Elastic scattering of electrons by Sr atom: a study of critical minima and spin polarization

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Abstract

Within the framework of the complex optical potential, the critical minima (CM) in the differential cross sections and the spin polarization in the elastic scattering of electrons by the Sr atom are studied in the energy range \( E_i = 1–1000 \text{ eV} \) using the Dirac and Schrödinger partial wave methods. The two methods are, respectively, termed as the optical potential method of Dirac (OPMD) and optical potential method of Schrödinger (OPMS). The differential cross sections (DCSs), total cross sections (TCs), momentum transfer cross sections (MTCs), integral elastic cross sections (IECs), viscosity cross sections (VCSs) and inelastic cross sections (INCs) for \( e^-\text{Sr} \) scattering are also calculated for the same energy range. In OPMD, the complex optical potential is composed of the static, exchange, polarization and absorption potentials. The OPMS potential, on the other hand, comprises the static, local exchange, polarization, spin-orbit, and absorption components. The number of CM points has been found to be respectively 7 and 5 with OPMD and OPMS methods in the DCSs of \( e^-\text{Sr} \) scattering. The number of maximum spin polarization points observed is 13 and 10 for the OPMD and OPMS methods respectively. The energy dependence of TCS, MTCS, IEC, VCS, and INC, studied in this work, show a non-monotonous pattern for energies beyond about 50 eV. So far as we are concerned, this is the first work for the study of CM in the DCSs of the \( e^-\text{Sr} \) scattering as there are neither experimental nor theoretical studies published in the literature for the same.

1. Introduction

The collision of electron with atoms is very important for the understanding, testing and refining of electron-atom interaction and collision dynamics. Apart from this fundamental importance, the various cross sections of electron-atom scattering are applied in such diverse fields as the modeling of various processes in laboratory plasmas, astrophysical processes, lasers, planetary atmospheres, pollution remediation, electron transports in materials of interest, etc [1]. The electron-atom collisions directly influence the atomic, molecular and optical physics, which have made tremendous contributions to our fundamental understanding of nature.

The critical minima (CM) [2] in differential cross-section (DCS) are the points, on the plane constituted by the scattering angle and projectile energy axes, where DCS attains its smallest values. In general, such minima exist for most of the atoms at one or more electron impact energies and scattering angles [3] and a small change in either of these two variables causes an increase of DCS. The role of CM is very important in electron-atom scattering as they are a sensitive test for the validity of experimental procedures, as well as theoretical predictions of DCS shapes, magnitudes and dependence on the spin polarization (SP) of scattered electrons [4]. The Sherman function, which is a measure of the spin polarization in a plane transverse to the scattering plane, also provides detailed information of the electron-atom collision process and the spin-dependent interactions in the scattering process [5]. It is useful in studies of high energy physics and the magnetism of surface and thin films [6].
The strontium (Sr), with $Z = 38$, is one of the six alkaline earth metals with electron valence configuration $5s^2$. The scattering of electrons from Sr atom has drawn considerable interest due to the presence of low-lying shape resonance (SR) structures and the existence of its negative ion $\text{Sr}^-$ [7]. To the best of our knowledge, there is no extensive experimental or theoretical study on DCS and other cross sections for $e$–Sr scattering in the literature. However, we found two experimental works on the total cross section (TCS) by Romanyuk et al. [8] and Kazakov et al. [9] for a narrow electron energy interval 1–10 eV that agree with the two-state close-coupling (CC2) theoretical calculations of Fabrikant [10]. In their work, Romanyuk et al. [8] observed a sharp increase of TCS as the scattering energy decreases to 0.1 eV. Kazakov et al. [9] found a $d$-wave shape resonance at 1.2 eV by studying the structure of electron spectra for the scattering of electrons by the Sr atom, but they also attributed a minimum structure in 0.3–0.4 eV.

Szymkowski and Sienkiewicz [11] have done theoretical calculations on TCS using the relativistic polarized orbital approximation for the elastic electron scattering by Sr in the energy range 0.2–10 eV. They calculated the static part of their interaction potential by solving the Dirac–Hartree–Fock (DHF) equations for the isolated target while the polarization potential was obtained by solving the coupled DHF equations for the target perturbed by an electric field produced by the projectile. Yuan et al. [12] performed the static exchange plus correlation–polarization calculations for the phase-shifts and cross sections (both partial and total) of $e$–Sr scattering from 0.1 to 4.0 eV. They found the existence of stable $\text{Sr}^-$ in the $5s^25p$ electronic configuration. In another paper, Yuan and Zhang [5] reported calculations for the spin polarization of elastic electron scattering from alkaline earth–metal atoms Ca and Sr in the Ramsauer-Townsend (RT) and low-lying shape resonance (SR) regions using a relativistic method. They showed that the SP effects of the collision of electrons with Sr in the RT region were significant in a considerable area on the energy-angle plane and that the spin-orbit interaction was well increased around the low-lying $d$-wave SR states. Another attempt was made by Yuan [13] to study the effect of intra–target relativistic effects on electron spin polarization for low-energy electron scattering from Ca, Sr, Ba, and Yb atoms. He found that the indirect relativistic effects, in particular the spin dependence of the Dirac–Fock one-electron orbitals, create quantitatively changes apparently in the spin polarization parameters around the $d$-wave shape resonances.

Yuan [14] calculated TCS and IECS for $e$–Sr scattering for low energy scattering up to 10 eV employing close coupling method within the frame-work of R-matrix. Bartschat and Sadeghpour [15] applied non-relativistic R-matrix scheme for the calculation of phase shifts, partial and summed angle integrated cross sections at ultra low energies for $e$–Sr scattering. Kumar et al. [16] calculated DCS, IECS, TCS and spin polarization parameters for $e$–Sr and $e$–Ba scattering systems over the energy range 2–300 eV, using a complex optical potential in the semi-relativistic approach.

Gribakin et al. [17] calculated the phase-shifts for the $p$-wave electron scattering by Ca, Sr, and Ba atoms. The MTCS for the elastic scattering of slow electrons on Ca, Sr and Ba were reported by Gribakin et al. [18] for energies below the ionization potential. To obtain the total potential they proposed a method based on the many-body theory. In 2004, Adibzadeh and Theodosiou [19] made an extensive study for the DCS, TCS, MTCS and Sherman functions for the elastic electron scattering by Ba and Sr atoms for the entire angular range and energies below 1keV. Kelemen et al. [20] have investigated the elastic and inelastic scattering of electrons by Ca, Sr, Ba and Yb atoms in the energy range $E \leq 200eV$ using a phenomenological complex optical potential. Theoretical calculations of the critical minima (CM) for the alkaline earth atom Be have been done by Kaushik et al. [21]. Khare et al. [22] performed theoretical calculations on CM for $e$–Ca elastic scattering. Very recently, Kumar et al. [23] have published an article in which a novel iterative procedure is developed to theoretically calculate the CM for an atom. A pilot application of the method was made on Mg atom. In their paper, they have studied the effective interaction between the electron and Mg atom that includes static, polarization, exchange and spin-orbit interaction with absorption effects. However, to the best of our knowledge, there is no theoretical or experimental work for the determination of CM for the Sr ($Z = 38$).

The DCS minima in the elastic electron–atom scattering are sensitive to the theoretical formalism used for prediction [23]. The exchange potential along–with the target polarization potential is crucial in this case. The process can conveniently be described by an effective optical potential (OP) in which the non-local OP is approximated by a local complex OP. As stated, the previous works are concerned with the determination of the DCS, TCS, MTCS and spin polarizations, but do not provide any calculation of CM in the DCS for $e$–Sr elastic scattering which is of present interest. In this paper, we have analyzed the CM positions as well as the Sherman functions in the vicinity of these minima in greater detail. Here we have employed the complex OP using the OPMD and OPMS partial wave methods to study the DCSs, MTCSs, integrated elastic cross sections (IECSs), inelastic cross sections (INCSs), viscosity cross sections (VCSs) and the Sherman function $S(\theta)$ with a special attention on CM in the DCSs for the elastic electron scattering by Sr atom at energies 1–1000eV. In OPMD, the complex OP is a combination of the components of OP with use of analytical electron density function of the target atom. Here the electron charge density for neutral atom, generated numerically by the Hartree–Fock method, is represented by a parametrized analytical form of Koga [24]. The correlation polarization potential is a
2. Theory

An atom is a composite system of electrons and the nucleus, and as such the interaction of an electron with the atom is a many-body non-local problem. It will be easy to solve the many-body problem if it can be reduced to a one-body problem. The beauty of the optical model approximation is that in this model, the system can be studied as a one-body problem which makes it tractable for solution of either the Schrödinger or the Dirac equation for the scattering observables. The microscopic optical potential model (OPM) is directly formulated from the exact many-body Schrödinger equation on the basis of the multichannel expansion. In this work, we have employed Dirac partial wave and Schrödinger partial wave methods to calculate different cross sections for e–Sr scattering with special attention for CM in DCS.

2.1. Dirac partial wave method

In Dirac partial wave method, the optical potential \( V_{\text{D}}(r) \) can be expressed [26] as

\[
V_{\text{D}}(r) = V_o(r) + V_{\text{ex}}(r) + V_{\text{cp}}(r) - iW_{\text{abs}}(r)
\]

where \( V_o(r) \), \( V_{\text{ex}}(r) \) and \( V_{\text{cp}}(r) \) are, respectively, the static, exchange and correlation polarization potentials. The fourth term with magnitude \( W_{\text{abs}}(r) \) is the imaginary potential which describes the loss of flux to inelastic channels. The potential given in equation (1) and all its components are spherical as the atomic charge distribution is spherically symmetric. The static potential \( V_o(r) \) is obtained using the procedure given in Salvat et al. [27] assuming the Fermi nuclear charge distribution [28] for proton density and Hartree–Fock analytical density function [24] for electron density. The exchange potential \( V_{\text{ex}}(r) \) is the semi-classical potential of Furness and McCarthy [29] generated from the non-local exchange interaction coupled with the Wentzel-Kramers-Brillouin (WKB) approximation for the wave functions, and is given by

\[
V_{\text{ex}}(r) = \frac{1}{2} [E_i - V_o(r)] - \frac{1}{2} [(E_i - V_o(r))^2 + 4\pi a_0 e^4 \rho_a(r)]^{1/2}.
\]

Here \( E_i \) is the incident energy of the projectile electron, \( a_0 \) is the Bohr radius, \( \rho(r) \) is the electron density function represented by an analytical function which is normalized to the atomic number as

\[
\int \rho(r) 4\pi r^2 dr = Z.
\]

According to the treatment given in [26], we have used the global correlation polarization potential \( V_{\text{cp}}(r) \) combining the parameter free long-range polarization potential \( V_{\text{cp}}(r) \) of Sun et al. [25] and a short-range local-density approximation (LDA) correlation potential \( V_{\text{co}}(r) \). The polarization potential is thus given by

\[
V_{\text{cp}}(r) = \begin{cases} 
\max\{V_{\text{co}}(r), V_{\text{cp}}(r)\} & \text{if } r < r_c \\
V_{\text{cp}}(r) & \text{if } r \geq r_c.
\end{cases}
\]

where \( r_c \) is the outer radius at which the short-range part \( V_{\text{co}}(r) \) crosses first with the long-range part \( V_{\text{cp}}(r) \). The long-range potential \( V_{\text{cp}}(r) \) at long electron–atom distances can be estimated [25] as

\[
V_{\text{cp}}(r) = -\frac{\alpha_d}{2(d^2 + d^2)^2},
\]

where \( \alpha_d \) is the atomic static polarizability of the target atom. The constant \( d \) in equation (5) is found from

\[
V_{\text{cp}}(0) = -\frac{\alpha_d}{2d^2} \approx V_o(0)
\]
According to the work of Perdew and Zunger [30], the correlation potential can be parametrized as

\[
V_{\alpha}(r) = \begin{cases} 
\frac{\delta_i}{a_0} (0.0311 \ln(r) - 0.0584 + 0.00133r \ln(r) - 0.0084r) & \text{for } r_s < 1 \\
\frac{\delta_i}{a_0} \left(1 + \frac{7\delta_i}{a_0} \right) (\frac{4f\delta_i}{a_0} + \frac{4\delta_i}{a_0}) & \text{for } r_s \geq 1.
\end{cases}
\]

(7)

with \(\delta_i = 0.1423, \delta_1 = 1.0529\) and \(\delta_2 = 0.3334\). The density parameter \(r_s\) is related to the local atomic electron density \(\rho(r)\), equal to the density of a free electron gas (FEG), as

\[
\rho_s = \frac{1}{a_0^3} \left(\frac{3}{4\pi\rho(r)}\right)^{\frac{1}{3}}.
\]

(8)

Following Salvat [26], the absorption potential is given by

\[
W_{\alpha\beta}(r) = A_{\alpha\beta} \left(\frac{\hbar}{2} \nu_L \rho(r) \sigma_{\alpha\beta}(E_i, \rho, \Delta)\right) \left(\frac{2(E_i + m_0 c^2)^2}{m_0 c^2 (E_i + m_0 c^2)^2}\right) \nu_L^2.
\]

(9)

Here \(m_0\) is the electron mass, \(c\) is the velocity of light in free space and \(\nu_L\) is the local velocity of an electron in the electron gas of density \(\rho(r)\) given by

\[
\nu_L = \left(\frac{2E_i}{m_0}\right)^{\frac{1}{2}}.
\]

(10)

in which \(E_i(r) = E_i - V_\alpha(r)\) is the local kinetic energy of the electron. \(\sigma_{\alpha\beta}(E_i, \rho, \Delta)\) is the cross section for the binary collision of electron with the degenerate FEG involving energy transfers greater than a certain energy gap \(\Delta\). In this work, the value of the empirical parameter \(A_{\alpha\beta}\) has been chosen \(A_{\alpha\beta} = 2\). The value of the energy gap \(\Delta\), equal to the first excitation energy of Sr atom \(\varepsilon = 0.97\), has been taken from the NIST Physics Reference Data [31].

In Dirac partial wave method, the cross sections are calculated from the direct scattering amplitude \(f(\theta)\) and the spin-flip amplitude \(g(\theta)\), respectively given [32] by

\[
f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \left(\begin{array}{c}
l + 1 \\
1
\end{array}\right) \left[1 + e^{i2\delta_{ki} - i(l+1)} - 1\right] P_l^i(\cos \theta),
\]

(11)

and

\[
g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \left[1 - e^{i2\delta_{ki} - i(l+1)}\right] P_l^i(\cos \theta).
\]

(12)

Here \(P_l^i(\cos \theta)\) and \(P_l^j(\cos \theta)\) are, respectively, the Legendre polynomials and associated Legendre polynomials. \(\kappa\) is the relativistic quantum number defined as \(\kappa = (1 - j)(2j + 1)\), where \(j\) and \(l\) are, respectively, the total and orbital angular momentum quantum numbers which are determined by the value of \(\kappa\) as

\[
j = |\kappa| - \frac{1}{2}, \quad l = j + \frac{\kappa}{|\kappa|}.
\]

(13)

In equations (11) and (12) \(k\) is the relativistic wave number of the electron which is related to the kinetic energy \(E_i\) as

\[
(kc)^2 = E_i + 2m_0 c^2.
\]

(14)

We have calculated the phase shifts \(\delta_\alpha\) from the numerical solution of the radial wave functions \(P_{\alpha\beta}(r)\) (large component) and \(Q_{\alpha\beta}(r)\) (small component) satisfying the coupled Dirac equations [33]:

\[
\frac{dP_{\alpha\beta}}{dr} = -\frac{\kappa}{r} P_{\alpha\beta} + \frac{E_i - V + 2m_0 c^2}{k c} Q_{\alpha\beta},
\]

(15)

\[
\frac{dQ_{\alpha\beta}}{dr} = -\frac{E_i - V}{k c} P_{\alpha\beta} + \frac{\kappa}{r} Q_{\alpha\beta}.
\]

(16)

The asymptotic form of the function \(P_{\alpha\beta}(r)\) can be expressed in terms of the complex phase shift \(\delta_\alpha\) by

\[
P_{\alpha\beta}(r) \approx \sin \left(kr - \frac{\kappa}{2} + \delta_\alpha\right).
\]

(17)

Equations (15) and (16) are numerically solved using the subroutine package RADIAL [34].
2.2. Schrödinger partial wave method

The interaction potential between the electron and Sr, in the Schrödinger method, is given [23] by

\[ V_S(r) = V_a(r) + V_{ex}(r) + V_p(r) + V_{s}(r) + iV_{abs}(r) \]  

(18)

Here, \( V_a(r) \) is the direct static potential having the expression given in [35]. \( V_{ex}(r) \) is the local exchange potential and in this work, we have used the asymptotically adjusted exchange potential of Riley and Truhlar [36]. \( V_p(r) \) is the polarization potential which has the form [37, 38]

\[ V_p(r) = - \left( \frac{\alpha_d r^2}{(r^2 + D^2)^3} + \frac{\alpha_q r^4}{(r^2 + D^2)^5} \right). \]  

(19)

Here, \( \alpha_d \) and \( \alpha_q \) are, respectively, the dipole and quadrupole polarizabilities of the target Sr which have the values \( \alpha_d = 199 \) [39], \( \alpha_q = 4577 \) [40]. In equation (19), \( D \) can be expressed as

\[ D = 0.75 \left( \frac{k}{L-1} \right). \]  

(20)

where the mean excitation energy \( L-1 \) is given [41] by

\[ L-1 = \exp \left[ \frac{L(-1)}{S(-1)} \right]. \]  

(21)

Here \( S(-1) = 18.77 \) and \( L(-1) = -21.49 \) [42] are, respectively, the dipole and logarithmic dipole sums that can be obtained from the dipole oscillator strength distribution of the atom. With these values of \( S(-1) \) and \( L(-1) \), the value of \( L_{-1} \) is found as \( L_{-1} = 0.3183 \). It is pertinent to mention that the above polarization potential overestimates the attractive potential for energies roughly less than \( k_r^2 = 3.56nL_{-1} \) [23]. Therefore, in the present, investigation we have taken \( k_r^2 = 3.56nL_{-1} \) as switch over energy and have replaced \( k \) by \( k_r = \sqrt{3.56nL_{-1}} \) in equation (20) for incident energies less than \( 3.56nL_{-1} \), where \( n \) is a adjustable parameter and, in the present investigation, we have taken \( n = 3 \).

Following the works of [43, 44], the spin-orbit potential of the electron–Sr scattering has been assumed to be of the form

\[ V_{s}(r) = \xi(j, l) \frac{\alpha^2}{2r} \frac{d}{dr} [V_a(r) + V_{ex}(r) + V_p(r)], \]  

(22)

where \( \alpha \) is the fine structure constant and

\[ \xi(j, l) = \begin{cases} \frac{j}{2} & \text{for } j = l + \frac{1}{2} \\ \frac{j+1}{2} & \text{for } j = l - \frac{1}{2} \end{cases} \]  

(23)

We have employed the absorption potential of Raj and Kumar [45] which has the following form

\[ V_{abs}(r) = \frac{V_s(r)}{k}. \]  

(24)

where \( V_s(r) \) is the absorption potential of Staszewska et al [46] and \( k \) is the non relativistic wave number of the electron. In Schrödinger method, the direct and spin-flip amplitudes are, respectively, given [47] by

\[ f(\theta) = \frac{1}{2ik} \sum_{l=0}^{M} [(l + 1)(e^{i2k} - 1) + l(e^{i2k} - 1)] P_l(\cos \theta) + f_{dp} - \frac{1}{k} \sum_{l=0}^{M} (2l + 1) \delta_l^e P_l(\cos \theta) \]  

(25)

and

\[ g(\theta) = \frac{1}{2ik} \sum_{l=0}^{M} [e^{i2k} - e^{i2k}] P_l(\cos \theta). \]  

(26)

Here, \( f_{dp} \) represents the first Born scattering amplitude and \( \delta_l^e \) are the semiclassical phase shifts for the long range polarization potential given in equation (19). \( M \) is an energy-dependent integer such that the phase shift for the \( M \) th partial wave, \( \delta_l^e \approx \delta_l^e \) (within 2%). For \( l = 0 \) to \( M \), the phase shifts \( \delta_l^e \) can be obtained by solving the radial Schrödinger equation

\[ \left[ \frac{d^2}{dr^2} + k^2 - V_S(r) - \frac{l(l + 1)}{r^2} \right] u_l(r) = 0. \]  

(27)

The elastic DCS can be expressed in terms of the direct and spin-flip amplitudes \( f(\theta) \) and \( g(\theta) \) by

\[ \frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2. \]  

(28)
The IECS, MTCS, VCS and TCS are:

\[
\sigma_t = 4 \pi \int_0^\pi \sigma_{t} d\Omega = 2\pi \int_0^\pi [ (|f(\theta)|^2 + |g(\theta)|^2) \sin \theta d\theta, \tag{29}
\]

\[
\sigma_m = 2\pi \int_0^\pi (1 - \cos \theta) (|f(\theta)|^2 + |g(\theta)|^2) \sin \theta d\theta \tag{30}
\]

\[
\sigma_v = 3\pi \int_0^\pi (1 - (\cos \theta)^2) (|f(\theta)|^2 + |g(\theta)|^2) \sin \theta d\theta. \tag{31}
\]

and

\[
\sigma_{tot} = \frac{4\pi}{k} \text{Im} f(0), \tag{32}
\]

Here \(\text{Im} f(0)\) denotes the imaginary part of the scattering amplitude \(f(0)\) at the forward direction. The spin polarization or the Sherman function \(S(\theta)\), which is a measure of the asymmetry of the spin-up and spin-down states of the electron, can be obtained from

\[
S(\theta) = \frac{i f(\theta) g^*(\theta) - f^*(\theta) g(\theta)}{|f(\theta)|^2 + |g(\theta)|^2}. \tag{33}
\]

3. Results and analysis

3.1. DCS and total cross sections

In figures 1–4, we present the differential cross sections (DCSs) for \(e–Sr\) elastic scattering in the range of incident energies \(E_i = 1–1000\) eV, obtained from the OPMD and OPMS methods. There is no experimental work on DCS for \(e–Sr\) elastic scattering, and so we compare our predictions with the available theoretical works of Kelemen et al [20] for energies 1.0 and 2.0 eV, Kumar et al [16] for 10.0 and 100 eV and Adibzadeh and Theodosiou [19]. To the best of our knowledge, the present work is the first one to predict the DCS at energies \(E_i = 60, 150, 250, 600, 800\) and 900 eV.

It is observed from figures 1–4 that the number of DCS minima depends explicitly on the incident electron energy. For calculations using OPMD, there exist two minima at energies 1–5 eV, three at 10 eV and again two at 15–70 eV. As the projectile energy increases, the DCSs again show three minima at 80, 90, 100, 150 and 200 eV. For further increase of collision energy, the number of minima decreases to two at 300 and 400 eV, and to one at 600 and 700 eV. For energies \(E_i \geq 800\) eV, the DCS varies monotonously with incident energy with a shallow minimum around the scattering angle \(\theta = 120^\circ\). The number of DCS minima for OPMS calculations (figures 1–4) is somewhat different from that for OPMD calculations. The number varies from two at 5 eV to three at 10 eV and then again to two at 15–100 eV. For energies greater than 100 eV the number of DCS minima increases to three at 150, 200 and 250 eV, then falls to two at 300, 400 and 500 eV. As the projectile energy increases further, the DCSs find just one minimum at 600, 700 and 750 eV.

Figures 1(a)–(c) clearly show that the angular distributions of the DCS obtained from the present calculations using OPMD for 1, 2 and 3 eV is completely different from the semiempirical calculations of Adibzadeh and Theodosiou [19]. While the number of DCS minima in our work is two, the [19] shows just one minimum for all three cases. Although at \(E_i = 5\) eV, the number of minima for OPMD, OPMS and [19] is the same, the positions of first minima predicted by the three methods are different. The positions are at \(\theta = 42^\circ\) for OPMD, \(\theta = 70^\circ\) for OPMS and, \(\theta = 82^\circ\) for [19]. The three calculations also do not agree with one another in the magnitude of the cross sections before the first minima as well as after \(105^\circ\) scattering angle. The qualitative as well as quantitative disagreement at most of angular points among the predicted DCSs of the three methods at the energy 10 eV is apparent from the figure 1(e). However, the present work with OPMD has a rough qualitative agreement with the work of Kelemen et al [20] at energies 1 and 2 eV, as observed from figures 1(a) and (b). It can be noticed from figure 1(e) that the OPMD calculations have also qualitative agreement with Kumar et al [16] for 10 eV incident energy. Furthermore, for 100 eV collision energy, OPMD and [16] produce similar cross sections both in trend and magnitude (figure 3(c)). As seen in the figure 1(f), the three predictions produce a good qualitative agreement with differences in the cross-section values, except for the low angles where a good agreement in trend and magnitude of DCS is noticeable. The difference in magnitude of DCS might be from the use of different potentials and procedures. It is evident from figures 2(a)–(f) that the positions of minima in DCSs predicted by OMPS and OPMD for incident energies 20–70 eV are the same as those of [19] except the case of OPMS calculation for 70 eV where it produces second minima at \(118^\circ\) scattering angle while OPMD and [19] at around \(107^\circ\). The set of cross sections by OPMD and OPMS for 70 eV is also a bit different from that of [19] except at \(\theta = 10^\circ\).
As seen in figures 3(a)–(f), present OMPD and [19] calculations of DCSs produce a close qualitative agreement, albeit differences in magnitude, at energies 80, 90, 100 and 200 eV. The OPMS calculations show disagreement, to some extent, in trend and magnitudes of the DCSs at energies 80–150 eV with OPMD or [19] or both particularly at large angles. However, at energies 200 and 250 eV the aforesaid differences are mitigated. The noticeable differences in the predictions of DCSs by the OPMS from those of OPMD and [19] at large angles might be due to the relativistic effect as the latter two methods use the relativistic dynamics. As apparent from figures 4(a)–(f) for energies 300–1000 eV, the number of minima in the DCSs is the same and these minima are
produced at almost the same positions for the three calculations. However, these two variables are energy dependent. It is noticeable that these three calculations, one non-relativistic and two relativistic, produce a close agreement with one another, barring the minimum positions where the non-relativistic calculation OPMS produce deeper minima. This observation reveals that the relativistic effect has bearing on the interference of scattered waves that produces minima in DCSs. These results can be useful to motivate further experimental and theoretical studies at these energies. Figure 4 shows that our two calculations and that of \[19\] produce almost similar quality of DCS for 1000 eV collision energy.

In Figure 5, we present our results of TCS, MTCS, IECS, VCS and INCS for $e$–Sr scattering in the range of energy $E_i = 1$–1000 eV in comparison with the available experimental data and other calculations. The results using the OPMD and OPMS calculations for TCS are compared in figure 5(a) with the experimental data of Romanyuk et al [8] and the theoretical calculations of Adibzadeh and Theodosiou [19], Kelemen et al [20], Kumar et al [16] and Yuan [14]. The above mentioned six calculations almost follow the same trend of energy variation with differences in magnitude of the cross-sections. The overestimation of both the relativistic calculations and more closeness of the OPMS calculation to the experimental data at low energies might be due

![Figure 2](image-url). The same as figure 1, but for the incident energies (a) 20, (b) 30, (c) 40, (d) 50, (e) 60, and (f) 70 eV.
to the overplay of relativistic effect. There is no experimental data for the MTCS, IECS, VCS and INCS and we have found three theoretical calculations [16, 18, 19] for MTCS and also three [14, 16, 20] for IECS. As seen in figure 5(b), all the five calculations for MTCS disagree in magnitude below around 50 eV energy, but agree in pattern beyond this region, differing in magnitude at most of the points of energy. For IECS all the calculations except [16] follow the same trend but slight disagreement in magnitude beyond 10 eV collision energy. So far as we are concerned, there are neither experimental nor theoretical data of the VCS and INCS for e−-Sr scattering. We calculate these quantities to examine the effect of the non-relativistic and relativistic collision dynamics on the cross sections. As expected, there is relativistic enhancement of IECS and VCS beyond the energy 50 eV. We present the IECS and VCS results respectively in figures 5(c) and (d) using both OPMD and OPMS methods whereas the INCS calculations are shown only with OPMD method in figure 5(e). The present results might be useful for normalizing future experimental data and/or testing and refining theories.

Figure 3. The same as figure 1, but for the incident energies (a) 80, (b) 90, (c) 100, (d) 150, (e) 200, and (f) 250 eV.
3.2. Spin polarization

The results of the calculations of spin polarization or the Sherman function $S(\theta)$ for energies 1–500 eV are displayed in figures 6 and 7, and compared with the available predictions of Adibzadeh and Theodosiou [19] at energies 1, 5, 10, 15, 20, 30, 40, 50, 100 and 500 eV, and Kumar et al citeKumar1994 at 10, 30, 100 and 300 eV. We are not aware of any experimental data for $S(\theta)$ at any energy in the literature. Although there are no other calculations for $S(\theta)$ at 200 and 300 eV, we calculate this quantity for comparison between our two calculations.

As apparent from figure 6(a), at energy of 1 eV, our OPMD prediction agrees fairly with that of [19], but the two predictions disagree remarkably in the angular region 45–140°. For 5.0 eV collision energy (figure 6(b)), the OPMD and OMPS calculations, and [19] produce the same number of positive and negative excursions of $S(\theta)$, albeit with shift in positions. As seen in the figure 6(c), the OPMD calculations produce close agreement with

Figure 4. The same as figure 1, but for the incident energies (a) 300, (b) 400, (c) 500, (d) 600 and 700, (e) 750, and (f) 800, 900 and 1000 eV. The curves are multiplied by the indicated factor.
those of[19] and[16] but the OPMS results are quite different in magnitude and pattern over around angles 22°–125°. The above four calculations are more or less closed to one another at energies 15, 20 and 100 eV (6(d)–(f)). The figure 7(a) shows that our two calculations and those of[16] agree with one another except around the angle 143° where both OPMS and[19] produce peaks in the positive excursion while the OPMD, in the negative excursion. Like the figure 7(f), the predictions of these three calculations follow the similar pattern except at around 137° where OPMS differ in magnitude and pattern from the other two predictions. It is noticed from

**Figure 5.** Energy dependence of (a) the total cross section (TCS), (b) momentum transfer cross section (MTCS), (c) integrated elastic cross section (IECS), (d) viscosity cross section (VCS) and (e) inelastic cross sections (INCS) for the e–Sr scattering. The thick-solid lines (red) and dash-dotted lines (pink) are the present results obtained using the OPMD and OPMS calculations respectively. Other theoretical predictions are broken lines (black) from[19], dash-dot-dotted lines (blue) from[20], dashed lines (olive) from[16] and dotted lines (magenta) from[14]. The solid circles are the experimental data from[8].
That the OPMD calculations are close to those of [16], whereas the OPMS disagree beyond 90° scattering angles. As seen in figure 7(e), the OPMD and [16] agree well with each other but the OPMS calculations show a slight variation for angles 65°–85° and 107°–140°. In the figure 7(d), the comparison between our two calculations at energy 200 eV are made as no other calculations or measurements are available, to the best of our knowledge.
3.3. Critical minima (CM) in DCSs

The energy dependence of minima in the DCSs for \(e^{-}\)-Sr scattering is shown in figure 8(a) for OPMD results. One can observe the appearance of the high angle minima in the DCSs for electron energies up to 1000 eV. The positions vary between 113° and 147° as can be seen from curve-3 of figure 8(a). Figure 8(a) also reveals that the appearance of the low angle minima (curve-1) exists between 3 and 200 eV collision energies. The angular positions of these minima vary from 58° at 3 eV to 40° at 200 eV. The intermediate angle minima are seen to exist between 1 eV to 600 eV, reaching its minimum position of 67° at 32 eV. There is neither any experimental nor theoretical values available in the literature on CM in DCSs for \(e^{-}\)-Sr collision to compare with.

The figure 8(b) presents the energy variation of cross section of the DCS minima corresponding to the curves 1, 2 and 3 of the figure 8(a). The present calculations using OPMD, as observed in figure 8(b), predict nine deep
minima in the DCSs. In curve-1 of figure 8(b), we observe two minima, but only one fulfills the criteria of CM in the low angle region. There is no such minimum found in the low angle region as depicted in the curve-1 of figure 8(b). For the intermediate angle region, as illustrated by curve-2 of figure 8(b), three deepest minima are noticeable at energies 20, 70 and 200 eV. Curve-3 of the same figure shows that, for the high angle minimum region, there exist four such deepest minima at energies 5, 50, 150 and 500 eV. In total we found seven CM out of nine deep minima. A DCS minimum has to satisfy two criteria to qualify for a CM point, namely: (i) the DCS values at that point will be generally (but it may be simply less than) several fold smaller than those at nearest energies and angles, (ii) the magnitude of the spin-flip scattering amplitude, \(|g(\theta)|\) will be greater than that of the direct scattering amplitude, \(|f(\theta)|\). In the present work, with OPMD calculations, all the seven CM shown in

Figure 8. For the elastic e–Sr scattering, (a) shows the plot of angular positions of the DCS critical minima versus energy; (b) depicts the energy dependence of DCSs; (c) and (d) show, respectively, the angular distributions of DCSs and spin-polarization \(S(\theta)\) at \(E_i = 3.4, 6.4\) and 7.4 eV in the vicinity of CM at [6.4 eV, 124°]; (e) and (f) show, respectively, the angular distributions of DCSs and spin-polarization \(S(\theta)\) at \(E_i = 482, 483\) and 484 eV with CM at [483 eV, 126.5°].
which varies from $Ec$ to examine the efficiency of our OPMD method, we show the angular dependence of DCS at higher energies large number of phase shifts contribute and DCS results no significant difference between the extremum values of $S(\theta)$ found, in the present OPMD calculations, is $E_c = 483.0$ eV at $\theta_c = 126.5^\circ$, and the highest critical angle is $\theta_c = 150.0^\circ$ at $E_c = 126.0$ eV. To examine the efficiency of our OPMD method, we show the angular dependence of DCS (figures 8(c) and (e)) as well as spin polarization (figures 8(d) and (f)) for some incident energies in the vicinity of two CM ($E_c = 6.4$ eV; $\theta_c = 124.0^\circ$ and $E_c = 483.0$ eV; $\theta_c = 126.5^\circ$). It is observed from figure 8(c) that the DCS value attains lowest at $E_c = 6.4$ eV. The DCS value increases if the energy is increased ($E_i = 7.4$ eV) or decreased ($E_i = 5.4$ eV) slightly from $E_i = 6.4$ eV. Similar result is found in figure 8(e) where the DCS value reaches its lowest at $E_i = 483.0$ eV than at its adjacent energies $E_i = 482.0$ eV and $E_i = 484.0$ eV.

The change in the number of minima with the impact energy is due to the dominance of one or two partial waves at that energy [44]. At higher energies large number of phase shifts contribute and DCS results no minimum.

Figures 8(d) and (f) illustrates the angular dependence of the Sherman function $S(\theta)$ for some energies in the vicinity of the CM. Figure 8(d) shows that in the vicinity of high angle CM at 6.4 eV, the Sherman functions $S(\theta)$ for three energies (6.4, 6.42 and 6.33 eV) are very close to each other which produce critical angle at $\theta_c = 124^\circ$. As observed in figure 8(d), a significant difference between the extremum values of $S(\theta)$ is found, which varies from $+0.0981$ at $123.5^\circ$ to $-0.0990$ at $124.5^\circ$ in the vicinity of $124.0^\circ$ for 6.4 eV. This happens also in figure 8(f), where two extremum values of $S(\theta)$ lies between $+0.0991$ at $126^\circ$ and $-0.0997$ at $127^\circ$ in the vicinity of $126.5^\circ$. These results agree with the work of Hasan et al [48] where they found the variation of $S(\theta)$ from $+0.54$ at $120.5^\circ$ to $-0.75$ at $121^\circ$ for $e$–Ca scattering at 139.5 eV and from $+0.64$ at $120.5^\circ$ to $-0.79$ at $121^\circ$ for 140 eV. This result profoundly reveals the success of OPMD calculations in determining the CM in DCSs for $e$–Sr scattering.

The positions of the maximum polarization points calculated with the OPMD method are tabulated in table 2. A total of 13 such points are found in this case. In table 2, $\Delta \theta$ is the difference between $\theta_i$ and the energy position for the extremal values of the Sherman function $S(\theta_i)$; $\Delta \theta$ is the difference between $\theta_c$ and the angular position of an extremum value of $S(\theta)$. The values of the Sherman function vary as $+0.672 2 \leq S(\theta) \leq 0.998 1$ and $-0.696 1 \geq S(\theta) \geq -0.999$. Among the 13 maximum polarization points, 10 satisfy the condition

| Energy, $E_c$ (eV) | Angle, $\theta_c$ (degree) | $|f(\theta)|$ ($a_0$) | $|g(\theta)|$ ($a_0$) | Remarks |
|------------------|-----------------|-----------------|-----------------|--------|
| 3.715            | 54.50           | 0.016 97        | 0.027 19        | $|g(\theta)| > |f(\theta)|$ |
| 6.400            | 124.0           | 0.003 17        | 0.060 73        |        |
| 49.90            | 136.5           | 0.004 65        | 0.010 72        |        |
| 71.05            | 108.0           | 0.004 16        | 0.015 60        |        |
| 126.0            | 150.0           | 0.002 82        | 0.006 92        |        |
| 199.0            | 84.00           | 0.006 56        | 0.017 06        |        |
| 483.0            | 126.5           | 0.001 26        | 0.012 10        |        |

| Maximum SP | Energy, $E_c$ (eV) | $\Delta E$ (eV) | Angle, $\theta$ (degree) | $\pm \Delta \theta$ (degree) |
|------------|------------------|-----------------|-----------------|-----------------|--------|
| +0.977 3   | 3.701            | 0.014           | 54.50           | 0.0              |
| -0.999 0   | 6.420            | 0.042           | 124.5           | 0.5              |
| +0.998 2   | 6.339            | 0.061           | 123.5           | 0.5              |
| -0.931 2   | 49.00            | 0.900           | 137.5           | 1.0              |
| -0.905 0   | 50.13            | 0.230           | 136.0           | 0.5              |
| -0.982 8   | 72.95            | 1.900           | 107.0           | 1.0              |
| -0.990 1   | 69.92            | 1.135           | 108.5           | 0.5              |
| -0.696 1   | 127.3            | 1.300           | 149.5           | 0.5              |
| +0.672 2   | 125.6            | 0.400           | 150.0           | 0.0              |
| -0.761 9   | 198.7            | 0.300           | 84.50           | 0.5              |
| +0.982 7   | 199.7            | 0.700           | 83.50           | 0.5              |
| -0.997 3   | 478.9            | 4.100           | 127.0           | 0.5              |
| -0.991 1   | 486.6            | 3.600           | 126.0           | 0.5              |
The spin polarization in the elastic scattering of electrons by the Sr atom have been studied systematically in the energy range \( E_i \), within the framework of the complex optical potential, the critical minima (CM) for the maximum polarization \( S(\theta) \) distribution depends on the value of the angular widths in the positive and negative excursions \( \Delta \theta^p \) and \( \Delta \theta^n \) for the maximum polarization \( S(\theta_{\text{CM}}) \). If the sum of the widths \( \Delta \theta^p \) and \( \Delta \theta^n \) is very small corresponding to \( S(\theta) \) distribution near \( |S(\theta)| = 1 \), then the angular DCS distribution at its CM and the corresponding \( S(\theta) \) can be assumed to be sharp. As seen in the last column of table 2, for all the cases the sum of the angular width \( \Delta \theta^p + \Delta \theta^n \) is nearly achieved and 3 fails to attain this condition. The sharpness of the angular DCS distribution at its CM and the corresponding \( S(\theta) \) distribution are both sharp for the case of OPMD calculations.

In table 3, we list the energy and angular position of CM in DCS along-with the corresponding values of \( f(\theta) \) and \( g(\theta) \) for \( e\)-Sr elastic scattering using OPMS calculations. Five qualified CM positions are found in this case. The highest critical energy, in this case, has been found to be \( E_c = 574.441 \) eV at \( \theta_c = 125.467^\circ \), and the highest critical angle found is \( \theta_c = 158.859^\circ \) at \( E_c = 124.758 \) eV. The positions of the 10 maximum polarization points, calculated with OPMS, are presented in table 4. Here, the Sherman function values vary as \( 0.999 \leq S(\theta) \leq 0.999 \), and \( -0.989 \leq S(\theta) \leq -0.999 \). All the 10 points achieve the condition \( |S(\theta)| \approx 1 \). It is, therefore, noticeable that for OPMS the DCS distribution at its CM and the corresponding \( S(\theta) \) distribution in all the cases are very sharp.

The three-dimensional plot of the Sherman function \( S(\theta) \) with OPMD in figure 9 shows the positions of the maximum polarization points tabulated in table 2. In figure 10, we have shown a three-dimensional plot of the CM which clearly indicates the positions of CM in DCSs.

4. Conclusions

Within the framework of the complex optical potential, the critical minima (CM) in the DCS distributions and the spin polarization in the elastic scattering of electrons by the Sr atom have been studied systematically in the energy range \( E_i = 1–1000 \) eV using the Dirac [OPMD] and Schrödinger [OPMS] partial wave methods. To the best of our knowledge, present study is the first work for the calculation of CM for \( e\)-Sr collision. The DCSs, TCSs, MTCSs, IECSs, VCSs and INCs for \( e\)-Sr scattering have also been calculated for the same energy range. The number of DCS minima has been found to vary from one to three for \( E_i = 1–700 \) eV, while no minima has been noticed for 800, 900 and 1000 eV projectile energies. A total of seven CM points have been observed in the DCSs of \( e\)-Sr scattering using OPMD method. The angular positions along-with the energy-widths and angular widths of these minima have been revealed and discussed. The critical energy \( E_c \), in this case, has been found to

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|S(\theta)| \geq 0.9 \quad \text{and the rest 3 fails to achieve it. One can thus notice that for 10 points the condition of total polarization } \quad |S(\theta)| = 1 \quad \text{is nearly achieved and 3 fails to attain this condition. The sharpness of the } S(\theta) \text{ distribution depends on the value of the angular widths in the positive and negative excursions } \Delta \theta^p \text{ and } \Delta \theta^n \text{ for the maximum polarization } S(\theta_{\text{CM}}). \text{ If the sum of the widths } \Delta \theta^p \text{ and } \Delta \theta^n \text{ is very small corresponding to } S(\theta) \text{ distribution near } |S(\theta)| = 1, \text{ then the angular DCS distribution at its CM and the corresponding } S(\theta) \text{ can be assumed to be sharp. As seen in the last column of table 2, for all the cases the sum of the angular width } \Delta \theta^p + \Delta \theta^n, \text{ which signifies that the angular DCS distribution at its CM and the corresponding } S(\theta) \text{ distribution are both sharp for the case of OPMD calculations.}

In table 3, we list the energy and angular position of CM in DCS along-with the corresponding values of } f(\theta) \text{ and } g(\theta) \text{ for } e\)-Sr elastic scattering using OPMS calculations. Five qualified CM positions are found in this case. The highest critical energy, in this case, has been found to be } E_c = 574.441 \text{ eV at } \theta_c = 125.467^\circ, \text{ and the highest critical angle found is } \theta_c = 158.859^\circ \text{ at } E_c = 124.758 \text{ eV. The positions of the 10 maximum polarization points, calculated with OPMS, are presented in table 4. Here, the Sherman function values vary as } 0.999 \leq S(\theta) \leq 0.999 \text{ and } -0.989 \leq S(\theta) \leq -0.999. \text{ All the 10 points achieve the condition } |S(\theta)| \approx 1. \text{ It is, therefore, noticeable that for OPMS the DCS distribution at its CM and the corresponding } S(\theta) \text{ distribution in all the cases are very sharp.}

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\begin{array}{cccccc}
\text{Energy, } E_c & \text{Angle, } \theta_c & |f(\theta)| & |g(\theta)| & \text{Remarks} \\
\text{(eV)} & \text{(degree)} & (\alpha_\theta) & (\alpha_\theta) & \\
6.566.75 & 125.231 & 0.002 007 & 0.083 30 & |g(\theta)| > |f(\theta)| \\
41.126 & 144.292 & 0.000 271 & 0.003 31 & \\
124.758 & 158.859 & 0.000 059 & 0.004 34 & \\
275.346 & 78.933 & 0.000 205 & 0.010 05 & \\
574.441 & 125.467 & 0.000 062 & 0.007 96 & \\
\end{array}
\]

\[
\begin{array}{cccccc}
\text{Maximum SP} & \text{Energy, } E & \pm \Delta E & \text{Angle, } \theta & \pm \Delta \theta \\
&(\text{eV})&(\text{eV})&(\text{degree})&(\text{degree}) \\
\text{–0.999 745} & 6.540 & 0 & 0.026 8 & 124.70 & 0.531 0 \\
\text{+0.999 996} & 6.590 & 0 & 0.023 3 & 125.75 & 0.519 0 \\
\text{–0.995 211} & 40.910 & 0 & 0.216 4 & 144.47 & 0.178 0 \\
\text{+0.999 705} & 41.410 & 0 & 0.283 6 & 144.06 & 0.232 0 \\
\text{–0.999 894} & 124.51 & 0 & 0.248 0 & 158.56 & 0.299 0 \\
\text{+0.999 302} & 125.00 & 0 & 0.242 0 & 158.90 & 0.291 0 \\
\text{–0.999 998} & 269.55 & 0 & 5.796 0 & 78.900 & 0.033 3 \\
\text{+0.999 980} & 281.44 & 0 & 6.094 0 & 78.930 & 0.003 3 \\
\text{–0.989 170} & 574.68 & 0 & 0.239 0 & 125.02 & 0.447 0 \\
\text{+0.999 986} & 572.13 & 0 & 2.311 0 & 125.95 & 0.483 0 \\
\end{array}
\]
vary between $3.715$ eV corresponding to $\theta_c = 54.5^\circ$ and $483.0$ eV corresponding to $\theta_c = 126.5^\circ$. The critical angle $\theta_c$ varies from $54.5^\circ$ at $E_c = 3.715$ eV to $150.0^\circ$ at $E_c = 126.0$ eV. For OMPS calculations, on the other hand, we have found five CM points. A total of 13 maximum polarization points are found in the vicinity of CM positions using the OPMD where the Sherman function varies as $0.672 2^{S(\theta)} 0.998 1$ and $-0.696 1^{S(\theta)} -0.999$. However, for calculations with the OPMS method, we reveal 10 maximum polarization points for which the Sherman function values vary from $0.999 302$ to $0.999 996$ in the positive excursion and $-0.989 17$ to $-0.999 998$ in the negative excursion. As there is no experimental data, the calculated DCS using the OPMD and OPMS methods have been compared with the available theoretical works of Adibzadeh and Theodosiou [19], Kelemen et al [20] and Kumar et al [16]. So far as we are concerned, this is the first work for the calculation of DCS at projectile energies $E_i = 60, 150, 250, 600, 800$ and $900$ eV for $e$-$Sr$ elastic scattering. The energy dependence of TCS, MTCS, IECS, VCS and INCS, studied in this work, show a non-monotonous pattern for energies beyond about $50$ eV. This work confirms the observation of Haque et al [49] that the positions of extremum spin-polarization are obtainable in the vicinity of CM.
The present work satisfactorily describes the DCS, TCS, MTCS, INCS, VCS and IECS for e–Sr scattering. The performance of the present optical potential analysis using the OPMD and OPMS methods have been shown to be satisfactory in generating the CM in DCS and maximum polarization. The outcome of the present study using the combination of the optical potential and the relativistic and non-relativistic dynamics makes these methods useful for fast generation of accurate cross sections which are needful in the areas of science, technology and industry.

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