact. The wave function is first expressed as a product of initial distorted waves which is a solution of the Schrödinger equation and the initial atomic wave function. Finally, the first term of the distorted wave is evaluated numerically utilizing partial wave expansions because the interaction is small.

Distortion potentials

The distortion potential adopted in this study is of the form

$$V_{opt}(r) = V_{st}(r) + V_{ex}(r) + V_{pol}(r) + iV_{abs}(r) \qquad (1)$$

where $V_{st}(r)$, $V_{ex}(r)$, $V_{pol}(r)$ and $iV_{abs}(r)$ are the static, exchange, polarization and absorption potentials respectively.

The static interaction between the electron and the target atom is attractive and contributes to electron-atom scattering. This interaction is short-range and decays exponentially as a function of the radial distance from the target. The static potential is derived from the lowest-order terms of the conventional multipole series expansion, which is given by

$$V_{st}(r) = -\frac{Z}{r} + \sum_{nl} v_a \int_0^{\infty} dr' \frac{p_{nl}^2(r')}{r_>} \qquad (2)$$

with $Z = 20$ for the nuclear charge of calcium atom, r is radial distance, $r_>$ is the greater of r' and r, n and l are quantum numbers while $P_{nl}(r) = \sum_{j=1}^{k} C_{jnl} f_{jnl}(r)$ is the ground state atomic radial wave function given by Bunge *et al.* (1993). The $f_{jnl}(r)$ and C_{jnl} are the normalized Slater-type orbitals and coefficients respectively.

The exchange interaction is also a short-range part of the optical potential, and thus has the tendency of becoming significant for low impact energies where the projectile electron is close to the target. At high impact energies, chances are that the projectile is far away from the target (beyond classical limit), and hence there is no interaction. The exchange interaction that results from exchange between the projectile electron and the target electron can be simplified to the exchange potential of Furness and McCarthy (1973), which is given by

$$V_{ex}(r,E) = \frac{1}{2}\left[\left(E - V_{st}(r)\right) - \left[\left(E - V_{st}(r)\right)^2 + 4\pi\rho(r)\right]^{\frac{1}{2}}\right] \qquad (3)$$

The electronic charge density of the target atom is given by

$$\rho(r) = \sum_{nl} 2(2l+1)\frac{p_{nl}^2(r)}{4\pi r^2}.$$

The polarization interaction is a long-range part of the optical potential that results from the distortion of the target atom by the charged projectile, and is also attractive (Hasan *et al.*, 2013). The net effect of the static and polarization interactions is that they add to each other, hence increasing the cross-section values in atomic scattering. In this study, the energy-dependent-type polarization potential advanced by Khare *et al.* (1985) was adopted which is given by

$$V_{pol}(r,d) = -\frac{1}{2}\left[\frac{\alpha_d r^2}{\left(r^2+d^2\right)^3} + \frac{\alpha_q r^4}{\left(r^2+d^2\right)^5}\right] \qquad (4)$$

where $d = \frac{3}{4}(1.78/\Delta)^{\frac{1}{2}}$ is the cut-off radius that allows convergence of the polarization potential at $r = 0$, $\alpha_d = 168.71$ is the static dipole polarizability obtained from the experimental results of Miller and Bederson (1976), $\alpha_q = 3356.96$ is the quadrupole polarizability obtained from the theoretical results of Sen and Schmidt (1981), and $\Delta = 0.14635$ a.u. is the mean excitation energy for a calcium atom

The least scattered electrons pass far away from the atomic charge cloud of the target; hence this potential dominates small scattering angles. In atomic collisions, the polarization potential is important in accounting for the distortion of the target charge cloud.

In order to account for loss of flux in the elastic channel, Staszewska *et al.* (1984) suggested a quasi-free absorption potential having the form

$$V_{abs}(r,E) = -\frac{1}{2} T_{loc}(r,E)\,\rho(r)\,\bar{\sigma}_b \tag{5}$$

where $T_{loc}(r,E) = \left(\frac{k^2}{2} - V_{se}\right)^{\frac{1}{2}}$ is the local kinetic energy of the incident electron, k is the electron momentum vector, V_{se} is the static and exchange potentials, and $\bar{\sigma}_b = \frac{32\pi^2 N}{15k^2} H(f_1 + f_2)$ is the average binary collision cross section with H being the Heaviside unit step function.

The distortion potentials discussed above result from the multipole expansion of the electron-electron interaction and the solution of the Schrödinger equation, where the wave functions are expanded in terms of Slater determinants.

The transition matrix element and cross sections

The DWBA transition matrix element adopted in this study for elastic scattering has two direct matrix elements and one exchange matrix element as given by Schiff (1968) with

$$T_{if}^{DWBA} = T_{if}^{D1} + T_{if}^{D2} - T_{if}^{E} \tag{6}$$

where

$$T_{if}^{D1} = -\left(4\pi^2 k\right)^{-1} \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin\delta_l P_l(\cos\theta) \tag{7}$$

and

$$T_{if}^{D2} = -\left[4(\pi k)^2\right]^{-1} \sum_{l=0}^{\infty} (2l+1) e^{2i\delta_l} \left[P_l(\cos\theta) \int_0^{\infty} \left[\chi_l(k,r)\bar{V}(r)\chi_l(k,r)\right] dr \right] \tag{8}$$

with $\bar{V} = -\left(V_{st} - V_{opt}\right)$ being the reduced residual potential, and the exchange T-matrix element is approximated by

$$T_{if}^{E} = \left[2(\pi k)^2\right]^{-1} \sum_{l=0}^{\infty} \sum_{n_\beta l_\beta} \sum_{\lambda=|l-l_\beta|}^{l+l_\beta} e^{2i\delta_l} \left[l_\beta\right][l]^2 \begin{pmatrix} l & \lambda & l_\beta \\ 0 & 0 & 0 \end{pmatrix}^2 R_{l_\beta}^{\lambda} P_l(\cos\theta) \tag{9}$$

where $R_{l_\beta}^{\lambda}$ is the Slater integral, P_l is a Legendre polynomial of order l, δ_l is the phase shifts, θ is the polar angle and χ_l is the radial distorted wave function.

In equation (9), we also have a Wigner 3-j symbol.
The DWBA differential cross sections are then calculated from T_{if} using

$$\frac{d\sigma_T}{d\Omega} = (2\pi)^4 \frac{k_f}{k_i} \left|T_{if}\right|^2 \tag{10}$$

where Ω is the solid angle, k_i and k_f are initial and final momenta of the incident and scattered particles respectively.

The total (elastic and inelastic) cross section (TCS) denoted by σ_T is evaluated using the optical theorem, with

$$\sigma_T = -\frac{2}{k_i} (2\pi)^3 \,\mathrm{Im}\, T_{00} \tag{11}$$

where T_{00} is the forward scattering part of the T-matrix element.
The absorption cross section, σ_{abs}, is determined using the relation

$$\sigma_{abs} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)\left(1 - e^{-4\beta_l}\right) \tag{12}$$

where β_l is the imaginary part of the complex phase shifts.
The total elastic cross section (TECS), σ_{el}, is given by

$$\sigma_{el} = \sigma_T - \sigma_{abs}\,. \tag{13}$$

RESULTS AND DISCUSSION

We present the DWBA DCS, TCS and TECS results for elastic scattering of electrons by a calcium atom at an intermediate energy region obtained using equations (10), (11) and (13) respectively. We have also analyzed the contribution of various potentials, namely the exchange, polarization and absorption potentials, effect in the electron-calcium scattering. The present results are compared with the experimental data of Milisavljevic *et al.* (2005) along with the R-matrix calculations of Zatsarinny *et al.* (2019).

The present results obtained using a complex potential fit the measured data for low energies especially at 20 eV. However, they overestimate the experimental values for high impact energies. The R-matrix calculations of Zatsarinny *et al.* (2019) underestimate the experimental values for low impact energies but are very good for high

energies. The current results with a complex potential are in good shape resonance with the calculations of Zatsarinny *et al*. (2019) at all impact energies considered.

The static interaction only yields result with two minima while inclusion of the exchange distortion potential increases the number of minima from two to three for low energies. The effect of exchange interaction becomes minimal for high energy as the observed number of minima decreases to two. This behavior is anticipated since a low-energy electron has a high chance of undergoing exchange with a target atom electron because of low kinetic energy hence more interaction time unlike a high energy-electron. The polarization potential raises the DCS values significantly for small angular regions. This is because it is the potential that affects electrons moving far away from the target atom, and hence is dominant at small scattering angles. The effect of the absorption interaction is significant for low impact energies, where it lowers the DCS values. Thereafter, it becomes marginal for high energies and large scattering angles. The minimal effect of absorption potential for low energy is attributed to the fewer open channels.

Differential cross sections

In this section, we report the differential cross section results calculated within the framework of a complex DWBA method for elastic scattering of electrons by a calcium atom at 10, 15, 20, 40, 60, 80 and 100 eV for an angular range of $\theta = 0^{\circ}$ to 180°.

In reference to figure 1 (a), at 10 eV, it is noted that the present results with a complex potential are in good shape agreement with the measured data of Milisavljevic *et al*. (2005). The calculations of Zatsarinny *et al*. (2019) underestimate the experimental values at this energy. This is attributed to their absorption potential which is overestimating the loss of flux to excited states for this energy. Hence, their model does not yield good results for low energy.

At 15 eV, there are no available measured or other calculated data for comparison. figure 1 (b) compares the present DWBA results obtained using various potentials. There are three minima at $\theta = 30^{\circ}$, 80° and 130° when an exchange interaction is incorporated in the potential. The static interaction only yields DCS results with two minima. The results obtained using a complex potential are lower than those obtained using static-exchange-polarization potentials. This is because the absorption potential accounts for the loss of flux at this low energy.

In figure 1 (c), at 20 eV incident energy, the present results obtained using a complex potential are a good fit to the experimental results of Milisavljevic *et al*. (2005). This indicates that our model is suitable at this impact energy. It is clearly seen that the theoretical results of Zatsarinny *et al*. (2019) underestimate the measured and present values.

At 40 eV electron-impact energy, the present DCS results in figure 1 (d) are overestimating the measured results of Milisavljevic *et al*. (2005) and theoretical predictions of Zatsarinny *et al*. (2019). This is attributed to the adopted absorption potential of Staszewska *et al*. (1984) which underestimates the loss of flux for this relatively high impact energy. The theoretical results of Zatsarinny *et al*. (2019) fit better to the experimental data of Milisavljevic *et al*. (2005). This is due to the inclusion of several excited states in their calculations.

In figure 2 (a), at 60 eV, the present differential cross section results obtained using various distortion potentials are in good shape resonance with both the experimental findings of Milisavljevic *et al*. (2005) and theoretical predictions of Zatsarinny *et al*. (2019). However, they are overestimating the values of these other studies.

At 80 eV, again there are no available measured or other calculated results for comparison. Figure 2 (b) compares the present DWBA results obtained using various potentials. The curves have similar structure and there is a little difference in the static, static-exchange, static-exchange-polarization and static-exchange-polarization-absorption approximations. This suggests that the static potential only is simply a good approximation for this energy.

Figure 2 (c) analyses the present DCS result at 100 eV obtained using various distortion potentials. The predictions of Zatsarinny *et al.* (2019) are in good accord with the measured data of Milisavljevic et al. (2005). This indicates that there is success in their model for high energy. The present DWBA_SEPA results overestimate both the measured and theoretical findings of Zatsarinny *et al.* (2019) especially for large angular region. This discrepancy may be resolved fully by employing the absorption potential which is highly accurate for high impact energies.

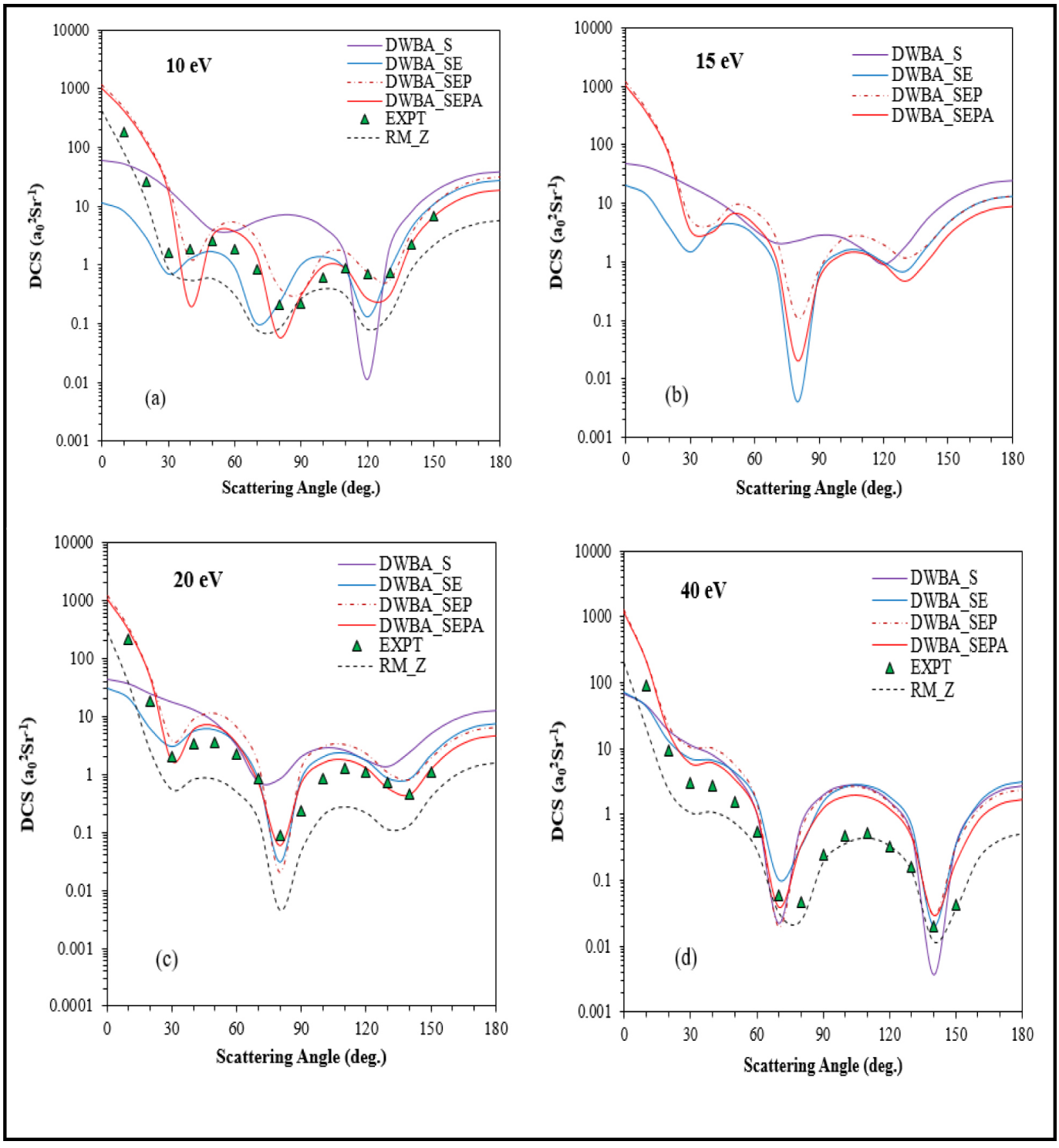

Figure 1: DCS ($a_0^2 Sr^{-1}$) for elastic e-Ca scattering for impact energies; (a) 10, (b) 15, (c) 20 and (d) 40 eV. Experimental: EXPT, Milisavljevic *et al.* (2005). Theoretical: DWBA_S, DWBA_SE, DWBA_SEP and DWBA_SEPA are the current DWBA models with static, static-exchange, static-exchange-polarization and static-exchange-polarization-absorption respectively; RM_Z, R-matrix (Zatsarinny *et al.*, 2019).

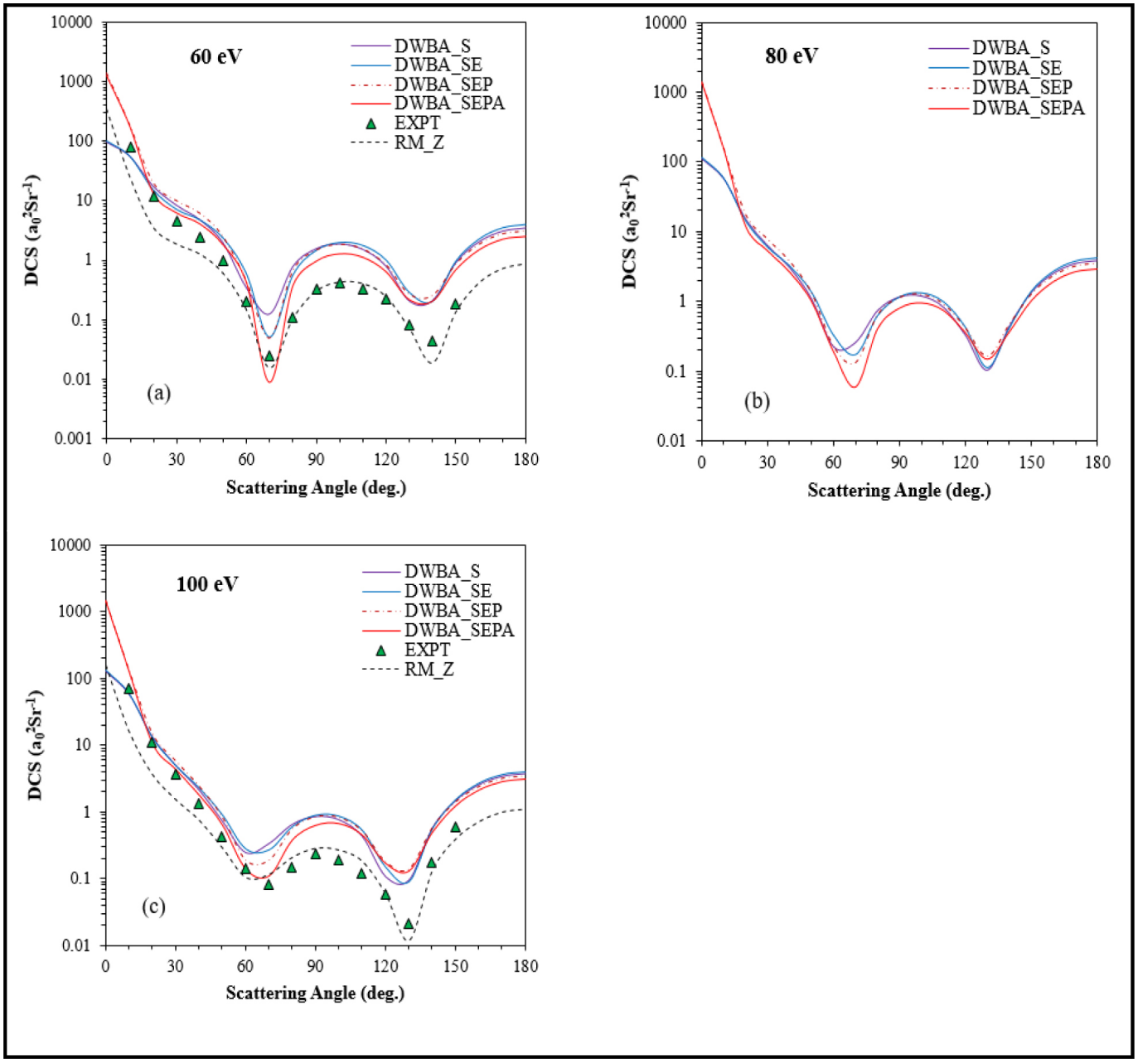

Figure 2: Same as figure 1 but for impact energies; (a) 60, (b) 80 and (c) 100 eV.

Total cross section

In this study the TECS and TCS for elastic scattering of electrons by a calcium atom were calculated using the DWBA method in the energy range from 10 – 100 eV.

Figure 3 (a) presents DWBA total cross sections for elastic scattering of electrons by a calcium atom obtained using Equation (13) for DWBA_S, DWBA_SE, DWBA_SEP and DWBA_SEPA along with the measured data of Milisavljevic et al. (2005). It is clearly seen that the DWBA_S and DWBA_SE total elastic cross sections differ considerably for low energy and converge for high energy. This disparity may be attributed to the exchange potential which is strong for low impact energy and vanishes for high energy. The DWBA_SEPA results underestimate the DWBA_SEP results because of the inclusion of the absorption potential in the DWBA_SEPA approximation which lowers the DCS values. The agreement between DWBA_S and experimental results shows that the exchange, polarization and absorption potentials are unnecessary in describing the measured cross sections in figure 3 (a).

Figure 3 (b) compares the present TCS results obtained using a complex potential and other theoretical predictions available. The present DWBA results are close to the theoretical optical potential results of Raj and Kumar (2007) and Khare et al. (1985) for low energy. However, they overestimate them for high electron impact energy. This may be due to the absorption potential adopted which underestimates the loss of flux in elastic channels at high energies. The present results and other calculated data considered for TCS, satisfy the theoretical prediction that the total cross sections should decreases with an increase in impact energy.

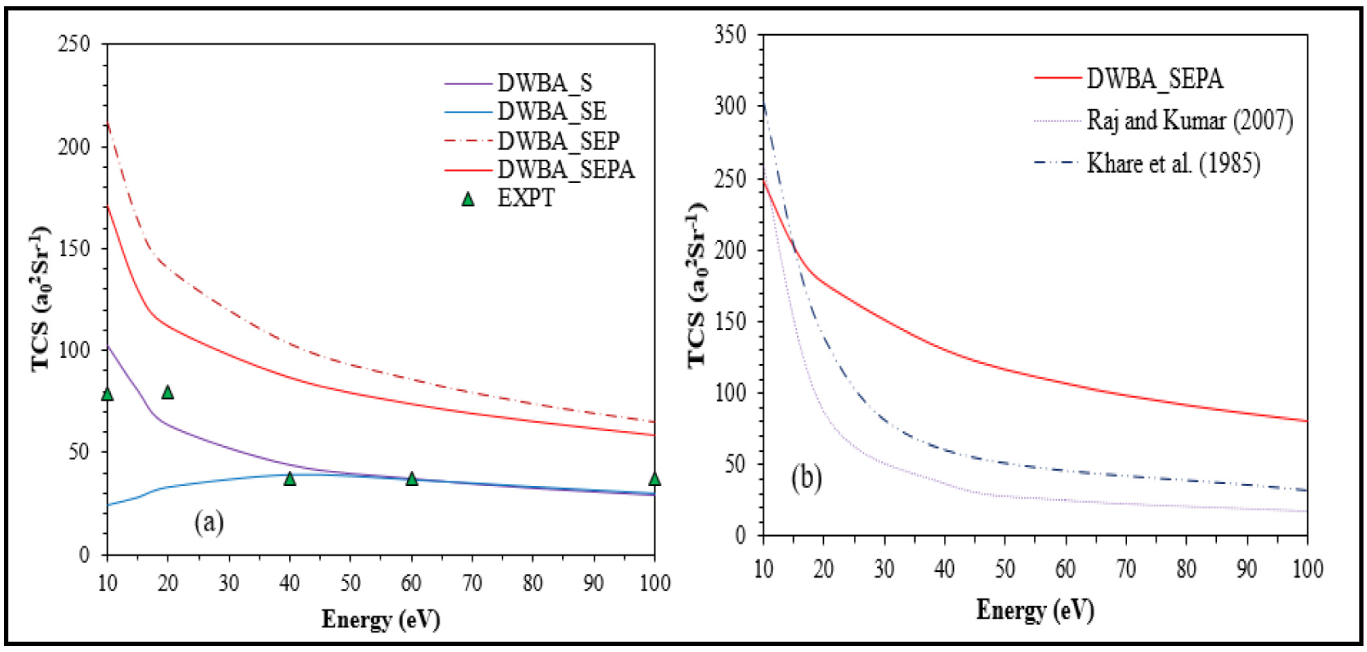

Figure 3: Total cross sections for elastic e-Ca atom scattering for impact energy $10 \le E \le 100$ eV; (a) Total elastic cross section. Experimental: EXPT, Milisavljevic et al. (2005). Theoretical: DWBA_S, DWBA_SE, DWBA_SEP and DWBA_SEPA and (b) total elastic + inelastic cross sections. Theoretical: DWBA_SEPA approximations compared with the OP calculations of Raj and Kumar (2007) and Khare *et al.* (1985).

CONCLUSION

Electron elastic scattering by a calcium atom has been studied theoretically employing the DWBA approximation with a complex potential. In our calculations we have used the polarization potential with an adjustable cut-off radius that allows convergence of the potential at $r = 0$, hence it can be applied from threshold to high impact energies. However, the absorption potential adopted is not highly accurate for high impact energies.

The shape agreement between the present calculated DWBA_SEPA results and the experimental data of Milisavljevic *et al.* (2005) is noticed in general. The SEPA approximation gives much better fit to the measured data than the DWBA_S, DWBA_SE and DWBA_SEP approximations for low energies. Also, the SEPA predictions are in good shape resonance with the R-matrix calculations of Zatsarinny *et al.* (2019) in the entire energy region considered. The exchange effect increases the number of minima for low electron impact energies. The present results obtained using real and complex potentials converge for high impact energy and large scattering angles.

REFERENCES

Bunge, C. F., Barrientos, J. A., and Bunge, A. V. (1993). Roothaan-Hartree-Fock Ground-State Atomic Wave Functions: Slater-Type Orbital Expansions and Expectation Values for Z = 2-54. *Atomic Data and Nuclear Data Tables*, *53*, 113 – 162.

Furness, J. B., and McCarthy, I. E. (1973). Semiphenomenological optical model for electron scattering on atoms. *Journal of Physics B: Atomic, Molecular Optical Physics*, *6*, 2280 – 2291.

Gregory, D., and Fink, M. (1974). Theoretical electron scattering amplitudes and spin polarizations: Electron Energies 100 to 1500 eV Part III. Li, Na, Mg, P, K, Ca, Sc, Mn, Ga, Br, Sr, Mo, Rh, Cd, Ba, W, and Os targets. *Atomic Data and Nuclear Tables*, *14*: 39 – 50.

Gu, L., Shah, C., and Zhang, R. (2022). Uncertainties in atomic data for modeling astrophysical charge exchange plasmas. *Sensors* 2022, *22*(3), 752. URL https://doi.org/10.3390/s22030752.

Hasan, M., Uddin, M. A., Hossain, M. I., Haque, A. K. F., and Basak, A.K. (2013). Elastic Scattering of Electrons by Calcium Atoms. *Canadian Journal of Physics*, *92*(3): 206 – 215. URL https://doi.org/10.1139/cjp-2013-0385. Kelemen, V. I., Remeta, E., and Sabad, E. P. (1995). Scattering of electrons by Ca, Sr, Ba and Yb atoms in the 0 – 200 eV energy region in the optical potential model. *Journal of Physics B: Atomic, Molecular Optical Physics*, *28*: 1527 – 1546.

Khare, S. P., Ashok, K., and Vijayshri (1985). Elastic scattering of electrons and positrons by the calcium atom. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *18*: 1827 – 1840.

Madison, D. H., and Barschat, K. (1996). *The Distorted wave method for elastic scattering and atomic excitation.*

In *Computational Atomic Physics*. ed. K. Barschat. Springer-Verlag, Berlin.

Milisavljevic, S., Sevic, D., Chauhan, R. K., Pejcev, V., Filipovic, D. M., Srivastava, R., and Marinkovic, B. P. (2005). Differential and integrated cross sections for the elastic electron scattering by calcium atom. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *38*: 2371 – 2384.

Miller, T.M., and Bederson, B. (1976). Measurement of polarizability of calcium. *Phys. Rev*. *A*, *14*, 1572.

Pandya, C. V., Patel, P. M., and Baluja, K. L. (2010). Differential scattering cross sections for elastic electron scattering by calcium atom. *Chinese Journal of Physics*, *48*: 451 – 459.

Raj, D., and Kumar, A. (2007). Cross sections for electron scattering by a Ca atom at intermediate energy. *Journal of Physics B: Atomic, Molecular and Optical Physics*, *40*: 3101 – 3111.

Schiff, L. I. (1968). *Quantum Mechanics*. 3rd Ed. (McGraw-Hill. Singapore).

Sen, K. D., and Schmidt, P. C. (1981). Static dipole and quadrupole polarizabilities of alkaline earth atoms. *Int. J. Quantum Chem*., *19*, 373.

Staszewska, G., Schwenka, D. W., Thirumalai, D., and Truhalar, D. G. (1983). Quasifree-scattering model for the imaginary part of the optical potential for electron scattering. *Phys. Rev. A*, *28*: 2740.

Staszewska, G., Schwenka, D. W., and Truhalar, D.G. (1984). Investigation of the shape of the imaginary part of the optical-model potential for electron scattering by rare gases. *Phys. Rev. A*, *29:* 3078–3091.

Zatsarinny, O., Parker H., and Barschat K. (2019). Electron-impact excitation and ionization of atomic calcium at intermediate energies. *Phys. Rev. A*, *99*, 012706.