A study of the critical minima and spin polarization in the elastic electron scattering by the lead atom

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Abstract

A complex optical potential, in the framework of Dirac partial wave analysis, is employed to study the minima in the differential cross sections (DCSs) and the spin polarization due to the elastic scattering of electron by Pb atom. In addition, integral, momentum-transfer, absorption, viscosity and total cross sections are also reported for the energy region 6 eV \( \leq E_i \leq 10 \) keV. This complex optical potential comprises the static, exchange, polarization and absorption components. We obtain, in total, 12 critical minima (CM) positions, where DCS attains its smallest values and 22 points with of the maximum values of spin polarization (MSP). CM and MSP are found to be correlated in terms of \( E_i \) and scattering angles where the spin-flip amplitude overrides the magnitude of their direct counterpart. As per as we know, there is neither any experimental nor any theoretical study exclusively on CM of e-Pb scattering available in the literature. A detailed comparison shows a good agreement between our predicted results with the available experimental and other theoretical findings.

1. Introduction

The critical minima [1] (CM) in the elastic electron scattering by atoms are those points on the plane formed by electron energy and scattering angle axes at which the differential cross section (DCS) attains the local minima. The role of CM [1, 2] in the electron–atom elastic scattering is important as the scattered electron undergoes total polarization in the vicinity of the deepest minima. Studies of spin asymmetries, which is associated with spin-polarized leptons perpendicular to the scattering plane (the so-called Sherman function), probe an additional degree of freedom and therefore provide more detailed information on the collision process. Spin polarized electron beam is useful in studies of high energy physics and the magnetism of surface and thin film [3]. Such precise scattering characteristics provide a recipe for a crucial test of both the experimental and theoretical studies. The lead (Pb) atom with atomic number \( Z = 82 \), one of the heaviest stable elements, has been detected in the stellar [4–13] and interstellar gas spectra [14, 15]. A systematic study of the collision of electrons with the Pb atoms has been a subject of current research interest to evaluate the abundances of lead in the solar photosphere from the various scattering cross sections.

Both experimental and theoretical studies on the elastic electron scattering by the heavy open-shell Pb atom are very limited in the literature. With open shell structure Pb atom is challenging as the fine structure effects are involved. To the best of our knowledge, neither any experimental nor any theoretical study exclusively on CM of this scattering system is yet unavailable in the literature. Measurements of spin-asymmetry function \( S(\theta) \) on the elastic e-Pb scattering were reported by Kaussen et al [16] for scattering angles \( \theta = 30^\circ–130^\circ \) in the energy range \( E_i = 6–180 \) eV and by Hamelbeck et al [17] for \( \theta = 30^\circ–135^\circ \) and \( E_i = 11–14 \) eV. Williams and Trajmar [18] measured DCS of this scattering system at a single energy \( E_i = 40 \) eV for the scattering angles from 0° to 140°.
Recently, Tošić et al.\textsuperscript{19} have carried out both experimental and theoretical studies on elastic e-Pb scattering and reported elastic DCS, integrated cross section (IECS), momentum-transfer cross section (MTCS), and viscosity cross section (VCS) in the energy range 10–100 eV. They employed Hartree–Fock (HF) and Dirac–Fock (DF) wave functions in their theoretical analysis.

Theoretical studies of DCS for the scattering of electrons by Pb atoms were also reported by Pandya and Baluja\textsuperscript{20} at projectile energies 10–100 eV using a complex optical potential model (OPM) formalism. At low-energies (2.5 ≤ \(E_i\) ≤ 14 eV), Zatsarinny et al.\textsuperscript{21} used the Dirac B-spline R-matrix method to evaluate both the DCS and the spin–symmetry function. Using the R-matrix method, Wijesundera et al.\textsuperscript{22} reported the total cross section (TCS) for the scattering of electrons by Pb atoms for \(0 < E_i < 4\) eV. Haberland and Fritsche\textsuperscript{23} used the generalized Kohn–Sham (GKS) one-particle theory including the relativistic effects to study the elastic scattering of low-energy electrons by Pb atoms. Semi-relativistic R-matrix method has been applied by Bartschat\textsuperscript{24} in the calculation of both the elastic and the inelastic TCSs for the e-Pb scattering in the energy range \(0 < E_i < 7\) eV. Kumar et al.\textsuperscript{25} calculated DCS, IECS, TCS, and MTCS for the e-Pb scattering system in the energy range \(2 \leq E_i \leq 200\) eV using a complex potential in the Dirac equation for scattered electrons. Using a spherical complex optical potential Jain et al.\textsuperscript{26} calculated DCS, MTCS and TCS for electron scattering from germanium and lead atoms in the energy range 100–5000 eV. With inclusion of both the fine-structure of the target atoms and the spin–orbit couplings of the scattered electron, Kaur et al.\textsuperscript{27} reported relativistic distorted wave DCS results for the electron impact scattering of thorium and lead atoms for \(11 \leq E_i \leq 40\) eV. All of these DCS results were published as a function of angle at well separated incident energy grids. But, they did not analyze the energy positions of CM. To the best of our knowledge, for the e-Pb scattering system, there is neither experimental nor theoretical calculation of the absorption cross section (ABSCS) available in the literature.

The positions of the minima in a DCS distribution depend, however, very sensitively on the theoretical method used for prediction. A proper treatment of the exchange potential coupled with a careful choice of the target polarization potential is rather crucial. The elastic scattering of electrons by heavier target atoms can conveniently be described by an effective optical potential (OP) in which the non-local OP is approximated by a local complex OP. We here have employed a suitable complex OP to study DCSs, IECSs, ABSCSs, VCSs, TCSs and S(\(\theta\)) along with a special emphasis on CM in the DCSs for the elastic e-Pb scattering at the incident energies 6 eV ≤ \(E_i\) ≤ 10 keV, using a combination of the components of OP and an analytical electron density function of the target atom. The numerical electron charge density for neutral atoms, generated by the Hartree–Fock method, is represented by a parametrized analytical form by Koga\textsuperscript{28}. The real part of the effective OP includes static\textsuperscript{29}, exchange\textsuperscript{30} and correlation-polarization potentials\textsuperscript{31} which are used to generate the various parts of OP.

Owing to the indistinguishability of the incident and target electrons, the role of exchange remains challenging for an electron scattering. The correlation polarization potential, in the present work, is a combination of the long-range polarization potential of Sun et al.\textsuperscript{32} and a short-range local-density approximation (LDA) correlation potential. The imaginary component of the optical potential, representing absorption, takes into account the loss of the incident flux to all energetically possible inelastic channels \textsuperscript{33} above their threshold. Here we use a parameter-free absorption potential derived, using Linhard dielectric theory\textsuperscript{34}, in free electron gas (FEG) considering electron hole and plasmon interactions. The results of our calculations for various scattering characteristics are compared with the available experimental measurements as well as with other theoretical findings.

The rest of the paper is organized as follows. Section 2 outlines our theory. In section 3, we provide the discussion of our results with the display of figures in comparison with the findings due to available measurements and other theoretical calculations. Section 4 comprises the conclusions on our findings. Atomic units are used throughout unless otherwise specified.

2. Outline of the theory

Electron interaction with atoms, a composite system of electrons and nucleus, is a well known many-body non-local problem. In the optical model approximation, it can, however, be reduced to a two-body problem to make it tractable for solution of either the Schrödinger or Dirac equation for scattering observables. The microscopic OPM is directly formulated from the exact many-body Schrödinger equation on the basis of multichannel expansion. The components of OP can be generated from the knowledge of the wave function of the target. To ease the mathematical problem, all or some of the components are represented by phenomenological analytical expressions. The complex optical potential \(V(r)\) for the e-Pb effective interaction used in our work is given by \[34\]
\[ V(r) = V_d(r) + V_a(r) + V_{qp}(r) - iW_{abs}(r). \]  

(1)

The real components \( V_d(r), V_a(r), V_{qp}(r) \) are, respectively, the static, exchange and correlation-polarization potentials, and \( W_{abs}(r) \) denotes the absorptive imaginary potential. The static potential \( V_d(r) \) has been generated from the procedure adopted in Salvat et al [35], assuming Fermi nuclear charge distribution [36] and Hartree–Fock analytical density function [28] for proton and electron densities, respectively. The exchange potential \( V_a(r) \) uses the semi-classical exchange potential of Furness and McCarthy [37]. Using the non-local exchange interaction coupled with the Wentzel-Kramers-Brillouin (WKB) approximation for the wave functions this exchange potential becomes

\[ V_a(r) = \frac{1}{2} \left[ E_i - V_a(r) \right] - \frac{1}{2} \left\{ \left[ E_i - V_a(r) \right]^2 + 4\pi a_o e^4 \rho(r) \right\}^{1/2}. \]  

(2)

Here \( E_i \) is the incident energy of electron, \( a_o \) is the Bohr radius, \( \rho(r) \) is the electron density function represented by an analytical function normalized to the atomic number as \( \int \rho(r) 4\pi r^2 dr = Z \).

The polarization potential stems from the displacement of the charges of the atom by the incident electron. As per the prescription of Salvat [34], this work uses a global correlation polarization potential \( V_{cp}(r) \) combining the parameter free long-range polarization potential \( V_{cp} \) of Sun et al [32] and the short-range correlation potential \( V_a \) formed from local density approximation (LDA). Thus, \( V_{cp}(r) \) can be expressed as

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

(3)

where \( r_c \) is the outer radius at which short-range \( V_a(r) \) and long-range \( V_{ps}(r) \) cross first.

The long range part \( V_{ps}(r) \) i.e. at long electron-atom distances, is approximated as [32]

\[ V_{ps}(r) = -\frac{\alpha}{2(r^2 + d^2)^{1/2}}, \]  

(4)

where \( \alpha \) is the atomic static polarizability for lead atom and the constant \( d \) can be determined from

\[ V_{ps}(0) = -\alpha/2d^4 \approx V_a(0) \]  

(5)

then

\[ d = (-\alpha/2V_a(0))^{1/2}. \]  

(6)

In LDA, the correlation energy of the projectile at \( r \) is the same as if it were moving within a free electron gas (FEG) of density \( \rho(r) \) equal to the local atomic electron density. Padial and Norcross [31] calculated the correlation potential as the functional derivative of the FEG correlation energy with respect to \( \rho(r) \). Introducing the density parameter

\[ r_s \equiv \frac{1}{a_o} \left[ \frac{3}{4\pi \rho(r)} \right]^{1/3}. \]  

(7)

Perdew and Zunger [38] parametrize the correlation potential as

\[ V_a(r) = -\sum_{n=1}^{\infty} \left( \frac{0.0311 \ln(r_s) - 0.0584 + 0.00133r_s \ln(r_s) - 0.0084r_s}{a_o} \right)^2 \]  

(8)

for \( r_s < 1 \) and for \( r_s \geq 1 \),

\[ V_a(r) = -\frac{e^2}{a_o} \frac{1 + (7/6)\beta_1 r_s^6 + (4/3)\beta_2 r_s^3}{(1 + \beta_1 r_s^6 + \beta_2 r_s^3)^{(2/3)}}, \]  

(9)

where \( \beta_0 = 0.1423, \beta_1 = 1.0529 \) and \( \beta_2 = 0.3334 \).

In this work, we use the absorption potential \( W_{abs}(r) \) originally proposed by Salvat [34] from LDA and then relativistically corrected. This is given by

\[ W_{abs}(r) = \frac{2(E_i + m_e c^2)^2}{m_e c^2 (E_i + 2m_e c^2)} \times A_{abs} \frac{\hbar}{2} \int r^2 \rho(r) \sigma_{bc}(E_i, \rho, \Delta). \]  

(10)

Here, \( m_e \) is the mass of the electron, \( c \) is the velocity of light in vacuum, \( V_i \) is the local velocity of the electron in the electron gas of density \( \rho \) and is given by \( \gamma = (2E_i/m_e)^{1/2} \) corresponding to the kinetic energy \( E_k(t) = E_i - V_a(t) - V_{ps}(t) \). \( \sigma_{bc}(E_i, \rho, \Delta) \) is the cross section for binary collision of electron with the degenerate FEG [37] involving energy transfers greater than a certain energy gap \( \Delta \). In the present calculation, the value of the empirical parameter \( A_{abs} \) is chosen to be 1.2 and the adopted value of the energy gap \( \Delta \) is the first excitation energy of lead atom, \( \epsilon_{1} = 0.97 \text{ eV} \), taken from NIST Physics Reference Data [39].

In the Dirac partial wave analysis, various scattering cross-sections for the electron-atom scattering are directly related to the direct and spin-flip amplitudes \( f(\theta) \) and \( g(\theta) \) respectively. These amplitudes are given [40]
by
\[ f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} [\exp(2i\delta_{l-1}) - 1] P_l(\cos \theta), \]  
(11)
and
\[ g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} [\exp(2i\delta_{l-1}) - \exp(2i\delta_{l-1})] \times P_l(\cos \theta). \]  
(12)

Here, \( P_l(\cos \theta) \) and \( P_l'(\cos \theta) \) denote, respectively, the Legendre polynomials and associated Legendre functions. The relativistic quantum number \( \kappa \) is defined as \( \kappa = (l - j)(2l + 1) \), where \( j \) and \( l \) are the total and orbital angular momentum quantum numbers that are both determined by the value of \( \kappa \); \( j = |\kappa| - 1/2, \ l = j + \kappa/(2|\kappa|) \). \( k \) is the relativistic wave number of the projectile that is in terms of the momentum \( p \) and the kinetic energy \( E_i \) by
\[ (ck)^2 = E_i(E_i + 2m_e c^2). \]  
(13)

In the present study, the phase shifts \( \delta_k \) are calculated from the numerical solution of the radial functions \( P_{E_k}(r) \) and \( Q_{E_k}(r) \) satisfying the following set of coupled Dirac differential equations [41]:
\[ \frac{dP_{E_k}}{dr} = -\frac{\kappa}{r} P_{E_k}(r) + \frac{E_i - V + 2m_e c^2}{ch} Q_{E_k}(r), \]  
(14)
and
\[ \frac{dQ_{E_k}}{dr} = -\frac{E_i - V}{ch} P_{E_k}(r) + \frac{\kappa}{r} Q_{E_k}(r). \]  
(15)

The asymptotic form of the large component \( P_{E_k}(r) \) of the scattering wave function which can be expressed in terms of the complex phase-shift \( \delta_k \), containing the scattering information, as
\[ P_{E_k}(r) \approx \sin \left( kr - \frac{\pi}{2} + \delta_k \right). \]  
(16)

The equations (14) and (15) satisfying the asymptotic condition (16) are solved numerically using the subroutine package RADIAL [42].

The elastic DCS is obtained from the expression
\[ \frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2, \]  
(17)

The IECS, MTCS, VCS and TCS are expressed in terms of the direct \( f(\theta) \) and spin-flip \( g(\theta) \) scattering amplitudes as
\[ \sigma_d = \int_0^{\pi} \int_0^{2\pi} (|f(\theta)|^2 + |g(\theta)|^2) \sin(\theta) d\theta, \]  
(18)
\[ \sigma_n = 2\pi \int_0^{\pi} (1 - \cos \theta)(|f(\theta)|^2 + |g(\theta)|^2) \sin(\theta) d\theta, \]  
(19)
\[ \sigma_s = 3\pi \int_0^{\pi} (1 - \cos \theta)^2(|f(\theta)|^2 + |g(\theta)|^2) \sin(\theta) d\theta, \]  
(20)
and
\[ \sigma_{tot} = \frac{4\pi}{k} \text{Im} f(0). \]  
(21)

Here, \( \text{Im} \) denotes the imaginary part of the expression that follows, and \( f(0) \) denotes the scattering amplitude in the forward direction.

From the relativistic treatment, one can obtain the spin polarization, a measure of the asymmetry of the spin-up and spin-down states of the electron. The expressions for the spin-polarization in terms of the scattering amplitudes is given by [43,44]
\[ S(\theta) = \frac{f(\theta)g^*(\theta) - f^*(\theta)g(\theta)}{|f(\theta)|^2 + |g(\theta)|^2}. \]  
(22)

This equation suggests that the behaviour of the scattering amplitudes \( f(\theta) \) and \( g(\theta) \), respectively, in equations (11) and (12) determines the total polarization points \( S = \pm 1 \) near CM in a DCS distribution. The minimum value of DCS at CM is attributed to the smallness of the direct amplitude from the electrostatic interaction even in comparison to the spin-flip amplitude from the spin-orbit interaction. This results in the total polarization.
3. Results and analysis

3.1. DCS and total cross sections

Figure 1 shows the sensitivity of the various components of the optical potential used in this investigation at incident energies $10^1$, $10^2$, $10^3$ and $10^6$ eV. It is evident from this figure that the static potential $V_{st}$ is the dominant contributor to DCS at all the energies. The contribution of each of the remaining components (exchange $V_{ex}$, polarization $V_{cp}$ and absorption $W_{abs}$) is rather very small in comparison to $V_{st}$ except at small scattering angles $\theta < 15^\circ$. In the forward direction the polarization potential enhances the DCS values, produced by $V_{st}$ noticeably at lower energies. This supports the fact that $V_{cp}$ is a weaker force, which decreases rapidly at higher energies. Absorption part lowers the $V_{st}$ contribution throughout the entire angular domain as it excites the inelastic channels for the scattered elastic electrons. At $E_i \geq 100$ eV, the contributions of the

![Figure 1](image-url)
exchange, absorption and polarization components start becoming negligible compared to that due to $V_{\text{sr}}$. Moreover, addition of these components do not change the positions and numbers of maxima and minima predicted by $V_{\text{sr}}$ only. A similar observation was reported earlier by Chen and Cui [45] for the elastic scattering of electron from Ne and Ar atoms.

In figures 2–4, our DCS results for the elastic electron scattering from lead atoms calculated over the energy range $6 \leq E_i \leq 10000$ eV are compared with the only experimental data of Tošić et al [19] at $E_i = 10, 20, 40, 60, 80$ and $100$ eV. In order to adjudge the effectiveness of our method, the present DCS results are also compared with other theoretical predictions due to the HF of Tošić et al [19] for the same sets of energy and the relativistic approach of Kumar et al [25] for $E_i = 6, 12.5, 17, 24, 50, 100$ and $180$ eV. As far as we know, for $E_i = 6, 12.5, 17, 24.5, 50, 180$ and 200–10000 eV, no experimental data are available in the literature for comparison. These calculations are presented in anticipation that this investigation will motivate future experimental and theoretical studies.

Figure 2. Angle dependent DCS in units of $a_0^2/S_i$ for elastic $e – \text{Pb}$ scattering at the incident energies (a) 6, (b) 10, (c) 12.5, (d) 17, (e) 20, and (f) 24 eV. The thick-solid lines (red) are the present results obtained within the framework of complex optical potential and relativistic Dirac partial wave analysis. Other theoretical predictions are shot-dash lines (blue) from [19] and dash lines (black) from [25]. Solid stars and circles are the experimental data from [18] and [19], respectively.
It is evident from figures 2–4 that the number and positions of the DCS minima show explicit energy dependency. The number of significant minima varies from one at 6 eV (figure 2(a)), 10 eV (figure 2(b)) and 12.5 eV (figure 2(c)) to three at 17 eV (figure 2(d)), 20 eV (figure 2(e)), 24 eV (figure 2(f)), 40 eV (figure 3(a)) and 50 eV (figure 3(b)), and then to two at 60 eV (figure 3(c)), 80 eV (figure 3(d)) and 100 eV (figure 3(e)). With increasing the collision energy the DCSs again reveal three minima at 180 eV (figure 3(f)) and 200 eV (figure 4(a)). With a further increase in collision energy the number of minima increases to four at 250 and 300 eV (figure 4(a)); 400, 450 and 500 eV (figure 4(b)); and 600 eV (figure 4(c)). However, at larger energies, the DCSs again show lesser number of minima, namely three at 700 and 800 eV (figure 4(c)); 900, 1000 and 1200 eV (figure 4(d)) then two at 1500 and 2000 eV (figure 4(e)) and finally one at 5000 eV (figure 4(e)); 7000, 9000 and 10000 eV (figure 4(f)). It is evident from figure 4(f) that, for \( E_i \geq 7000 \) eV, the variation of DCSs with angle is almost monotonous with a shallow minimum in DCSs.

The comparison, in figure 2(b), shows that our DCS results, at \( E_i = 10 \) eV, follow the pattern of the experimental data [19] with an overestimation before and after the minimum position near the scattering angle of 100°. The DF predictions of [19] also overestimate the cross sections at higher scattering angles, while doing better around the range 55°–100°. As seen in figure 2(e), the present results produce a close agreement...
qualitatively as well as quantitatively with the data except a bit of underestimation in the angular region $30^\circ \leq \theta \leq 130^\circ$. It is worth mentioning that the present predicted positions of the three minima near $45^\circ$, $90^\circ$, and $130^\circ$ almost coincide with those of the experimental data. At $E_i = 12.5, 17$ and $24$ eV, respectively, in figures 2(c), (d) and (f) the present results and theoretical values of Kumar et al [25] exhibit oscillations at about the same scattering angles with differences in magnitude. A possible explanation for this discrepancy is likely to be due to the different choices of the interaction potentials and different procedures adopted by these two theoretical studies.

As evident from figures 3(a) at $40$ eV, (c) at $60$ eV, (d) at $80$ eV and (e) at $100$ eV, our DCS results reproduce closely the experimental data of Tosić et al [19] and seem to be comparable to their theoretical predictions [19]. However, the latter calculations significantly underestimate the cross section values of the minima at about

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**Figure 4.** The same as figure 1, but for the incident energies (a) 200, 250 and 300; (b) 400, 450 and 500; (c) 600, 700 and 800; (d) 900, 1000 and 1200; (e) 1500, 2000 and 5000; and (f) 7000, 9000 and 10000 eV. The curves are multiplied by the indicated factor.
\[ \theta = 140^\circ \text{ for } 60 \text{ eV and } \theta = 132^\circ \text{ for } 80 \text{ eV. It is noticeable that at all these energies, our predictions lie closer to the experimental data [19] than those of the other calculations at higher angles. However, at } E_i = 40 \text{ eV, the experimental DCS results of Williams and Trajmar [18] overestimate our calculations and the experimental data of Tošić et al [19] throughout the entire angular range. In figures 3(b) and (f), we compare our DCSs with those of Kumar et al [25]. It is evident that the results due to these two calculations exactly follow the same pattern of variation in the whole angular domain except around } \theta = 80^\circ \text{ for } 50 \text{ eV and } \theta = 110^\circ \text{ for } 180 \text{ eV with shifts in positions of the minima.}

Figure 5 shows the present results of IECs, ABSCS, MTCS, VCS and TCS in the energy range \( 1 \leq E_i \leq 10^3 \text{ eV} \) for e-Pb scattering. We compare our results with the available experimental data from [19], other theoretical findings due to HF and DF of Tošić et al [19] and from the relativistic approach of Kumar et al [25]. As seen in figure 5(a), our results of IECs produce more or less quantitative agreement with the experimental data. Whereas IECs from the other calculations [19, 25] decrease almost monotonically, our
predictions show the maximum, albeit with a shift in position, in line with the experimental data. For MTCS of the e-Pb scattering, in figure 5(b), we obtain a reasonable agreement with the features of the experimental data at the intermediate energy region. However, at about $E_i = 30\text{ eV}$, our present results slightly underestimate both experimental and other theoretical values and overestimate the experiment beyond $E_i = 40\text{ eV}$. It is evident from figure 5(c), our VCS results show reasonable agreement with both the experimental data and other theoretical findings up to 70 eV. At higher energies, our VCS values, although overestimate the experimental data and other theoretical predictions, agree in trend of the DF results [19] with energy variation. As shown in figure 5(e), the present TCS results agree fairly well with those due to Kumar et al [25]. We have found neither experimental nor theoretical results of ABSCS for e-Pb scattering available in the literature for comparison.

3.2. Spin-polarization

Our calculated results for Sherman function $S(\theta)$ in the energy range 6–200 eV are shown in figures 6 and 7 to compare with the experimental data of Kaussen et al [16] and the predictions due to GKS one-particle theory of Haberland and Fritsche [23] at 6, 9, 11, 11.5, 12.2, 12.7, 14, 17, 24 and 180 eV; semi-relativistic R-matrix method of Bartschat [24] at 6 and 9 eV; and relativistic approach of Kumar et al [25] at 6, 9, 11, 14, 17, 24 and 180 eV. We have not found any experimental data as well as any theoretical prediction, at $E_i = 100$ and 200 eV, available in the literature for spin-polarization of e-Pb scattering to compare with.

As seen in figures 6 and 7, our results depict an overall agreement with the experimental data for the incident energies of 6, 9, 17 and 180 eV except for the regions of the absolute maxima in the positive and negative excursions. At these energies, the present results and other theoretical and experimental findings exhibit oscillations at about the same scattering angles but with differences in magnitude. At $E_i = 11, 11.5, 12.2, 12.7, 14$ and 17 eV, our predicted cross sections agree well with the experiment at and beyond the first minimum position with a slight overestimation from this minimum to lower scattering angles. Our results show a mixture of agreement and disagreement with those due to [25]. At 24.0 eV, in figure 7(c), it is revealed that our results produce a reasonable agreement with the experimental data for lower angles ($\theta \leq 80^\circ$) but overestimate the experiment beyond those angles. Nevertheless, our findings provide the best overall description of the experimental data in comparison to other theoretical results [23–25] considered herein.

3.3. CM in DCSs

Figure 8(a) shows the energy dependence of the angular positions of the minima in DCSs. The high angle minima are seen to appear in the DCSs for collision energies up to 10000 eV (figure 8(b)) and their angular positions vary in the range $105^\circ–164^\circ$ (see curve 4). Figure 8(a) also shows that the low angle minima (curve 1) are not found in the DCSs below 17 eV and maintains its appearance up to 600 eV and the angular positions vary from $48.5^\circ$ at 17 eV to $33^\circ$ at 600 eV reaching its minimum at $31.5^\circ$ in the interval 19–22 eV. At all energies below 3000 eV, DCSs show the presence of intermediate angle minima. There is only one minimum in DCSs up to 16 eV, three minima in the range 17–50 eV, two minima in 50–150 eV, three minima in 150–250 eV, four minima in 250–600 eV, three minima in 600–1200 eV and two minima in 1200–3000 eV. Finally, within the wide energy range 3000–10000 eV, the DCSs show only one minimum. As compared to the experimental data of [19] our results show fairly good agreement.

There are some deepest minima which remain conspicuous among the minimal DCS values. In the present calculations, as evident in figure 8(b), predict 13 deep minima in the DCS distributions. Two of such deepest minima are visible at 24 and 250 eV for the low-angle minimum region, depicted in curve 1. For the intermediate-angle minimum regions, corresponding to curves 2 and 3 in figure 8(b), there are six deepest minima at 24, 150, 250, 350, 500 and 1000 eV. And, finally, for high-angle minimum region (curve 4 in figure 8(b)), there are 5 such deepest minima at 20, 150, 250, 600 and 1750 eV. To qualify for a CM point, a DCS minimum must satisfy two important criteria: (i) the DCS values will be several fold smaller than those at the nearest energies and angles, and (ii) the spin-flip scattering amplitude is larger in magnitude than the direct scattering amplitude i.e. $|g(\theta)| > |f(\theta)|$.

Our predicted 12 critical minima qualified among the 13 deepest minima in figure 8(b) are listed in table 1 along with their respective critical energy $E_i$ and critical angle $\theta_c$. The DCS minimum at $[E_i = 250\text{ eV}, \theta_c = 38^\circ]$ does not qualify to be a CM for inclusion in table 1 as it fails to satisfy the second criterion with $|g(\theta)| = 3.8383 \times 10^{-10}$ lesser than $|f(\theta)| = 3.7775 \times 10^{-9}$. In the present calculations, the highest critical energy occurs at $[E_i = 1760\text{ eV}; \theta_c = 137^\circ]$ and the highest critical angle, at $[E_i = 155.3\text{ eV}; \theta_c = 162.5^\circ]$. As no experimental and theoretical data are available in literature, to our knowledge, we compare our results for CM (table 1) with those of the neighboring atom Hg provided by Kelemen and Remeta [46]. At $E_i > 24\text{ eV}$, this comparison shows that the positions of CM in both energy and angle remain very close to those of CM of Hg [46]. This is due to the minor difference in the components of the optical potentials caused by different densities of the above two atoms.
In order to establish the effectiveness of our present model we show the angular dependence of DCS as well as spin polarization for some incident energies in the vicinity of the two critical minima $E_c = 20.2$ eV; $\theta_c = 130.5^\circ$ and $E_c = 155.3$ eV; $\theta_c = 162.5^\circ$. The thick solid (red) lines are the present calculations described in the text. The solid circles are the experimental data of Kaussen et al [16]. Other theoretical predictions are in dash-dotted (green) lines [23]; shot-dash (blue) lines, [24] and dash (black) lines [25].

Figure 6. Angular dependence of spin-polarization $S(\theta)$ for the $e^-\text{Pb}$ scattering at impact energy (a) 6, (b) 9, (c) 11, (d) 11.5, (e) 12.2 and (f) 12.7 eV. The thick solid (red) lines are the present calculations described in the text. The solid circles are the experimental data of Kaussen et al [16]. Other theoretical predictions are in dash-dotted (green) lines [23]; shot-dash (blue) lines, [24] and dash (black) lines [25].
$E_c = 20.2 \text{ eV}$, the $S(\theta)$ values vary from $+0.8$ at $127^\circ$ to $-0.85$ at $133^\circ$. A similar behaviour is also observed for the CM at [$E_c = 155.3 \text{ eV}; \theta_c = 162.5^\circ$] in figure 8(f). All these results demonstrate the profound success of the present electron-atom optical potential in determining the CM positions precisely.

As mentioned earlier, table 1 lists 12 CM positions obtained from our OPM analysis. The importance of determining the CM positions is that the total polarization ($S(\theta) = \pm 1$) of the scattered electrons is obtained in the vicinity of the CM. The positions of the total polarization points calculated in the present study are presented in table 2. We have found a total of 22 points, at each of which, a large polarization ($\geq 90\%$) is achieved in the vicinity. Table 2 also presents the energy widths $\Delta E$ and angle widths $\Delta \theta$, where $|S(\theta)| \geq 0.9$. $\Delta E$ is defined as the difference between $E_c$ and the energy position for the maximum value of $|S(\theta)|$. Similarly $\Delta \theta$ denotes the difference between $\theta_c$ and the angular position of an extremum value of spin-polarization. For example, in

Figure 7. The same as figure 5, but for the impact energy (a) 14, (b) 17, (c) 24, (d) 100, (e) 180 and (f) 200 eV.
table 1, CM occurs at \( E_c = 486.7 \text{ eV}; \theta_c = 68.0^\circ \), the corresponding extremum values are found to appear at:

(i) \( E_m^p = 461.4 \text{ eV}; \theta_m^p = 68.0^\circ \) for \( S(\theta_m^p) = +0.9892 \) with energy width \( \Delta E^p = |E_c - E_m^p| = 486.7 - 461.4 = 25.3 \text{ eV} \) and angular width \( \Delta \theta^p = |	heta_c - \theta_m^p| = 68.0 - 68.0 = 0.0^\circ \); and

(ii) \( E_m^n = 510.1 \text{ eV}; \theta_m^n = 68.0^\circ \) for \( S(\theta_m^n) = -0.9996 \) with energy width \( \Delta E^n = |E_c - E_m^n| = 486.7 - 510.1 = 23.4 \text{ eV} \) and angular width \( \Delta \theta^n = |	heta_c - \theta_m^n| = 68.0 - 68.0 = 0.0^\circ \). It is also evident from tables 1 and 2 that for the CM at
is related to the width of the DCS valley at the corresponding CM position. Similarly, a sum of the angular widths for the maximum polarization for Pb are found very close to those of Hg, a neighboring atom, in absence of available data. Our predicted energy and angular positions of the critical minima in DCSs for the elastic e-Pb scattering. Also are shown the CM results of e-Hg scattering predicted by Kelemen and Remeta [46].

| \( E_c (eV) \) | \( \theta_c (deg) \) | \( |f(\theta)| \) cm | \( |g(\theta)| \) cm | Remark | \( E_c (eV) \) | \( \theta_c (deg) \) |
|---------------|----------------|----------------|----------------|--------|---------------|----------------|
| 20.2          | 130.5          | 8.15E-11       | 1.07E-09       |        | 14.6          | 64.69         |
| 23.8          | 39.5           | 1.01E-10       | 1.22E-09       |        | 17.2          | 124.03        |
| 23.9          | 88.0           | 4.55E-10       | 1.05E-09       |        | 31.3          | 84.22         |
| 148.8         | 113.0          | 9.85E-11       | 4.12E-10       |        | 146.0         | 113.20        |
| 155.3         | 162.5          | 8.11E-12       | 1.44E-10       |        | 157.8         | 161.33        |
| 235.1         | 83.5           | 5.81E-11       | 4.83E-10       |        | 236.4         | 83.12         |
| 274.6         | 146.5          | 5.06E-11       | 1.90E-10       |        | 264.6         | 146.81        |
| 341.5         | 119.0          | 5.85E-11       | 2.77E-10       |        | 334.0         | 119.10        |
| 486.7         | 68.0           | 5.82E-11       | 3.73E-10       |        | 482.1         | 67.92         |
| 580.9         | 153.0          | 1.07E-11       | 1.06E-10       |        | 555.6         | 153.21        |
| 971.0         | 99.0           | 4.64E-11       | 2.73E-10       |        | 916.2         | 99.67         |
| 1760.0        | 137.0          | 1.47E-11       | 1.76E-10       |        | 1656.6        | 137.14        |

Table 1. Calculated maximum polarization \( S(\theta_m) \) points and deviation from critical points for e-Pb scattering in the present study.

| \( S(\theta) \) | \( E_c (eV) \) | \( \pm \Delta E_c (eV) \) | \( \theta_c (deg) \) | \( \pm \Delta \theta_c (deg) \) | \( E_c (eV) \) | \( \theta_c (deg) \) |
|---------------|---------------|----------------|----------------|----------------|---------------|----------------|
| -0.9991       | 20.9          | 0.7            | 132.5          | 2.0           | 17.9          | 126.66        |
| +0.9998       | 19.3          | 0.9            | 127.5          | 3.0           | 15.7          | 119.38        |
| -0.9995       | 27.7          | 3.9            | 36.5           | 3.0           | ...           | ...           |
| +0.9994       | 30.0          | 6.1            | 85.5           | 2.5           | 26.0          | 82.95         |
| -0.8735       | 152.0         | 3.2            | 114.5          | 1.5           | ...           | ...           |
| +0.9988       | 151.1         | 2.3            | 110.5          | 2.5           | ...           | ...           |
| -0.9998       | 157.1         | 1.8            | 161.0          | 1.5           | 159.5         | 160.32        |
| +0.9772       | 153.8         | 1.5            | 164.0          | 1.5           | 156.5         | 162.22        |
| -0.9850       | 252.2         | 17.1           | 82.5           | 1.0           | 248.3         | 82.43         |
| +0.9938       | 217.1         | 18.0           | 85.5           | 2.0           | 224.2         | 84.17         |
| -0.9944       | 271.5         | 3.1            | 147.5          | 1.0           | 264.0         | 147.40        |
| +0.9822       | 275.7         | 1.1            | 146.0          | 0.5           | 265.0         | 146.15        |
| -0.9993       | 368.0         | 26.5           | 117.0          | 2.0           | 349.8         | 118.02        |
| +0.9886       | 327.9         | 13.6           | 120.5          | 1.5           | 322.0         | 120.22        |
| -0.9996       | 510.1         | 23.4           | 68.0           | 0.0           | 502.9         | 67.72         |
| +0.9892       | 461.4         | 25.3           | 68.0           | 0.0           | 462.3         | 68.04         |
| -0.9391       | 585.4         | 4.5            | 152.5          | 0.5           | 560.6         | 152.92        |
| +0.9624       | 577.4         | 3.5            | 153.5          | 0.5           | 551.8         | 153.48        |
| -0.9848       | 969.5         | 1.5            | 100.5          | 1.5           | 939.4         | 100.09        |
| +0.9797       | 951.0         | 20.0           | 98.0           | 1.0           | 894.5         | 99.20         |
| -0.9641       | 1702.0        | 58.0           | 138.5          | 1.5           | 1601.3        | 138.59        |
| +0.9856       | 1812.0        | 52.0           | 135.5          | 1.5           | 1712.1        | 135.59        |

\[ E_c = 23.8 \, eV; \theta_c = 39.5^\circ \] and the corresponding \( S(\theta_m) = -0.9995 \) at \( [E'_c = 27.7 \, eV; \theta'_m = 36.5^\circ] \), the widths are \( \Delta E \theta = 3.9 \, eV \) and \( \Delta \theta = 3.0^\circ \).

The sum of energy widths for the maximum polarization \( S(\theta_m) \) in the positive and negative excursions \( \Delta E \) and \( \Delta \theta \) is related to the width of the DCS valley at the corresponding CM position. Similarly, a sum of the angular widths \( \Delta \theta \) and \( \Delta \theta \) at the extremum values of spin-polarization denotes the angular width of the DCS dip at CM. If we consider CM at \( E_c = 486.7 \, eV \) in table 1 and from table 2 the corresponding \( S = -0.9996 \) at \( E_c = 510.1 \, eV \) with \( \Delta E = 23.4 \, eV \) and \( \Delta \theta = 0.0^\circ \) and \( S = +0.9892 \) at \( E_c = 461.4 \, eV \) with \( \Delta E = 25.3 \, eV \) and \( \Delta \theta = 0.0^\circ \), then the widths of the DCS valley at the CM are \( \Delta E = 23.4 + 25.3 = 48.7 \, eV \) along the energy-axis and \( \Delta \theta = 0.0^\circ + 0.0^\circ = 0.0^\circ \) along the angular axis. However, the latter suggests that the angular DCS distribution at its CM and the corresponding \( S(\theta) \) distribution near \( S = \pm 1 \) are both very sharp. In table 2, we also compare our calculations for maximum spin-polarization with those of Kelemen and Remeta [46] for Hg, a neighboring atom, in absence of available data. Our predicted energy and angular positions of the maximum spin-polarization for Pb are found very close to those of [46] for Hg at \( E_c \geq 30.0 \, eV \) like the situation
for the CM positions in table 1. It is important to note here that our recent results on the $e^-\text{-Hg}$ scattering [2] agree closely with those due to [46].

4. Conclusion

The critical minima in the DCS distributions and the total spin-polarizations in the elastic scattering of electrons by the Pb atoms have been studied systematically for the first time in the energy range $6 \text{ eV} \leq E_c \leq 10 \text{ keV}$ within the framework of relativistic Dirac partial wave analysis using a complex OP. Depending upon the collision energy, the number of minima in the DCSs are found to vary from one to four. The energy and angular positions of 12 CM in DCSs have been revealed and discussed. The critical angle $\theta_c$ varies from 39.5° at the critical energy $E_c = 23.8 \text{ eV}$ to 162.5° at $E_c = 155.3 \text{ eV}$. On the other hand, the critical energy varies from 20.2 eV at $\theta_c = 130.5^\circ$ to 1760 eV at $\theta_c = 137^\circ$. In the proximity of CM positions, 22 maximum polarization points are determined, for each of which the spin-polarization becomes $|S(\theta)| \geq 0.9$. The present DCS results produce a close agreement with the experimental data over the entire scattering angles. Calculated energy dependence of IECS, MTCS, VCS and TCS in the present study show a non-monotonous pattern of the minimum-maximum type for the energies $E_c > 3 \text{ eV}$. These are found to be better, to the best of our knowledge, than other calculations using different electron-atom optical potentials and/or methods. This work confirms the observation of Haque et al. [2] that the positions of extremum spin-polarization are obtainable from the derivative of DCSs in the proximity of CM. The positions of CM and the maximum slopes in the DCS valley provide the respective positions of $S = 0$ and $S = \pm 1$.

The satisfactory performance of our OPM analysis using an effective OP and the relativistic treatment of the collision dynamics clearly unfolds the intriguing aspects of the relation between the CM in DCS and the maximum polarization $|S| \geq 0.9$. Moreover, the non-monotonous energy-variations of IECS, MTCS and VCS from our OPM analysis, conforming to those of the experimental data for the electron elastic scattering on the heavy Pb atom with open-shell configuration. This outcome makes the present method useful for the fast generation of accurate cross sections needed in the areas of science, technologies and industries. More experimental data on electron scattering from other heavier target atoms are required for testing and refining the optical potential, target description and collision dynamics.

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