e± Ar scattering in the energy range 1 eV ≤ E_i ≤ 0.5 GeV

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Abstract
A theoretical investigation on differential, integral, momentum transfer, viscosity cross sections and spin polarization for elastically scattered electrons and positrons from Ar atoms in the energy range 1 eV ≤ E_i ≤ 0.5 GeV is presented. In addition, we have studied the critical minima in the elastic differential cross sections, and the absorption, total and ionization cross sections. Two different theoretical approaches, depending upon the incident energy, are employed for solving the relativistic Dirac equation with the partial-wave decomposition. The solution of the relativistic equation involves the use of either complex optical-model potentials or only nuclear potentials at higher energies. A comparison of the present results with the available experimental data and other theoretical findings produces a reasonable agreement throughout the investigated energy range.

1. Introduction
The study of elastic and inelastic scattering of electrons and positrons from neutral atomic targets is of fundamental importance in understanding not only the complex projectile—atom interaction [1], but also the dynamics of the collision process, structures of atoms, molecules and matters in bulk. The elastic differential cross section (DCS) provides an accurate test for the e± — atom (e− and e+ refer, respectively, to electron and positron) collisions. However, for comparing the theoretical predictions with the experimental observations, the critical minimum (CM) positions in the energy- and angular distribution of the DCS have the advantage over DCSs as the former requires cross sections at fewer energies and angles. Furthermore at CM, the spin polarization S(θ), the so-called Sherman function, attains its extremum values that can provide a more detailed information on the collision process. The spin polarization associated with leptons spin-polarized perpendicular to the scattering plane is of particular interest since it is most easily accessible to experiment and so serves to measure the beam polarization [2, 3]. Electron-impact ionization of atoms and molecules is also a fundamental collision process that occurs in a wide variety of natural and laboratory plasmas. The knowledge of the accurate estimation of the above scattering characteristics is required in such diverse areas as Auger-electron spectroscopy, electron microscopy, microbiological and material science research, etc.

The Ar atom is a dominant constituent of noble-gas discharge plasmas and plays an important role in rare-gas halide lasers and proportional scintillator counters [4]. In the scattering problems, a rare-gas atom is of advantage both for the experimental and theoretical studies. In experimental studies, Ar atoms are often used as an ideal specimen as they are non-reactive, easier to handle and inexpensively available in high purity. Moreover, owing to their closed shell structure, their theoretical treatment is relatively easy. So, the lepton scattering by the atomic Ar, using the relativistic Dirac partial-wave analysis, justifies its importance for the determination of various useful scattering characteristics.
Since the first electron-atom scattering experiments in 1931 [5], many theoretical and experimental studies on $e^\pm$-Ar have been available in the literature [6–8]. Apart from these investigations, the experimental works of Ranković et al [9], Zecca et al [10], Jones et al [11], Kurokawa et al [12], Cho and Park [13], Hargreaves et al [14], Milasavljević et al [15], Mielewska et al [16] and Gilbert et al [17], and the theoretical calculations of Ranković et al [9], Bartchat et al [18], Green et al [19], Fursa and Bray [20], Jones et al [11], Mohan et al [21], MeCharron and Stauffer [22], Bote et al [23], Gargioni and Grosswendt [4], Adibzadeh and Theodosiou [24], Yousif Al-Mulla [25], Jablonski et al [26], Salvat [27], Stepanek [28], Blanco and García [29, 30], Paikday and Alexander [31], Kelemen [32], Bartlett and Stelbovics [33], Sienkiewicz et al [34] and Panda and Shah [35], are worth mentioning among the important works.

In recent years, the theoretical studies on the scattering of electrons and positrons from atoms, employing various model potentials and methods, have enjoyed much interest. In particular, the $e^\pm$-Ar scattering, due to its relatively high excitation threshold, can be well described by a potential scattering model, such as the model-dependent potential [31] based on the dipole polarizability of the target atom, the relativistic optical potential (OP) approximation [11, 32], the OP model (OPM) [23, 27] with or without adjustable parameters, the \textit{ab initio} OP [22], and the spherical OP approach [21]. However, due to the existence of open inelastic channels, the simple potential scattering model becomes inadequate at high incident energies. In order to account for these inelastic channels, we use a complex OPM where the atomic $e^\pm$-Ar interaction potential is valid for $1 \text{ eV} \leq E_i \leq 1 \text{ MeV}$. And for $E_i > 1 \text{ MeV}$, we employ the nuclear structure approach (NSA). In the NSA, for $E_i > 10 \text{ MeV}$, the phase shift analysis for nuclei with spin is supplemented with the distorted-wave Born approximation (DWBA) to account for the magnetic scattering from the nucleus [36]. In the present work, however, we select the most abundant argon isotope, $^{40}\text{Ar}$, which has spin zero and hence the magnetic scattering is absent. Employing both of these methods, we have investigated here the elastic DCS, the integrated elastic cross section (IECS), the momentum transfer cross section (MTCS), the viscosity cross section (VICS), the absorption cross section (ABSCS), the total cross section (TCS), the total ionization cross section (TICS) and the spin polarization for electrons and positrons scattering from Ar atoms. In addition, we also have studied the CMs in DCSs and determined 6 points with maximum values of the spin polarization.

The paper is organized as follows. Section 2 gives a short outline of the theory. In section 3, we present and compare our results systematically with available measurements and other theoretical findings. The conclusion is provided in section 4. Atomic units are used throughout unless otherwise indicated.

2. Outline of the theory

2.1. The OPM method

In the present study, for low and intermediate energies, the effective interaction between a projectile and the target at a distance $r$ from the atomic target is described by means of a complex optical potential as suggested in [27],

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{op}(r) - iW_{ab}(r).$$  (1)

Here, $V_{st}(r)$ is the static potential, $V_{ex}(r)$ is the exchange potential, $V_{op}(r)$ is the correlation-polarization potential and $W_{ab}(r)$ is the modulus of the imaginary absorption potential. For positron scattering, we use the same optical potential as in (1) omitting the exchange part, as the incident positron is not identical to the bound target electrons. The static potential is of opposite sign for electrons and positrons. The correlation-polarization potential accounts for the polarization of the target electron cloud by the impinging projectiles. The imaginary component incorporates the loss of beam intensity to various inelastic channels during the collision.

The static potential $V_{st}$ represents the electrostatic potential of the target atom, which can be expressed as

$$V_{st}(r) = Z_0\varphi(r),$$  (2)

where $Z_{e,\bar{e}}$ is the charge of the projectile ($Z_{e,\bar{e}} = -1$ for electrons and $Z_{e,\bar{e}} = 1$ for positrons). As in [27], the electrostatic potential $\varphi(r)$ is the sum of the electrostatic interactions due to the nucleus $\varphi_n(r)$ and the electron cloud $\varphi_e(r)$. We have

$$\varphi_n(r) = \left(\frac{1}{r} \int_0^r \rho_n(r') 4\pi r'^2 dr' + \int_r^\infty \rho_n(r') 4\pi r'^2 dr'\right)$$  (3)

and

$$\varphi_e(r) = -\left(\frac{1}{r} \int_0^r \rho_e(r') 4\pi r'^2 dr' + \int_r^\infty \rho_e(r') 4\pi r'^2 dr'\right),$$  (4)

where $\rho_n$ and $\rho_e$ are, respectively, the nuclear and electronic charge densities.

This work uses the semi-classical exchange potential of Furness and McCarthy [37], which is derived directly from the non-local exchange interaction by using a WKB-like approximation for the wave functions. This is
Here $E_i$ is the incident energy of electron. The electron density $\rho_e(r)$, represented by an analytical function $F(r)$ due to Koga [38], was calculated from the numerical Hartree–Fock (HF) wave functions, subject to the following approximations

$$\rho_e(r) \equiv F(r) = f_0(r) + \sum_{i=1}^{N_f} c_i f_i(r),$$

where

$$f_0(r) = \rho_e(0) \exp(-2Zr)$$

and

$$f_i(r) = r^n \exp(-\zeta_i r), \quad (i = 1, \ldots, N_f),$$

with $n_i > 0$ and $\zeta_i > 0$.

The assumption (6) for the electron density consists of $N_f + 1$ terms and includes linear $\{c_i\}$ and nonlinear $\{n_i, \zeta_i\}$ fit parameters taken from [38]. For a neutral atom, $\rho_e(r)$, satisfying the following normalization condition,

$$\int_0^{\infty} \rho_e(r) 4\pi r^2 dr = Z,$$

with $Z$ being the atomic number of the target, is used throughout this investigation.

In the present work, we have chosen a global polarization potential $V_{cp}$ due to Salvat [27], which is a combination of the parameter-free long-range polarization potential $V_{cps}$ and the local-density approximation (LDA) correlation potential $V_{co}$. Accordingly, following [27] $V_{cp}$ is given by

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

where $r_c$ is the outer radius at which the short-range potential $V_{co}(r)$ and the long-range potential $V_{cps}(r)$ intersect first.

The long-range part $V_{cps}(r)$, extending to distances where the projectile is far from the atom, is approximated [39] as

$$V_{cps}(r) = -\frac{\alpha}{2(r^2 + d^2)},$$

where $\alpha = 5.1 \times 10^{-24}$ cm$^3$ is the static polarizability for the Ar atom. The constant $d$ can be obtained from [39]

$$V_{cps}(0) = -\alpha/2d^4 \approx V_{co}(0).$$

Thus

$$d = (-\alpha/2V_{co}(0))^{1/4},$$

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 $\rho_e(r)$ equal to the local atomic electron density. Following Padial and Norcross [40], the correlation potential is calculated as the functional derivative of the FEG correlation energy with respect to $\rho_e(r)$. It is convenient to introduce the density parameter

$$r_i \equiv \left[ \frac{3}{4\pi \rho_e(r)} \right]^{1/3}.$$

For electron scattering, the parameterization of the correlation potential due to Perdew and Zunger [41] as adopted in the ELSIPA code [42] is

$$V_{co}(r) = [0.031 \ln(r_c) - 0.058 4 + 0.001 33r_c \ln(r_c) - 0.008 4r_c]$$

for $r_i < 1$, and

$$V_{co}(r) = \beta_0 \frac{1 + (7/6)\beta_1 r_i^2 + (4/3)\beta_2 r_i}{1 + \beta_1 r_i^2 + \beta_2 r_i^2}$$

for $r_i \geq 1$, where $\beta_0 = -0.142 3$, $\beta_1 = 1.052 9$ and $\beta_2 = 0.333 4$. 

\[ V_{co}(r) = \frac{1}{2} [E_i - V_o(r)] - \frac{1}{2} ([E_i - V_o(r)]^2 + 4\pi\rho_e(r))^{1/2}. \]
For positron impact scattering, we use the correlation polarization potential of Jain [43] as given by

$$V_{\alpha}^{(+)}(r) = \frac{1}{2} [1 - 1.82 r_s^{-1/2} + 0.051 \ln(r_s) - 0.115 \ln(r_s) + 1.167],$$

for $r_s < 0.302$,

$$V_{\alpha}^{(+)}(r) = \frac{1}{2} [-0.923 05 - 0.090 98 r_s^{-2}]$$

for $0.302 \leq r_s < 0.56$, and

$$V_{\alpha}^{(+)}(r) = \frac{1}{2} \left[ -8.786 4 n_s \frac{1}{(r_s + 2.5)^2} - 13.151 + 0.955 2 n_s \frac{1}{(r_s + 2.5)^2} + 2.865 5 \frac{1}{(r_s + 2.5)^2} - 0.629 8 \right]$$

for $0.56 \leq r_s < 8.0$.

As the asymptotic region $r_s \gtrsim 8$ is the range beyond the crossing point the polarization potential is accurately given by equation (11). It is, however, important here to note that a misprint in $V_{\alpha}^{(+)}(r)$ has occurred in our previous papers [44–47].

The absorption potential $W_{ab}(r)$ depends on the cross section for binary collisions between the projectile and target electron. Such collisions raise the target electron to a higher energy state and contribute to the absorption of the incident energy. For electron scattering, $W_{ab}(r)$, originally proposed by Salvat [27], is derived by means of a relativistically corrected LDA [42] with

$$W_{ab}(r) = \frac{2(E_k + m_a c^2)^2}{m_a c^2 (E_k + 2m_e c^2)} \times A_{ab} \frac{1}{2} [v_L \rho_e(r) \sigma_{bc}(E_k, \rho_e, \Delta)].$$

Here, $v_L$ is the velocity with which the projectile of rest mass $m_a$ interacts as if it were moving within a homogeneous gas of density $\rho_e$. This velocity of interaction is given by $v_L = (2E_k / m_a)^{1/2}$ corresponding to the local kinetic energy $E_k(r) = E_k - V_{\alpha}(r) - V_{\alpha}(r)$. $\sigma_{bc}(E_k, \rho_e, \Delta)$ is the cross section for the binary collision of the electron with the degenerate FEG [37] involving energy transfers greater than a certain energy gap $\Delta$. In the present electron scattering calculations, the value of the empirical parameter $A_{ab}$ is needed to be 2 for the calculations of the various elastic cross sections and 4.5 for the inelastic cross sections.

The factor 1/2 in equation (21) for the absorption potential for electrons arises from the exchange effect in the binary collision of the incident electron with the electron gas. For positron scattering, the same expression (21) for $W_{ab}(r)$ is used with the omission of the factor 1/2 due to the absence of the exchange effect between the projectile positrons and the target electrons during the collision. For positron scattering, the value of $A_{ab}$ is taken as 0.0 and 2.75, respectively, for the calculations of elastic and inelastic cross sections.

The energy gap $\Delta$, in equation (21), accounts for the energy lost by the projectile and is larger than the first inelastic threshold. For the present computation, the energy gap $\Delta$ is adopted as

$$\Delta = \begin{cases} \epsilon_1 & \text{for electrons,} \\ \max \{ I - 6.8 \text{ eV}, 0 \} & \text{for positrons.} \end{cases}$$

Here $\epsilon_1$ and $I$ are, respectively, the first excitation energy and the ionization potential of the target atom. The value of $\epsilon_1$ for the atomic Ar is taken as $11.55$ eV from NIST Physics Reference Data. The quantity $6.8$ eV is the ground-state binding energy of the positronium atom.

The relativistic Dirac equation for a projectile moving at a velocity $v$ in a central field $V(r)$ following [48] is given as

$$[i \hbar \mathbf{\alpha} \cdot \mathbf{p} + \beta m_e c^2 + V(r)] \psi(r) = E \psi(r).$$

Here $E = m_e c^2 - E_k + m_a c^2$ is the total energy, $\gamma = (1 - v^2/c^2)^{-1/2}$, and $c$ is the velocity of light in vacuum. $E_k$ is again the kinetic energy of the incident particle, while $\mathbf{\alpha}$ and $\beta$ represent the usual $4 \times 4$ Dirac matrices. The relativistic wave function $\psi(r)$, a four-component spinor with quantum numbers $(\kappa \mu \sigma)$, represents the motion of the scattered projectile and is given [49] by

$$\psi_{\text{Exm}}(\mathbf{r}) = \frac{1}{r} \left[ \begin{array}{c} P_{\kappa \sigma}(r) \Omega_{\kappa \mu}(\mathbf{r}) \\ i Q_{\kappa \sigma}(r) \Omega_{\kappa \mu}(\mathbf{r}) \end{array} \right].$$

Here $P_{\kappa \sigma}(r)$ and $Q_{\kappa \sigma}(r)$ represent, respectively, the radial parts of the large and small components of the scattering wave function and $\Omega_{\kappa \mu}(\mathbf{r})$ are the spherical spinors. 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 $\kappa$ as $j = |\kappa| - 1/2$, $l = j + |\kappa|/2$. The large and small components, $P_{\kappa \sigma}(r)$ and $Q_{\kappa \sigma}(r)$, respectively, satisfy the following set of coupled differential equations [49]:
The scattering information is determined from the asymptotic form of the large component $P_{E_{n}}(r)$ of the scattering wave function, which can be expressed in terms of the complex phase-shift $\delta_{\kappa}$ as

$$
P_{E_{n}}(r) \approx \sin \left( kr - \frac{\pi}{2} + \delta_{\kappa} \right).
$$

Here $k$ is the relativistic wave-number of the projectile. The equations (25) and (26) are solved numerically using the subroutine package RADIAL \[30\] to obtain the asymptotic solution in (27).

The scattering amplitude for electrons and positrons, used in the OPM, consists of a direct part $f(\theta)$ and a spin-flip part $g(\theta)$, which are given by

$$
f(\theta) = \frac{1}{2ik} \sum_{l=1}^{\infty} \left[ (l + 1) \{ \exp(2i\delta_{l_{n-1}}) - 1 \} + l \{ \exp(2i\delta_{l_{n-1}}) - 1 \} \right] P_{l}(\cos \theta)
$$

and

$$
g(\theta) = \frac{1}{2ik} \sum_{l=1}^{\infty} \left[ \exp(2i\delta_{l_{n-1}}) - \exp(2i\delta_{l_{n-1}}) \right] \times P_{l}(\cos \theta).
$$

Here, $P_{l}(\cos \theta)$ and $P_{l}^{(1)}(\cos \theta)$ denote, respectively, the Legendre polynomials and associated Legendre functions. $\theta$ is the scattering angle.

The elastic DCS for unpolarized particles and the spin-polarization or Sherman function $S(\theta)$ are obtained in terms of $f(\theta)$ and $g(\theta)$ as

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

and

$$
S(\theta) = i \frac{f(\theta)g^{*}(\theta) - f^{*}(\theta)g(\theta)}{|f(\theta)|^{2} + |g(\theta)|^{2}}.
$$

The integrated elastic, momentum transfer, viscosity and total cross sections are, respectively, defined \[32\] as

$$
\sigma_{el} = \int d\Omega \frac{d\sigma}{d\Omega} = \int_{0}^{\pi} (|f(\theta)|^{2} + |g(\theta)|^{2}) \sin(\theta) d\theta,
$$

$$
\sigma_{m} = 2\pi \int_{0}^{\pi} (1 - \cos \theta)(|f(\theta)|^{2} + |g(\theta)|^{2}) \sin(\theta) d\theta,
$$

$$
\sigma_{v} = 3\pi \int_{0}^{\pi} (1 - \cos \theta)^{2}(|f(\theta)|^{2} + |g(\theta)|^{2}) \sin(\theta) d\theta,
$$

and

$$
\sigma_{tot} = \frac{4\pi}{k} \text{Im} f(0).
$$

Here, $\text{Im} f(0)$ denotes the imaginary part of the direct scattering amplitude in the forward direction at $\theta = 0$.

During the scattering process not only elastic, but also inelastic (absorption) scattering occurs due to the presence of the imaginary part of the optical potential. Therefore, for a given target, the total cross section $\sigma_{tot}$ can be written as

$$
\sigma_{tot}(E_i) = \sigma_{el}(E_i) + \sigma_{abs}(E_i),
$$

where the terms on the RHS denote, respectively, the integrated elastic and total absorption cross sections. As the inelastic channels in $e^\pm$ -atom scattering consist of excitation to discrete states and of ionization, the second term of equation (35) can be further divided,

$$
\sigma_{abs}(E_i) = \sum \sigma_{exc}(E_i) + \sigma_{ion}(E_i).
$$

A fraction or all of the energy lost to the nonelastic channel may be used for the ionization of the target electrons. The first term on the RHS of the above equation arises mainly from the low-lying dipole-allowed transitions and, therefore, the excitation cross sections become progressively smaller beyond the ionization threshold $I$. With increasing incident energy, the second term plays a dominant role due to the availability of infinitely many open channels during the collisions. Therefore, the quantity $\sigma_{abs}(E_i)$ can be employed to compute $\sigma_{ion}(E_i)$. In view of equation (36), these two quantities satisfy the following inequality.
\[ \sigma_{\text{els}}(E_i) \geq \sigma_{\text{ion}}(E_i). \]  

For obtaining an approximation to \( \sigma_{\text{ion}} \) in the present study, we define the energy-dependent ratio of the above two cross sections,

\[ R(E_i) = \frac{\sigma_{\text{ion}}(E_i)}{\sigma_{\text{els}}(E_i)}, \]

with \( 0 \leq R \leq 1 \).

In order to compute \( \sigma_{\text{ion}} \) from \( \sigma_{\text{els}} \), the empirical formula of [51], shown below, has been used

\[ R(E_i) = 1 - A \left\{ \frac{B}{U + C} + \frac{\ln(U)}{U} \right\} \]

where \( U = E_i / I \) is the reduced energy. It is observed in a number of experiments [7, 52–54], that the value of \( R(E_i) \) rises steadily as the energy increases above the threshold, and approaches unity at very high energies. All the above adjustable parameters \( A, B \) and \( C \) are, therefore, determined using the following simple conditions

\[ R(E_i) = \begin{cases} 0 & \text{for } E_i \leq I \\ R_p & \text{for } E_i = E_p \\ R_E & \text{for } E_i \geq E_p > E_p \end{cases} \]

The first of the above three expressions in (41) suggests that no ionization takes place below the ionization threshold. Here, \( R_p [51] \) is the value of \( R \) at \( E_i = E_p \) with \( E_p \) being the incident energy at which the maximum absorption occurs. The present study observes the maximum absorption at \( R_p = 0.75, E_p = 80 \text{ eV} \) for electron scattering and at \( R_p = 0.75, E_p = 28 \text{ eV} \) for positron scattering. At impact energies \( E_i \geq E_p \), well above the peak position \( E_p \), the value of \( R \) increases to \( R_p \) (very close to 1). Here, we obtain \( R_E \approx 0.9 \) at \( E_p = 1000 \text{ eV} \) for electron and \( E_E = 400 \text{ eV} \) for positron scattering. The optimum values of the parameters \( A, B \) and \( C \) are, respectively, found to be \(-1.929, -9.462\) and \(17.256\) for electron scattering; \(-2.163, -6.780\) and \(13.666\) for positron scattering.

### 2.2. NSA method for spin-zero nuclei

In the case of higher energies beyond \( E_i \approx 1 \text{ MeV} \), the projectile passes close to the nucleus, and so only the nuclear interaction part \( V_{\text{nuc}} \) is retained, such that \( V_{\text{ex}}(r) = V_{\text{nuc}}(r) \). It is generated from the nuclear ground-state charge distribution \( \rho_n(r) \), which is normalized to \( Z \),

\[ V_{\text{nuc}}(r) = \int d\mathbf{r}' \frac{\rho_n(r')}{|\mathbf{r} - \mathbf{r}'|}. \]

The phase shift analysis [55, 56] remains the same as applied at the lower energies, using equations (27) and (28) for the calculation of \( f(\theta) \) and \( g(\theta) \). However, for energies \( E_i > 1 \text{ MeV} \), the sum has to be carried out with the help of a multiple convergence acceleration [57]. In our results we have disregarded any loss of beam intensity which may arise either from nuclear excitation or fission.

### 3. Results and analysis

We recall that, in the OPM computation, the electrostatic potential of the electron cloud entering into \( V_{\text{ex}}(r) \) is generated from the Dirac–Fock numerical density [58] following Salvat et al [42]. The exchange potential \( V_{\text{ex}}(r) \) uses the semi-classical exchange potential of Furness and McCarthy [37]. The global correlation–polarization potential \( V_{\text{cp}}(r) \) is the combination of the parameter–free long-range polarization potential \( V_{\text{cp}} \) of Sun et al [39] and the short-range correlation potential \( V_{\text{cor}} \) generated from the local density approximation (LDA) given by Perdew and Zunger [41] for electrons and by Jain [43] for positrons. The absorption potential \( W_{\text{abs}}(r) \) due to Salvat [27] is derived from the relativistically corrected LDA [42].

#### 3.1. Integral, total and ionization cross sections

Figure 1 presents our OPM results for the integral elastic \( \sigma_{\text{el}} \), momentum transfer \( \sigma_{\text{mt}} \), viscosity \( \sigma_v \), absorption \( \sigma_{\text{abs}} \), total \( \sigma_{\text{tot}} \) and total ionization \( \sigma_{\text{ion}} \) cross sections for electron impact scattering at \( 1 \text{ eV} \leq E_i \leq 10 \text{ keV} \) in comparison with the available experimental data and other theoretical results. As seen in figure 1(a), the present \( \sigma_{\text{el}} \) results are in good agreement both qualitatively and quantitatively with the experimental data [59–61] as well as with other theoretical findings [18, 43, 62] with a slight underestimation below around 2 eV. Figure 1(b) compares our OPM predictions for \( \sigma_{\text{mt}} \) with the experimental data [59–61] and the calculations of [18, 63]. As evident from this figure, our cross sections reveal almost the same energy variation pattern and level of agreement with the experimental data and other calculations. Figure 1(c), comparing our result for \( \sigma_v \), with the
and the theoretical prediction of $[64]$, shows that our findings follow the same pattern as the experimental data and other values with a slight overestimation of the latter in magnitude.

In figure 1(d), our results of the absorption cross section $\sigma_{\text{abs}}$ are compared with those from the complex-optical-potential (COP) approach of Jain $[43]$. However, there exist no available experimental data of $\sigma_{\text{abs}}$ to compare with. The comparison of the theoretical results for $\sigma_{\text{abs}}$ reveals a similar energy dependence, except for the energy region below about 20 eV. However, the results of [43] show both a maximum and a minimum, while our cross sections exhibit only one maximum whose position almost coincides with the minimum point of [43]. Our results seem to be consistent with the energy variation of $\sigma_{\text{tot}}$ and $\sigma_{\text{el}}$ which show no minimum point. As seen in figure 1(e), our $\sigma_{\text{tot}}$ results produce reasonably good agreement with the experimental data $[12, 65]$ and other theoretical values $[18, 43, 62, 63]$ apart from the low-energy region below about 3 eV. The inclusion of the absorption part is found to improve the quality of agreement with the experimental data. As expected, beyond

![Figure 1](image-url)
the first excitation energy of 11.55 eV for Ar, \( \sigma_{\text{tot}} \) is greater than \( \sigma_{\text{el}} \), signifying the absorption of some particles into the inelastic channels.

In both atomic and molecular physics, the electron-impact ionization is a fundamental collision process. Ionization cross section data are required in many applied fields such as plasma physics, semiconductor etching, biological and medical sciences, Auger electron spectroscopy, etc. Figure 1(f) shows our ionization cross section \( \sigma_{\text{ion}} \) along with the experimental data [66–71] and the theoretical results due to Bartlett and Srivastava [33]. From this figure, it is evident that our results produce overall good agreement with the experiments, except for a slight discrepancy at lower energies \( E_i < 40 \) eV, but fairly close agreement with the calculations of [33]. The higher experimental values in the threshold region might be due to some indirect processes involved in the ionization.

Figure 2 displays the same quantities as figure 1, but for positron scattering. As apparent from figure 2(a), our results for \( \sigma_{\text{el}} \) produce poor agreement in magnitude, but not in pattern, with the experiment data from [10, 72–77] and other theoretical calculations are due to Green et al [19], Campeanu et al [78] and Laricchia [79].

![Figure 2](image-url)
scattering is considerably different from its electron counterpart. And the cross section values are lower for positron scattering than the corresponding electron scattering. This results basically from the repulsive static potential and the missing exchange potential for positron projectiles. Figures 2(b), (c) and (d) show, respectively, our results of $\sigma_{m}$, $\sigma_{v}$ and $\sigma_{abs}$ for positron scattering. The energy variation of these quantities are almost the same as those due to the electron scattering. So far as we are aware, there are neither experimental data nor theoretical positron results available in the literature to compare with.

Figure 2(e) compares our $\sigma_{tot}$ results for positron scattering with the experimental data [11, 73–75]. As evident, our result follows the same trend in energy variation over the entire energy region and produces a very close quantitative agreement with the experimental data beyond around 20 eV. It is noticeable that the TCS curve for positron scattering is different in shape from that due to the electron scattering. This stems from the differences in electron-atom and positron-atom interacting potentials. In figure 2(f), we compare our $\sigma_{ion}$ results with the experimental data [76, 77] and other theoretical results [78, 79]. Our results produce a good agreement with the experimental data and the other theoretical results.

![Figure 3](image-url)

Figure 3. Angular dependence of the differential cross section of the $e^{-}$-Ar scattering at the incident energies (a) 3, (b) 5, (c) 7.5, (d) 10, (e) 15 and (f) 20 eV. Theory: thick-solid lines (red), the present calculations; broken line (black), [86]; broken line (olive), [87]; das-dot-dashed (blue), [88]. Experimental data are from [13, 16, 59, 61, 80, 81].
agreement with one or another data set in and beyond the peak region. But, below the peak region, our calculated values lie between other theoretical and experimental data.

3.2. DCS for electron scattering

The angular dependence of the DCSs for $e^-\text{-Ar}$ scattering calculated over a wide range of energies, $3 \text{ eV} \leq E_i \leq 10 \text{ keV}$, within the framework of the present complex OPM, is presented in figures 3–9. As seen in these figures, the number of minima in the DCS distributions varies with energy from 2 at $3 \leq E_i \leq 5 \text{ eV}$ to 1 at $7.5 \leq E_i \leq 10 \text{ eV}$ and again to 2 at $15 \leq E_i \leq 150 \text{ eV}$. With a further increase in the collision energy, the DCSs again reveal 1 minimum at $200 \leq E_i \leq 950 \text{ eV}$. For $E_i \geq 1 \text{ keV}$, the DCSs decrease monotonously with energy, without yielding minimum or maximum. Our DCS results are compared with the experiments of Panajotović et al.\cite{59} at $E_i = 10, 15, 30, 40, 60, 75, 80$ and 90 eV; Iga et al.\cite{60} at 400, 800 and 1000 eV; Srivastava et al.\cite{61} at 3, 5, 7.5, 10, 15, 20, 30, 50, 75 and 100 eV; Ranković et al.\cite{9} at 40, 150 and 300 eV; Cho and Park [13] at 5, 10 and 30 eV; Mielewska et al.\cite{16} at 5, 7.5 and 10 eV; Gibson et al.\cite{80} at 3 eV; Dubois and Rudd\cite{81} at 20, 50, 100, 200, 500 and 800 eV; Vušković and Kurepa\cite{82} at 60, 70, 80, 90, 100, 110, 120, 130, 140 and 150 eV; Jansen et al.\cite{83}
at 100, 200, 300, 400, 500, 750, 1000, 2000 and 3000 eV; Williams and Wills [84] at 30, 40, 50, 150, 200, 250, 300 and 400 eV; and Bromberg [85] at 200, 300, 400, 500 and 700 eV.

The present DCS results are also compared with the findings of the modified quasifree-scattering model potential of Blanco and Garcia [30] at $E_i = 800$ eV; the pseudopotential approach of Plenkiewicz et al [86] at 3, 5, 7.5, 10, 15 and 20 eV; the model potential approach of Nahar and Wadehra [87] at 3, 5, 10, 15, 20, 30, 40, 50, 75, 100, 150, 200, 250 and 300 eV; and the OPM calculations of McCarthy et al [88] at 20, 40, 50, 60, 100, 150, 200, 300, 400, 500, 750, 1000, 2000 and 3000 eV. To the best of our knowledge, at energies $E_i = 350, 450, 550, 600, 650, 850, 900, 950$ and 4000–10000 eV, there are neither any measured data nor any other theoretical values for DCSs available in the literature to compare with.

The comparison shows that our results at $E_i = 500$ eV (figures 7–9) produce very close agreement with the experimental data. At low and intermediate energies (at $E_i < 500$ eV; figures 3–6), our results reproduce the experimental data at all angles fairly well, except in the regions of the largest extrema. These deep minima at energies $E_i = 110–140$ eV are not clearly understood. More data and calculations might be helpful to shed light on the presence of these abrupt minima. At the latter energies, all results, including ours and the experiments,
exhibit oscillations at about the same scattering angles but with differences in the magnitude. These differences show the sensitivity of the theoretical models involving different interaction potentials. At \( E_i = 5 \text{ eV} \) in figure 3, the poor agreement of our results with the experiment may be due to the onset of the inelastic threshold that interplays between the real and imaginary components of the OP due to dispersion; this however, could affect the smooth variation in the OP parameters with energy. Nonetheless, at 3 eV, our DCS produces a good agreement with the data for the scattering angles \( 20^\circ \leq \theta \leq 90^\circ \) and shows correctly the oscillatory behavior.

The present DCS results are also in reasonable agreement with those from the model potential [87] at 15, 20 and 30 eV and the OPM calculations [88] at 400, 300, 1000, 2000 and 3000 eV. Although the calculations of ours and [88] employ OPM the components of OPM in the two cases are different. Figure 8(c), at 800 eV, reveals that the modified quasifree scattering model results [30] severely underestimate the experimental data. Figure 10 displays the energy dependence of the DCS and of the Sherman function \( S(\theta) \) for electron scattering at the four scattering angles 50°, 60°, 90° and 120° over the energy range 1 eV \( \leq E_i \leq 0.5 \text{ GeV} \). To cover the full energy domain, two different models, namely OPM for low to intermediate energies \( (E_i \leq 1 \text{ MeV}) \) and NSA for high...
energies ($E_i > 1$ MeV), are employed. For the NSA results in this figure (and also in figure 12), a Fourier-Bessel expansion is taken for the nuclear ground-state charge density [89].

Our DCS results computed with the OPM are compared with the experimental data of Panajotović et al [39], Iga et al [60], Srivastava et al [61], Riley et al [90] and Jansen et al [83]. The NSA predictions for the DCS are compared with the experimental data of Helm [91] at $\theta = 50^\circ$ and $60^\circ$, the experimental data of Ottermann et al [92] and Wendling and Walther [93] at $\theta = 50^\circ$, $60^\circ$ and $90^\circ$ and the experimental data of Schütz et al [94] at $\theta = 90^\circ$ and $120^\circ$. Note that Schütz et al measured the DCS for the scattering angles $\theta = 92.91^\circ$ and $117^\circ$.

Because of the very closeness we have included those data in the plots for the angles $90^\circ$ and $120^\circ$, respectively. The energy-dependent $S(\theta)$ predicted by our OPM is compared with the only experimental data of Beerlage et al [95]. No other experimental data of $S(\theta)$ for higher energies are available to compare with our NSA cross sections.

It is evident from figure 10 that both our present DCS and $S(\theta)$ results from OPM and NSA merge smoothly at the matching point of 1 MeV and show very close agreement with the experimental measurements. But our results of $S(\theta)$ agree less satisfactorily with the experimental data of Beerlage et al [95]. However, as expected, the
minima in $S(\theta)$ below 500 eV relate to the minima in the DCSs. The structures in $S(\theta)$ are much more pronounced than those in the DCS, because of the greater sensitivity of $S(\theta)$ to the choice of the potentials and methods for the calculations. It is also evident that for most energies the magnitude of $S(\theta)$ increases with scattering angle. This may be, for a particular scattering process, due to the significant influence of the stronger nuclear field on $S(\theta)$ at a smaller projectile-nucleus distance.

3.3. DCS for positron scattering
The angular dependence of the DCSs predicted by our OPM theory for positron scattering is depicted in figure 11. We recall that $V_{ct}$ and $V_{nuc}$ for positrons are opposite in sign to those of electrons, while $V_{ex}$ is absent for positron impact scattering. The changes in $V_{cp}$ and $W_{abs}$ are nontrivial. The present results are compared with the experimental data of Dou et al [96] at $E_i = 100$ and 300 eV; Hyder et al [97] at 100, 200 and 300 eV and also with the theoretical cross sections from the model potential approach of Nahar and Wadehra [87]. Our results agree very well with those of [87] except for energies $E_i < 200$ eV at the low scattering angles where there exist

Figure 8. The same as figure 3, but for the incident energies (a) 700, (b) 750, (c) 800, (d) 850, (e) 900 and (f) 950 eV. The experimental data are from [60, 81, 83, 85].
differences, which increase with decreasing positron energy. At large scattering angles, the present DCS results along with those of [87] agree well with the experimental data of [97], but both theoretical cross sections underestimate the data of [96].

Figure 12 provides the energy dependence of the DCSs and of the corresponding spin polarization $S(\theta)$ for positron scattering. The present OPM-predicted DCS results are compared with the experiments of Dou et al [96] at $\theta = 60^\circ, 90^\circ$ and $120^\circ$ and Finch et al [98] at $60^\circ$. Our DCS results agree reasonably well with the experimental measurements. Similar to the case of electron scattering, the magnitude of $S(\theta)$ increases with increasing scattering angles. However, in the low-to-intermediate energy region, the positron spin polarization is considerably smaller than that for electrons. This points to a Coulomb-dominated behavior of the positron potential as discussed in [99]. There are no experimental or theoretical results of the spin polarization for this positron scattering process to compare with. It is anticipated that this investigation might motivate future experimental and more theoretical investigations.

Figure 9. The same as figure 3, but for the incident energies (a) 1000, (b) 2000, (c) 3000, (d) 4000, (e) 5000, 6000, 7000 and (f) 8000, 9000 and 10000 eV. The experimental data are from [60, 83].
3.4. Positions of critical minima in the electron DCS

The angular positions of the low-angle and high-angle minima in the DCS distributions as a function of incident electron energy are shown in figures 13(a) and (b). In order to assess the reliability of our results, a comparison is made with experiments from [59, 61] for both low- and high-angle minima and from [60, 81] for the high-angle minima only. The experimental angles of the minima for the energies 10.3–100 eV are taken from [59]; for $E_i = 100$ eV from [60, 81]; and for $E_i < 10$ eV from [61].

As seen in figure 13(a), the angular position of the low-angle minima ($\theta \leq 80^\circ$) first increases rapidly with energy, reaching a maximum of $72^\circ$ at 19 eV and then falls monotonously to $58^\circ$ at 120 eV. It is worth mentioning that special attention was given to the determination of the location of those minima at energies 10.3–20 eV. Several careful repetitions of the calculations in this study reconfirms their existence. This careful exercise in determining the DCS minima is of interest for the polarization analysis of the scattered electrons.

Figure 10. Energy dependence of DCS and Sherman function $S(\theta)$, in respective order, for electron scattering from the Ar atom at scattering angles $50^\circ$ in insets (a) and (b); at $60^\circ$ in (c) and (d); at $90^\circ$ in (e) and (f); and at $120^\circ$ in (g) and (h). The experimental data for DCS are from [59–61, 83, 90–94] and for $S(\theta)$ from [95].
Starting from 3 eV, our calculated results follow closely the trend of the experimental data with a slight underestimation near the highest scattering angle. Figure 13(b) shows that the position of the high-angle minima reaches its largest value of 140° at around 35 eV. As the electron energy increases above or decreases below 35 eV, the angular position of the minima decreases almost monotonously to a value of 98° at 600 eV and 119° at 10 eV. A further increase in electron energy above 600 eV or decrease below 10 eV leads again to a gradual increase of the position of the high-angle DCS minima. The present results are in close agreement with the experimental data from [61] in the energy region of 10–100 eV and from [81] for 20–850 eV. Our cross sections also follow closely the experiment of Panajotović et al [59], but exhibit a slight underestimation at the highest scattering angle.

With the help of the DCS minima in the angular distribution, the positions of the absolute critical minima with respect to both angle and energy can be traced by plotting the energy dependence of the DCS minima. We display in figures 13(c) and (d) the variation of the low-angle and high-angle minima with energy, as calculated in the present study. As seen in figure 13(c), the number of low-angle deepest minima is only one. In the high-

Figure 11. The same as figure 3, but for the e⁻-Ar scattering at the incident energies (a) 50, (b) 100, (c) 150, (d) 200, (e) 250, and (f) 300 eV. Comparison is made with the theory [87] and the experiments [96, 97].
angle minimum region (figure 13(d)), there are 3 such deepest minima. As a result, there exist in total 4 deepest minima of all minimal DCS values over a wide energy domain up to 1 keV. The energy and angular positions of these deepest minima, denoted respectively by the critical energies $E_c$ and the critical angles $\theta_c$, are listed in table 1. An important criterion for a minimum point in the energy-dependent DCS to be a critical one is that $|g(\theta)|$ must be larger than $|f(\theta)|$, since $f(\theta)$ should be close to a zero \[100\]. Among the 4 deepest minima, obtained in this study, only two (at $E_c = 9.27 \text{ eV}, \theta_c = 117^\circ$ and $E_c = 38.21 \text{ eV}, \theta_c = 141^\circ$) satisfy the preceding criterion of CM. In the present calculations, the deepest minimum, located at $E_c = 124.9 \text{ eV}, \theta_c = 118.5^\circ$ with $|f(\theta)| = 2.36 \times 10^{-11}$ and $|g(\theta)| = 1.87 \times 10^{-11}$, does not qualify to be a CM.

As mentioned earlier, the DCS attains its smallest value at a CM point to be adjudged with a careful scrutiny in the analysis. Figures 13(e) and (f) depict the angular dependence of the DCS for some incident energies in the vicinity of the two critical minima at (9.27 eV, 117°) and (38.21 eV, 141°). As seen in figure 13(e), the DCS reaches its lowest value exactly at the incident electron energy of 9.27 eV. A slight increase to 10.00 eV or

\[
\begin{align*}
\text{Figure 12.} \quad \text{The same as figure 10, but for the e^+ - Ar scattering. The experimental data are from [96, 98].}
\end{align*}
\]
decrease to 8.00 eV affects the DCS values considerably. A similar behavior is also noticed in Figure 13, where the DCS is much lower at 38.21 eV than at $E_i = 36.0$ and 40.0 eV.

Table 1 gives a comparison of our computed positions of the deepest minima in the DCS with those of six experimental [15, 59, 81, 84, 102, 104] and eight other theoretical [15, 22, 32, 34, 88, 101, 103, 105] predictions. It is evident from this table that the angular positions of the deepest DCS minima reported here produce an overall good agreement with the experimental data. As the DCS values are usually reported with a step of 5° in the literature, one may infer that the angular position of any CM is not determined better than ±2.5°. The maximum deviation in angular position between our result and experiment is $|\Delta \theta| = |144° - 143.8°| = 2.8°$ for the critical point at $E_i = 38.21$ eV, $\theta_c = 141°$. This difference, however, remains outside the expected uncertainty. It may be ascribed to the error bar in the experimental DCS deduced from the measured phase shifts.

Figure 13. For $\text{e}^{-}$-Ar elastic scattering, (a) and (b) show the energy dependence of the angular positions, respectively, for the low-angle and high-angle minima in the DCS distributions; (c) and (d) show, respectively, the energy dependence of the low-angle and high-angle minima of DCSs; (e) and (f) show the angular distribution of DCS at $E_i = 8, 9.27, 10$ eV with CM at ($E_c = 9.27$ eV, $\theta_c = 117°$) and $E_i = 36, 36.83, 38$ eV with CM at ($E_c = 36.83$ eV, $\theta_c = 67.5°$), respectively. Experimental data are taken from [59–61, 81].
taken from [22], and to the uncertainty in the theoretical values computed from the relativistic approximation of [34].

Concerning the energy position of the high-angle CMs, our results agree well with the experimental values except those from [102] for $(E_c = 38.1 \text{ eV}, \theta_c = 141^\circ)$. However, a significant difference in the energy position is observed in the case of the low-angle deepest minimum at $(E_c = 36.83 \text{ eV}, \theta_c = 67.5^\circ)$. It may be argued that the angular positions of the DCS low-angle CM for energies between 30 and 40 eV gradually vary from 69° to 66° and are within the experimental angular error bar. Moreover, for this minimum, there are large discrepancies between the experimental values. For example, the positions of the low-angle deepest minimum between [59] and [102] differ in energy by 14.8 eV.

### 3.5. Electron spin polarization

One of the important features of the deepest minima, including the CM, is the fact that in the vicinity of these minima the maximum polarization of the scattered electrons can be found. We performed calculations in the neighborhood of the individual deepest minima to find the energy $E_d$ and angle $\theta_d$ at which the spin polarization $S(\theta)$ reaches extremal values of both signs. Table 2 presents the positions of such maximum polarization points for the three high-angle deepest minima calculated in this study. Comparing tables 1 and 2, we find that for these minima there are pairs of points with extremum polarizations located symmetrically on both sides of the individual position of the above-mentioned deepest minima at the energy position $E_d$ and the angular position $\theta_d$. As seen in table 2, the polarization $S(\theta)$ is found to vary between $+0.54 < S(\theta) < +0.99$ in the positive excursion and $-0.64 < S(\theta) < -0.79$ in the negative one. Thus the required total polarization values of

### Table 1. Energy $E_c$(eV) and angle $\theta$ (degree) positions of the deepest minima in the DCS for elastic $e$-Ar scattering. There exist two CM at the positions $(E_c = 9.27 \text{ eV}, \theta_c = 117.0^\circ)$ and $(E_c = 38.21 \text{ eV}, \theta_c = 141.0^\circ)$ (see text for details).

| Present calculation | Experimental data | Theoretical calculations |
|---------------------|-------------------|--------------------------|
| $E_c$(eV) | $\theta$(deg.) | $E_c$(eV) | $\theta$(deg.) | Reference | $E_c$(eV) | $\theta$(deg.) | Reference |
| 9.27 | 117.0 | — | — | — | 8.76 | 119.22 | [22] |
| & | | — | — | — | 8.44 | 119.89 | [32] |
| 36.83 | 67.5 | 41.3 $\pm$ 0.2 | 68.3 $\pm$ 0.3 | [59] | 31 | 70.4 | [22] |
| & | 47.7 | 66.1 | [81] | 39.3 | 68.5 | [34] |
| & | 56.1 $\pm$ 0.7 | 65.73 $\pm$ 0.05 | [102] | 37.0 | 66.6 | [68] |
| 38.21 | 141.0 | 37.3 $\pm$ 0.2 | 143.5 $\pm$ 0.3 | [59] | 38.29 | 140.83 | [22] |
| & | 42.3 $\pm$ 0.9 | 143.8 $\pm$ 0.2 | [102] | 39.5 | 141 | [34] |
| & | 39.5 | 142.2 | [84] | 38.2 | 141.3 | [68] |
| & | 39.4 | 140.7 | [101] |
| 124.9 | 118.5 | 129.4 $\pm$ 0.5 | 119.4 $\pm$ 0.5 | [15] | 118.0 $\pm$ 0.5 | 118.9 $\pm$ 0.3 | [15] |
| & | 126.1 | 118.9 | [102] | 126.33 | 118.12 | [32] |
| & | 126.9 | 119.0 | [104] | 124.2 | 118.3 | [101] |
| & | 125.2 | 117.3 | [105] |

### Table 2. Calculated maximum polarization points $S_d(\theta)$ and deviation from the critical points for $e$-Ar scattering.

| Present calculation | Walker [103] |
|---------------------|-------------|
| $S_d(\theta)$ | $E_d$(eV) | $\pm \Delta E$(eV) | $\theta_d$(deg.) | $\pm \Delta \theta$(deg.) | $E_d$(eV) | $\theta_d$(deg.) |
| $-0.793 \pm 0.2$ | 9.30 | 0.03 | 117.0 | 0.0 | 11.15 | 115.1 |
| $+0.536 \pm 0.3$ | 9.29 | 0.02 | 116.5 | 0.5 | 11.15 | 114.9 |
| $-0.635 \pm 0.5$ | 38.29 | 0.08 | 141.0 | 0.0 | 42.0 | 141.0 |
| $+0.621 \pm 0.7$ | 38.15 | 0.06 | 141.0 | 0.0 | 42.25 | 140.8 |
| $-0.774 \pm 0.9$ | 123.30 | 1.60 | 119.0 | 0.5 | 137.0 | 118.65 |
| $+0.590 \pm 0.8$ | 124.54 | 0.36 | 118.5 | 0.0 | 138.0 | 118.3 |
$S(\theta) = \pm 1$ are not found for $e^-\text{Ar}$ scattering. However, according to Walker [103], the points with $|S| > 0.5$ could be considered as total polarization. His calculated values for total polarization are also listed in Table 2.

To correlate the positions of the maximum values $S_m(\theta_m)$ of the Sherman function with the position $(E_d, \theta_d)$ of a deepest minimum in the DCS, the energy shift or deviation $\Delta E$ and the angle shift $\Delta \theta$ are introduced. We define the energy shift $\Delta E$ as the distance of the energy position of a maximum value of $|S_m|$ from $E_d$, and similarly $\Delta \theta$ as the angular distance of the position of a maximum value of $|S_m|$ from $\theta_d$. Table 2 lists those deviations for both positive and negative values of the maximum $S_m(\theta_m)$ with respect to the corresponding deepest DCS position. Denoting the deviations from the maximum $S_m(\theta_m)$ with positive and negative values, respectively, by $\Delta E^p$ and $\Delta E^n$, the sum $\Delta E^p + \Delta E^n$, which is the energy distance between the positive and negative polarization maxima, is ascribed to the width in energy of the DCS valley. Similarly, with an equivalent notation of the angular shifts or deviations, the sum $\Delta \theta^p + \Delta \theta^n$ refers to the angular distance between the positive and negative maxima of the spin polarization, corresponding to the angular width of the DCS valley. For

![Figure 14](image-url)
example, in the case of the high-angle DCS valley centered at \( E_c = 38.21 \) eV, \( \theta_c = 141^\circ \), the corresponding \( S_m^0(\theta_m) = -0.635 \) at \( E_m^0 = 38.29 \) eV with \( \Delta E_n = 0.08 \) eV and \( \Delta \theta_n = 0.0^\circ \), while \( S_m^0(\theta_m) = +0.621 \) at \( E_m^0 = 38.15 \) eV with \( \Delta E_n = 0.06 \) eV and \( \Delta \theta_n = 0.0^\circ \). From this, the widths of the DCS valley are \( \Delta E = 0.08 + 0.06 = 0.14 \) eV along the energy axis and \( \Delta \theta = 0.0^\circ + 0.0^\circ = 0.0^\circ \) along the angular axis. The latter suggests that the angular DCS distribution at its CM and the corresponding \( S(\theta) \) distribution near the extremum values of \( S(\theta) \) are both very sharp.

Figure 14 depicts the angular dependence of the spin polarization \( S(\theta) \) for three nearby incident energies in the vicinity of each of the four deepest DCS minima, including the two CMs observed in this study. An important feature of the position \( (E_c, \theta_c) \) of these deepest DCS minima is that only in its proximity \( S(\theta) \) attains both its maximum and minimum. As seen in figure 14(a), our results show that in the vicinity of \( \theta_c = 117^\circ \) at \( E_c = 9.27 \) eV, \( S(\theta) \) varies from +0.54 at \( \theta_m = 116.5^\circ \) to −0.79 at \( \theta_m = 117^\circ \). A similar behavior is observed in the case of \( \theta_c = 67.5^\circ \) at \( E_c = 36.83 \) eV in figure 14(b), \( \theta_c = 141^\circ \) at \( E_c = 38.21 \) eV in figure 14(c) and \( \theta_c = 118.5^\circ \) at \( E_c = 124.90 \) eV in figure 14(d). Figure 14(d) also provides the relative positions of the DCS pattern in addition to the spin polarization \( S(\theta) \) near the DCS minimum. The maximum values \( S_m^0(\theta_m) \) of either sign occur at the maximum slopes in the DCS valley with \( S(\theta) = 0 \) located at the DCS minimum. This suggests that \( S(\theta) \) is determined by the derivative of the DCS in the valley, which lends confirmation to the observation made in Bühring [100] and Haque et al [44]. All these results demonstrate the efficacy of the present electron-atom optical potential in determining accurately the deepest DCS valley and CM positions.

3.6. High-energy considerations

The correspondence between the minima in the differential cross section and the extrema in the Sherman function holds also at energies beyond the MeV region, where diffraction effects from the leptons scattering off individual protons in the target nucleus come into play.

Figure 15 shows the angular dependence of the DCS and of the spin polarization for 248 MeV electrons and positrons colliding with a \(^{40}\text{Ar}\) nucleus, together with the electron scattering data from [92] and [93]. The results for two different nuclear charge densities are shown: the first one provided in terms of a Fourier-Bessel expansion and the second one being a Fermi distribution, \( \rho_F(r) = \rho_0 (1 + e^{-(r/c)^a})^{-1} \) with \( c = 3.53 \) fm\(^{-1} \), \( a = 0.542 \) fm\(^{-1} \) and \( \rho_0 \) the normalization constant [89]. At scattering angles \( \theta \gtrsim 100^\circ \), both DCS and \( S \) become very sensitive to the details of the nuclear charge distribution. In particular, the third minimum in the DCS for electrons is absent for the Fermi distribution. This corresponds to a monotonous behavior of \( S \) in the angular region above \( 130^\circ \). On the other hand, for a Fourier-Bessel type density, the second minimum in the angular distribution is replaced by a shoulder (for positrons) or eventually dies out (for electrons) when the collision energy is increased beyond 250 MeV. In this context one has to keep in mind that the fit of a Fourier-Bessel expanded density, used in the theoretical framework, to experimental scattering data has only been carried out for momentum transfers \( q \) less than 1.8 fm\(^{-1} \) (which for 248 MeV corresponds to angles below \( 92^\circ \)), and hence is not reliable at much higher \( q \). Although the Fermi distribution reproduces the low-\( q \) data less well, its functional dependence is smooth (in contrast to the superposition of oscillating sine terms in the Fourier-Bessel expansion). Hence, for very large momentum transfers, it will still provide reasonable qualitative predictions.
For positrons, as compared to electrons, the onset of the diffraction structures is shifted to higher angles. This can be explained by the repulsive positron-nucleus force, which requires relatively a higher energy. However, for the same energy $E_i$, with a repulsive positron potential, the diffraction pattern moves to larger angles with the decrease of the effective particle momenta. From figure 15(b) it is evident that for high energies the spin polarization oscillates, but keeps globally increasing with scattering angle and reaches its maximum close to 180° (whereas $S = 0$ at 180° due to symmetry reasons [106]). It should be noted that the sign of $S$ in this backmost extremum depends on the choice of the charge distribution, as well as on the lepton energy. This confirms that $S$ is a sensitive probe for nuclear structure properties.

The energy dependence of the minima is displayed in figure 16. In contrast to the low-energy behavior of figure 13, the position of each of the minima (which start to appear near 150 MeV, see figure 16(a)) decreases monotonously with collision energy. The reason is that the nuclear diffraction pattern is determined by the momentum transfer, which for high-energy elastic scattering is given by $q \approx 2(E_i/c) \sin(\theta/2)$. Thus the consequence of an increase of $E_i$ is a decrease of $\theta$ in order to keep $q$ fixed. Figure 16(b) provides the DCS in these minima. We see that in all cases, there is an increase of this minimum DCS with energy, while any critical minima (like those in figures 13(c), (d) are absent. We note, however, that the criterion for the critical minima, namely that the spin-flip part $|g(\theta)|^2$ of the cross section is dominant, holds for all angles above 90° − 95°, irrespective of the lepton energy (for $E_i \geq 150$ MeV).

Another striking difference from the low-energy behavior is the fact that, although $S$ has a resonance structure at the DCS minima, the spin polarization is far below its maximum value 1. In fact, when the rest energy of the projectile becomes negligible, its helicity is conserved during the collision [107]. Thus $|S| \to 0$ as $E_i \to \infty$ [106].

4. Conclusion

We have reported the DCS and the spin polarization $S(\theta)$ calculated for elastically scattered electrons and positrons from the argon atom at collision energies from 1 eV to 0.5 GeV in the framework of the relativistic Dirac partial-wave phase-shift analysis. We have chosen two theoretical approaches: the atomic optical potential for low to intermediate energies (1 eV ≤ $E_i$ ≤ 1 MeV) and the nuclear potential for high energies beyond $E_i = 1$ MeV. The predictions of these two models were shown to match within 1% near $E_i = 1.0$ MeV. It is noticeable that the OPM and NSA methods overlap with each other at the transition energy, predicting accurately the cross section as well as the Sherman function over a broad energy range.

The reported DCS results obtained by the above two approaches produce reasonable agreement with the available experimental data over the entire range of scattering angles. We find, in total, 4 (one low-angle and three high-angle) deepest DCS minima including 2 CM positions, where the DCS attains its smallest value. The energy and angular positions of these DCS valleys have been determined and discussed. The angular position $\theta_d$ of the DCS minima varies from 67.5° at the energy position $E_c = 36.83$ eV to 141° at $E_c = 38.21$ eV. On the other hand, the energy position $E_c$ at the deepest minimum varies from 9.27 eV at $\theta_c = 117°$ to 124.9 eV at

**Figure 16.** (a) Position $\theta_{\min}$ of the first three minima in the DCS and (b) cross section $\frac{d\sigma}{d\Omega}(\theta_{\max})$ for leptons scattering elastically from $^{40}$Ar as a function of collision energy. The positions of the $i$th minima ($i = 1, 2, 3$) are arranged from bottom to top, the DCS in the $i$th minima are arranged from top to bottom. Fourier-bessel type charge density: ——, electrons; ——, positrons. Fermi distribution: ——, electrons; ——, positrons. For the first minimum (bottom lines in (a), top lines in (b)), the results from the two charge distributions are indistinguishable.
In the proximity of the deepest minima, the positions of the six maximum polarization points are determined, where the spin polarization \( S(\theta) \) varies from \( +0.54 \leq S(\theta) \leq +0.99 \) and \( -0.64 \leq S(\theta) \leq -0.79 \). The distance between the positions of the two extrema of spin polarization represents the width of the DCS valley as can be seen in figure 14(d). Experimental DCS values in the valley may offer a sensitive test of the dynamics involved in the scattering process. In the high-energy diffractive regime, beyond 150 MeV, an investigation of the energy dependence of the DCS valleys shows a monotonous decrease of their positions with energy, as well as a monotonous increase of the DCS in these valleys. Hence no additional critical minima are present at energies above 1 keV. The calculated energy dependence of the integral elastic (IECS), momentum transfer (MTCS), viscosity (VCS), total (TCS), absorption (ABSCS) and total ionization cross sections (TICS) in the present study is characterized by the low-energy maximum and the oscillatory pattern in conformity with the trends of the experimental data (see figure 1), except in the case of the ABSCS where we are not aware of experimental data.

The Ar atom with a high excitation energy is found ideal to study the dynamics of \( e^+ \) elastic scattering at low energies and to reveal the details of intricacies involved in the spin polarization in the region of the DCS valley including a deepest minimum. Our predicted results are found to be better, to the best of our knowledge, than other calculated values obtained by using different electron-atom optical potentials and/or methods. We have studied the positron impact scattering as well and have furnished all findings elaborately since experimental results are very sparse. The positron results are expected to be reliable too as evident from their electron counterpart predictions, which agree nicely with the available experimental data. This outcome makes our present method useful for the fast generation of accurate cross sections needed in various application areas of science, technologies and industries.

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