Molecular Physics
An International Journal at the Interface Between Chemistry and Physics

ISSN: (Print) (Online) Journal homepage: https://www.tandfonline.com/loi/tmph20

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To cite this article: Ahmed Abdullah & A. H. Hussain (04 Jan 2024): Critical positions and spin polarisation for electrons scattered by potassium atoms, Molecular Physics, DOI: 10.1080/00268976.2023.2300323

To link to this article: https://doi.org/10.1080/00268976.2023.2300323

MOLECULAR PHYSICS e2300323
https://doi.org/10.1080/00268976.2023.2300323

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RESEARCH ARTICLE

Critical positions and spin polarisation for electrons scattered by potassium atoms

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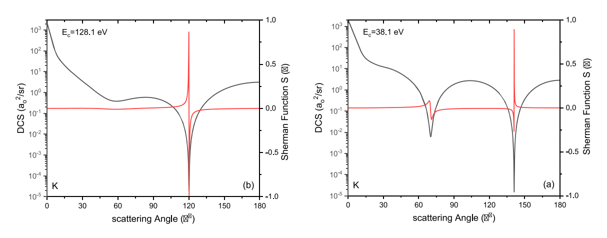
ABSTRACT

The critical points were calculated using the Dirac equation and real optical potential model, in addition to calculating differential, integrated elastic, transfer momentum and viscosity cross sections, and Sherman function for elastic scattering of Potassium atoms at the range 4 to 150 eV and in the angular range $\theta = 0$–180°. We obtained two critical positions (38.1 eV, 141.1°) and (128.1 eV, 120.2°) at these positions we obtained the highest polarisation of spin, and the amplitude of the spin–flip is greater than the amplitude of the direct scattering. This study is considered the first calculation of the critical points in the differential cross sections for electron scattering by potassium atom.



ARTICLE HISTORY
Received 4 October 2023
Accepted 22 December 2023

KEYWORDS
Angular distribution; critical position; DCS; Sherman function; potassium atom

1. Introduction

Electron scattering experiments have an important role in understanding the basic laws of nature [1]. It represents the main tool of modern physics to identify the structure of matter by analysing the results of collisions, and we can extract useful information about the composition of the target from which the electrons are scattered [2]. In addition to their fundamental significance, the collision results are used in many other scientific disciplines, industries, technological advancements, including atomic physics, radiation physics, plasma physics, electronic gas, astrophysics, materials science, electronic spectrum analysis, and many other applications that we cannot mention [3].

The angular distributions of the DCS appear in the electron elastic scattering by the atoms maximum and minima values. The minima are of special importance because, at these small boundaries of the DCS, critical points are formed. The critical energy E_c is the energy of the incident electron at this point, and the critical angle θ_c is the corresponding angle of incidence [4]. One important result of studying critical points in the differential cross sections (DCS) is that, at these points, electrons scattering from atomic targets become completely polarised. The function describing this polarisation is called the Sherman Function, serving as a measure of the degree of spin polarisation. Furthermore, critical points and spin polarisation coefficients provide valuable information for experimental methods and theoretical models [5]. It should be noted that these minima typically exist at one or more electron collision energies and scattering angles for the majority of atoms. Thus, a minor change in either results in an increase in DCS. After scattering, the unpolarised electron beam transforms into a polarised state due to the spin-dependent potential offered by the atomic target to the incident electrons. With an increase in atomic number Z in the spin-dependent potential, the degree of polarisability rises, reaching its maximum at critical points [6].

The focus on studying critical points for scattering electrons from atoms has been shared among numerous researchers, the first researcher to indicate the existence

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of critical points in atoms was the researcher Buhring [7], during his study of spin polarisation in of heavy atoms. Kollath and Lucas [8] presented a practical study to calculate the critical point for scattering electrons from a neon atom. Khare and Raj [9] presented a computational method to calculate critical points for atoms with atomic numbers (6–10) by determining phase shift values at three different energies. Kaushik et al [10] calculation of critical points for the beryllium atom at collision energy (5–30) eV. Khare et al [11] conducted a study to calculate differential and total cross-sections for electrons and positrons from the calcium atom, the results included the determination of critical points and polarisation parameters S(θ), T(θ), and U(θ) at energy levels ranging from (10–500) eV. Milosavljevic et al [12] presented a practical study to determine critical minima in the differential cross-sections for electrons scattered from argon atoms over the energy range (90–150) eV and the angular range (40–126°). Hasan et al [13] conducted a theoretical study to identify critical minima in the calcium atom within the range of (1-2000) eV. Raj and Kumar [14] enabled us to find the critical points for the zinc atom. Sienkiewicz et al [15] presented a theoretical study to determine the critical minima for the zinc and argon atoms. The study of critical points for the argon atom is associated with many researchers such as Lucas [16], M M Haque et al [17], and Panajotovic et al [18]. As for the lead atom, the critical minima and spin polarisation for it have already been identified by A K F Haque et al [19]. The critical points for the copper atom have also been calculated M. Shorifuddoza et al [2].

In this manuscript, we conducted a study to calculate the critical points in differential cross sections when scattering electrons from potassium atoms. For the first time, critical points for the potassium atom have been computed. Additionally, a comparison of the cross-section results was made with various researchers.

The minima observed in the differential cross section (DCS) are highly dependent on the chosen theoretical description method. Utilising relativistic methods allows for the precise determination of both the minima in the DCS and the degree of spin polarisation. Various researchers have demonstrated the important role of relativistic effects in electron scattering from atoms.

2. Outline of the theory

2.1. Partial-wave analysis

In these papers, to investigate the scattering, we used the Dirac equation for a projectile with rest mass m_0 travelling at a velocity v in a central field (r) is given as [20]:

$$[c\boldsymbol{\alpha}.\boldsymbol{p} + \beta m_0 c^2 + V(r)]\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}) \tag{1}$$

When $E = m_0\gamma c^2 = E_i + m_0c^2$ is the total energy, $\gamma = (1 - v^2/c^2)^{-1/2}$ m_0 is the rest mass of the electron, c is the velocity of light in vacuum, E_i is the kinetic energy of the incident electrons, $\boldsymbol{\alpha}$ and β are the usual (4×4) Dirac matrices.$\Psi(\boldsymbol{r})$ is the relativistic wave function with a four-component spinor with quantum numbers κ,m describing the motion of the scattered electron and is given by [21]:

$$\Psi_{Ekm}(\boldsymbol{r}) = \frac{1}{r}\begin{pmatrix} P_{Ek}(r)\Omega_{k,m}(\hat{\boldsymbol{r}}) \\ iQ_{Ek}(r)\Omega_{-k,m}(\hat{\boldsymbol{r}}) \end{pmatrix} \tag{2}$$

Here $P_{Ek}(r)$ and $Q_{Ek}(r)$ represent, the radial parts of the large and small components of the scattering wave function, and $\Omega_{Ek}(r)$ are the spherical spinors, the relativistic quantum number κ is defined as $k = (l - j)(2j + 1)$, where l and j are the orbital and total angular momentum quantum numbers, are both calculated by the value of κ as $j = |k| - 1/2$ and $l = j + k/2|k|$. The radial functions $\mathrm{P_{Ek}(r)}$ and $\mathrm{Q_{Ek}(r)}$ are solved numerically to determine the phase shifts. The pair of coupled differential equations that are satisfied by the large and small components are as follows [22]:

$$\frac{dp_{Ek}}{dr} = -\frac{k}{r}p_{Ek} + \frac{E - V + 2m_ec^2}{c\hbar}Q_{Ek} \tag{3}$$

And

$$\frac{dQ_{Ek}}{dr} = -\frac{E - V}{c\hbar}p_{Ek} + \frac{k}{r}Q_{Ek} \tag{4}$$

The scattering information is calculated using the asymptotic from $r \to 0$ of the large component P_{Ek} of the scattering wave function, which is defined in terms of the phase shift δ_k [23].

$$P_{Ek} \cong \sin\left(kr - l\frac{\pi}{2} + \delta_k\right) \tag{5}$$

Using ELSEPA code [24], Numerical solutions are found for the equations (3) and (4) are satisfying condition (5).

Elastic scattering cross sections for e-atom scattering in the Dirac partial wave analysis are directly related to the direct and spin–flip amplitudes $f(\theta)$ and $g(\theta)$, respectively. These amplitudes come from:

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\{(l+1)[\exp(2i\delta_{k=-l-1}) - 1] + l[\exp(2i\delta_{k=l}) - 1]P_l(cos\theta)\} \tag{6}$$

And

$$g(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}[\exp(2i\delta_{k=l}) - \exp(2i\delta_{k=-l-1})]P_l^1(\cos\theta) \tag{7}$$

Here,$P_l(cos\theta)$ and $P_l^1(\cos\theta)$ denote the Legendre polynomials and associated Legendre functions, respectively. The projectile's relativistic wave number k is correlated with its kinetic energy E_i and momentum p, by:

$$\hbar k = p, \quad (c\hbar k)^2 = E_i(E_i + 2mc^2) \tag{8}$$

2.2. Cross sections and Sherman function

The equation below may be used to calculate the differential cross section (DCS) after determining the phase shift and scattering amplitudes [25]:

$$I(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2 \tag{9}$$

Also, integrate the DCS to produce the elastic cross section (IECS) as follows:

$$\sigma_{el} = \int \frac{d\sigma}{d\Omega}d\Omega = 2\pi\int_0^{\pi}[|f(\theta)|^2 + |g(\theta)|^2]\sin\theta d\theta \tag{10}$$

The elastic momentum transfer cross sections (MTCS) are represented by the following equation:

$$\sigma_m = 2\pi\int_0^{\pi}[1-\cos\theta]\left(\frac{d\sigma}{d\Omega}\right)\sin\theta d\theta \tag{11}$$

The viscosity cross sections (VCS) are represented by the following equation:

$$\sigma_v = 3\pi\int_0^{\pi}[1-(\cos\theta)^2]\left(\frac{d\sigma}{d\Omega}\right)\sin\theta d\theta \tag{12}$$

The Sherman function is considered a measure of the degree of polarisation of atoms when electrons are scattered from atoms, and useful parameter for understanding the spin-dependent interactions between incoming electrons and atomic targets. It's determined by the scattering amplitudes [4]:

$$S(\theta) \equiv i\frac{f(\theta)g(\theta)^* - f(\theta)^*g(\theta)}{|f(\theta)|^2 + |g(\theta)|^2} \tag{13}$$

2.3. Interaction potential

To eliminate the non-local many-body problem and transform it into a one-body problem, we require an interaction potential at electrons incident on an atomic target [1]. The interaction potential $V(r)$ used for the Potassium atom is components of the static $V_{st}(r)$, exchange V_{ex}, and polarisation-correlation potential:

$$V(r) = V_{st}(r) + V_{ex}(r) + V_{cp}(r) \tag{14}$$

Salvat et al [24] method, used to create the static potential $V_{st}(r)$, used the static field approximation to describe the elastic scattering of electrons by treating the target as a uniform distribution of charge. At a distance r of the target nucleus, given by:

$$V_{st} = Z_o e\varphi(r) \tag{15}$$

The electrostatic potential $\varphi(r)$ is the sum of the electrostatic interactions caused by the nucleus $\varphi_n(r)$ and the electron cloud $\varphi_e(r)$ [24]. Z_o is the charge of the scattered particle, which is the charge of an electron ($Z_o = -1$), which expresses the sum of the electrostatic potentials produced from the electronic and nuclear charge distribution. We have:

$$\varphi_n(r) = e\left(\frac{1}{r}\int_0^r \rho_n(r')4\pi r^2 dr' + \int_r^{\infty}\rho_n(r')4\pi r' dr'\right) \tag{16}$$

And

$$\varphi_e(r) = e\left(\frac{1}{r}\int_0^r \rho_e(r')4\pi r^2 dr' + \int_r^{\infty}\rho_e(r')4\pi r' dr'\right) \tag{17}$$

where ρ_e and are ρ_n, respectively, electrons and nuclear charge densities.

We have used the semi-classical exchange potential of Furness and McCarthy [26], which was obtained directly from the formal description of the non-local exchange interaction, by using a WKB-like approximation for the wave functions [27].

$$V_{ex,FM} = \frac{1}{2}[E - V_{st}(r)] - \frac{1}{2}\{[E - V_{st}(r)]^2 + 4\pi a_0\rho_e(r)\}^{1/2} \tag{18}$$

where E represents the electron incident energy. The analytical function developed by Koga represents the electron density ρ_e.

During this calculation, the polarisation-correlation potential model is a combination of the long-range polarisation potential and the short-range correlation potential derived from local density approximation (LDA)

[28]. This potential is expressed in Equation (14) as follows:

$$V^{-}_{cp.LDA}(r) \equiv \begin{cases} max\{V^{-}_{cp}(r), V_{cp.B}(r)\} & if\ r < r_c \\ V_{cp.B}(r) & if\ r \geq r_c \end{cases} \tag{19}$$

$$r_c = 9.47976a.u$$

where the term r_c refers to the outer radius separating the polarisation potential long-range and short-range $V^{-}_{cp}(r)$ as:

$$V_{cp,B}(r) = -\frac{\alpha_d e^2}{2(r^2 + d^2)^2} \tag{20}$$

The value of dipole polarisability of potassium atom $\alpha_d = 4.340 \times 10^{-23} cm^3$ and the constant d denote the phenomenological cut-off parameter serves to prevent the polarisation potential from diverging at $r = 0$. We employ the formulation by Mittleman and Watson [29]. We may get the constant d from:

$$d^4 = \frac{1}{2}\alpha_d a_0 Z^{-1/3} b^2_{pol} \tag{21}$$

where b_{pol} is an adjustable parameter whose value lowers as the projectile rises. As shown by the empirical formula below [17]:

$$b^2_{pol} = max\{(E - 50eV)/(16eV), 1\} \tag{22}$$

According to Padial and Norcross [30], the correlation energy In LDA for a projectile at r is the same as the projectile energy when moving in the FEG at r. The density parameter is easily introduced.

$$r_s \equiv \frac{1}{a_0}\left[\frac{3}{4\pi\rho_e(\mathrm{r})}\right]^{1/3} \tag{23}$$

It is the radius of the sphere containing one in the gas electron, in Bohr radius a_0 units for electrons, the correlation potential model used is the model presented by Perdew and Zunger [31]. Which gives the following:

$$V^{(-)}_{co}(r) = -\frac{e^2}{a_0}(0.0311lnr_s - 0.0584 + 0.00133r_s lnr_s - 0.004r_s) \tag{24}$$

For $r_s < 1$, and $r_s \geq 1$.

$$V^{(-)}_{co}(r) = -\frac{e^2}{a_0}\beta_0\frac{1 + (7/6)\beta_1 r_s^{1/2} + (4/3)\beta_2 r_s}{(1 + \beta_1 r_s^{1/2} + \beta_2 r_s)} \tag{25}$$

When $\beta_0 = 0.1423$, $\beta_1 = 1.0529$ and $\beta_2 = 0.3334$.

3. Results and discussion

The plots below show the angular distribution of the DCS and Sherman function. In addition to IECS, MTCS and VCS, that was estimated for collision of electrons with Potassium atom 4-150 eV at scattering angle of 0-180°. Relativistic calculations are done on the results using an interaction potential in the Dirac equation. All calculations were performed using the ELSEPA code [24]. Figure 1 represents our results for the DCS of electron scattering from potassium atoms at different electron incident energies $E = 7$, 20, 40, 54.4, 100, and 150 eV. Our results were compared with the theoretical results of Madison et al [32], Ratnavelua and Ong [33]. as well as with the experimental results of Buckman et al [32], Srivastava and Vuskovics [34,35]. It was found that the results are consistent with both the theoretical and experimental data. By analysing the differential cross-sectional data, it becomes evident that of critical points are contingent upon factors such as, potential interaction and the methodologies employed in generating the DCS data. The results also indicate the presence of several critical minima in the cross-sectional areas at all energies, with the depth minima reached by the differential cross-section occurring at the critical energy and angles, as illustrated in the Figure 2. These critical points are created as a result of destructive interference between the scattered waves from the bound electrons, so it is DCS very small. Critical points show at low energies. Where our note a regression in the values of the cross-sections when the energies are in Figures 3 and 4, these 2 critical positions along with their respective E_c and θ_c are listed in Table 1, we drew the DCS when the critical energy is fixed and angles change as in Figure 3, as well as when the energy change and the critical angle are constant as in Figure 4 for accuracy in the calculated results. We find that at critical points in DCS, the value of the scattering amplitude spin flip is larger than direct scattering amplitude $|g(\theta)|^2 > |f(\theta)|^2$, this indicates that the dominant interaction at resonant points is the spin–orbit interaction. The E_c and θ_c, located at $(E_c, \theta_c) = (38.1eV, 141.1°)$ with $|f(\theta)|^2 = 0.444 \times 10^{-5} a_o^2/sr$ and $|g(\theta)|^2 = 0.107 \times 10^{-4} a_o^2/sr$, and $(E_c, \theta_c) = (128.1eV, 120.2°)$ $|f(\theta)|^2 = 0.507 \times 10^{-6} a_o^2/sr$ and $|g(\theta)|^2 = 0.183 \times 10^{-4} a_o^2/sr$. Which indicates that the relative effects are clear at critical points.

As the argon atom with an atomic number (Z = 18) is close to the potassium atom with an atomic number (Z = 19), we will compare the critical positions in the differential cross-section with the argon atom. A.R. Milosavljevi´c et al [12] found that the critical positions of experimental results for the argon atom are (129.4 ± 0.5 eV, 119.4° ± 0.5°), similarly, with the

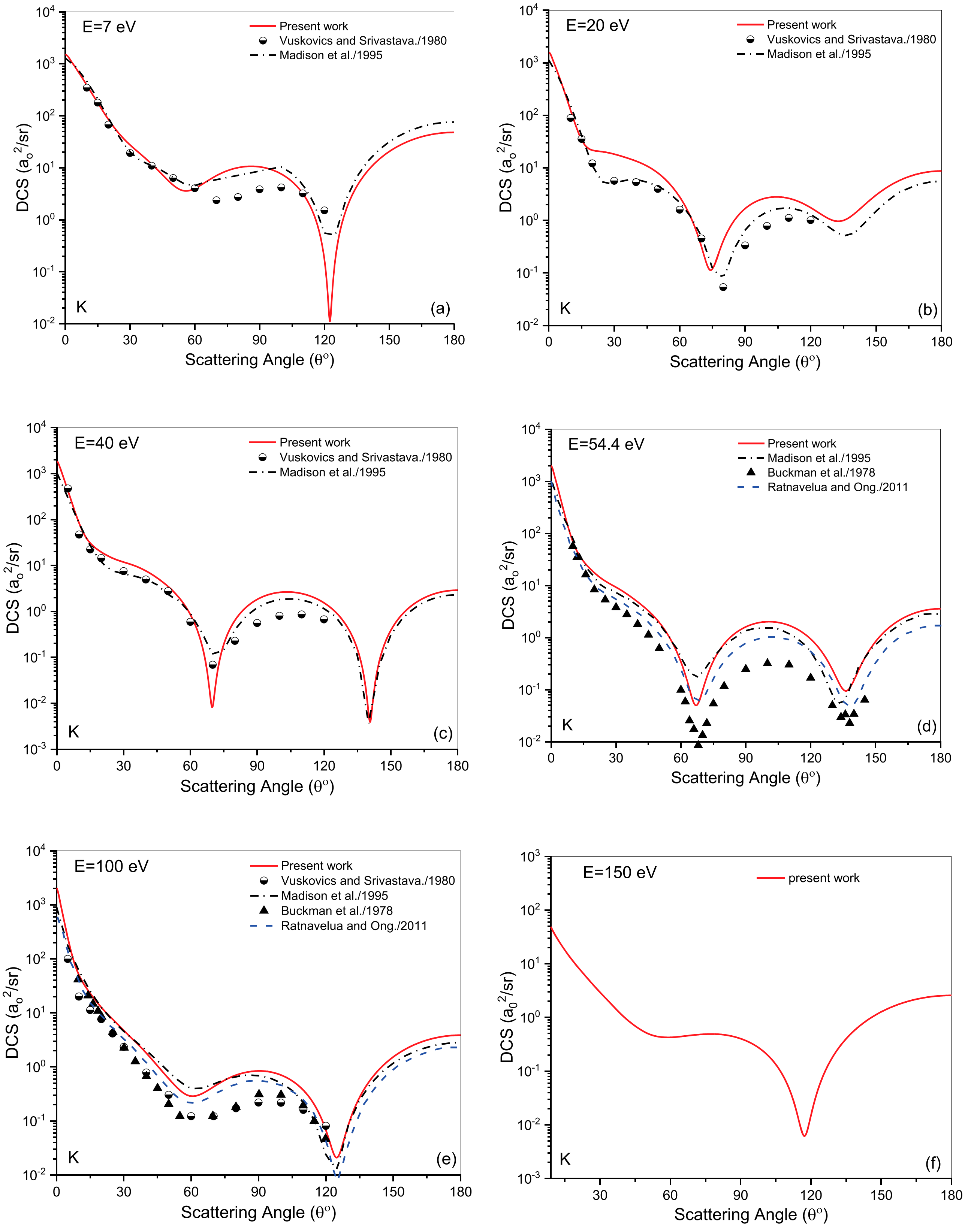

Figure 1. Angular distribution of differential cross section for electron scattering by potassium atoms (a) 7 eV, (b) 20 eV, (c) 40 eV, (d) 54.4 eV, (e) 100 eV, and (f) 150 eV.

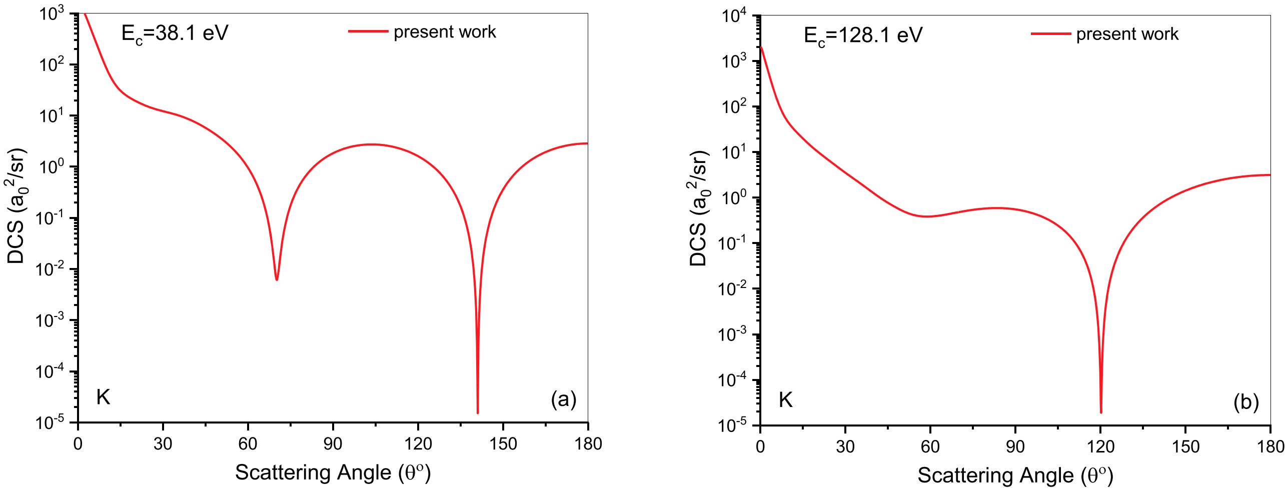

Figure 2. Angular distribution of differential cross section at critical energy for electron scattering by potassium atoms $E_c = 38.1$ eV and $E_c = 128.1$ eV.

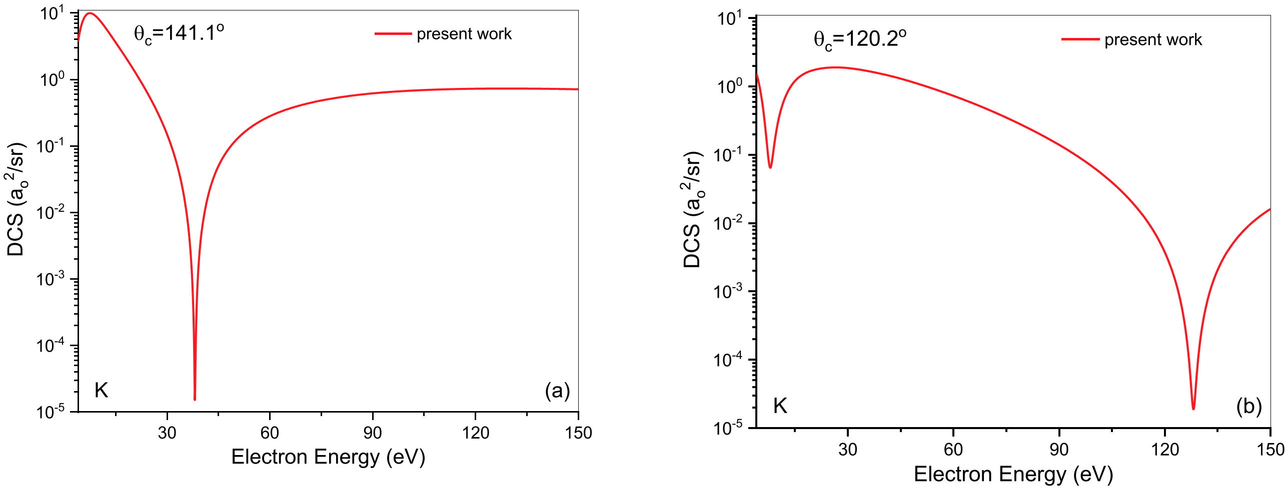

Figure 3. Energy dependence of differential cross section at critical angle for electron scattering by potassium atoms $\theta_c = 141.1°$ and $\theta_c = 120.2°$.

theoretical results of M M Haque et al [17] show critical positions at (38.21 eV, 141°) and (124.9 eV, 118.5°). Finally, the theoretical results of V. I. Kelemen [36] indicate values for critical energy and angle as (38.25 eV, 140.67°) and (126.33 eV, 118.12°). The results indicate that the critical positions of the potassium atom are similar to those of the argon atom because the atomic number of this atom is very close to that of the potassium atom. This comparison was conducted due to the unavailability of data for the critical positions of the potassium atom.

The results of our study are presented in Figure 4 of integrated elastic, momentum transfer and viscosity cross sections for range energy 4 eV $\leq E \leq$ 150 eV electrons scattering from potassium atoms. We correlated our results with the theoretical results of Ratnavelua and Ong [33] and the experimental results of Buckman et al [32], Srivastava and Vuskovics [34], found that the results are in good agreement with the experimental findings.

Table 1. The critical positions (E_c, θ_c) in DCS, $|f(\theta)|^2$ and $|g(\theta)|^2$.

E_c (eV)	θ_c (deg)	$\lvert f(\theta)\rvert^2 a_0^2/sr$	$\lvert g(\theta)\rvert^2 a_0^2/sr$
38.1	141.1	0.444×10^{-5}	0.107×10^{-4}
128.1	120.2	0.507×10^{-6}	0.183×10^{-4}

These cross sections have high values at low energies, which is because the potential of an atom has a greater effect than the incident energy. However, at higher energies, the potential's impact on the incident electron beam weakens, resulting in lower values of the cross section.

It is possible to obtain total electron polarisation for electrons scattered close to these positions, as was already mentioned makes it useful to identify critical positions. To create critical positions in DCS interference must be destructive. Therefore, the spin–flip amplitude $g(\theta)$ larger than the direct amplitude $f(\theta)$. Consequently, the spin polarisation reaches a maximum value. So, total

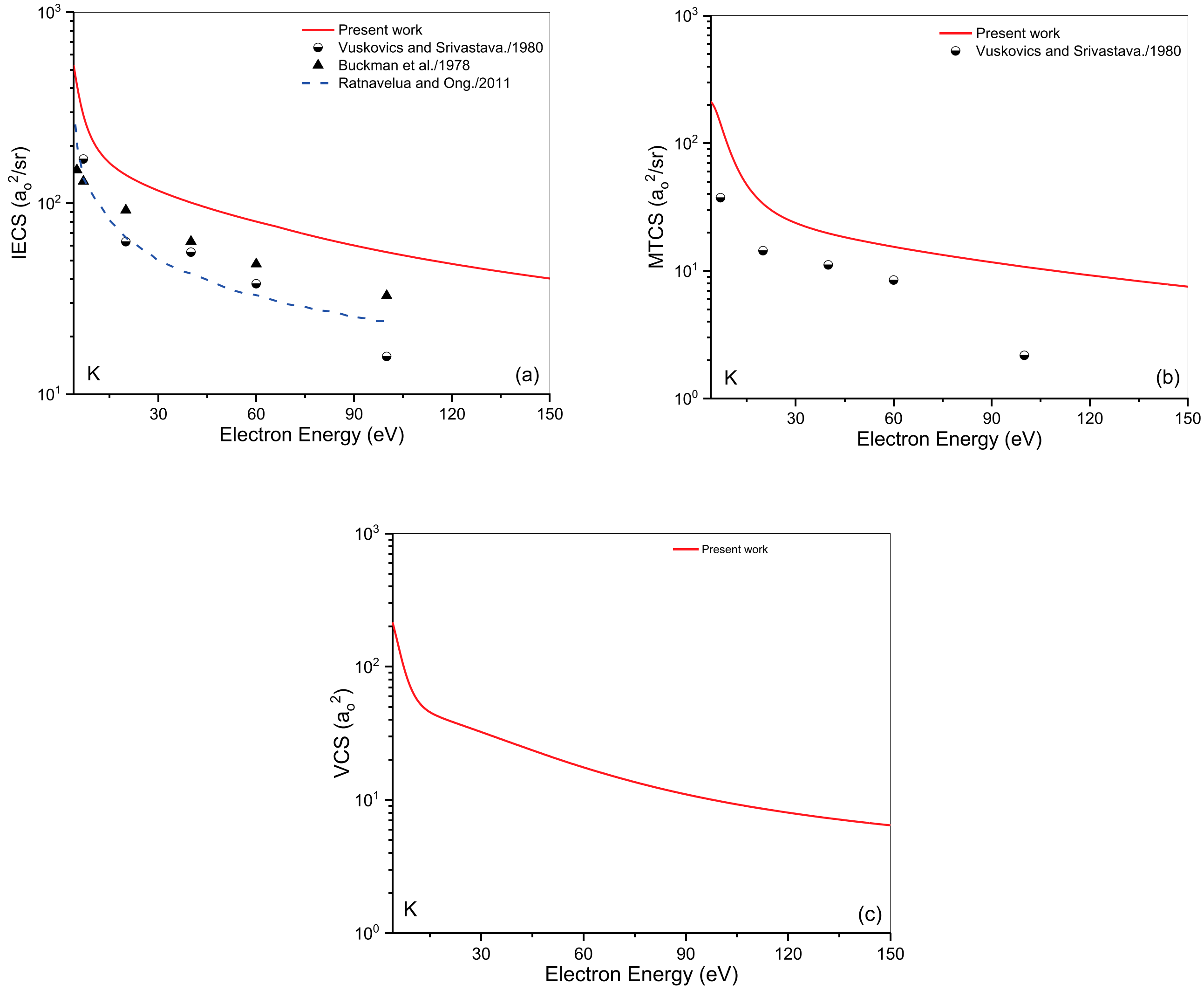

Figure 4. (a) integrated elastic, (b) momentum transfer and (c) viscosity cross-sections for electron scattering by Potassium atoms at range energy $E = 4$–150 eV.

polarisation happens near the critical positions. Our results for Sherman function S(θ) for e-K scattering at incidence energies between 4 and 150 eV are shown in Figure 5. These figures demonstrate the close relationship between the maxima in S(θ) and the minima in the angular distributions of DCS. Several different energies are used to determine the spin-asymmetry parameter, it is clear from the figures that the Sherman function for all energies corresponding to the large differential cross-sections spin polarisation is very weak, while we notice at critical points that the Sherman function is very high, in which the polarisation reaches its maximum value. Figure 6 shows the angular distribution of the Sherman function (spin polarisation) S(θ) at two incident energies near each of the two DCS minima. The location of the innermost DCS minimum has the fundamental property that S(θ) can reach maximum and minimum in its vicinity. Figure 6(a) shows our results that at critical energy $E_c = 38.1$ eV the value of S(θ) $> +0.8$. A similar in Figure 6(b) at critical energy $E_c = 128.1$ eV the value of S(θ) $> +0.95$. This is because the exchange potential has the effect of deepening the DCS. Therefore, the shapes in S(θ) are more obvious in DCS. S(θ) exhibits sharp positive and negative regions close to a critical point, to be more precise Our calculations clearly show that from Figure 6(a,b), near the critical points [$E_c = 38.1$ eV, $\theta_c = 141.1°$] and [$E_c = 128.1$ eV, $\theta_c = 120.2°$].

4. Conclusion

In this article, we present the result of computations for the electrons throughout the collision energy range of 4–150 eV for spin asymmetry parameters, critical points, IECS, MTCS and VCS. These scattering observables were computed using partial wave analysis. We discovered that the cross-section theoretical data is reasonably consistent

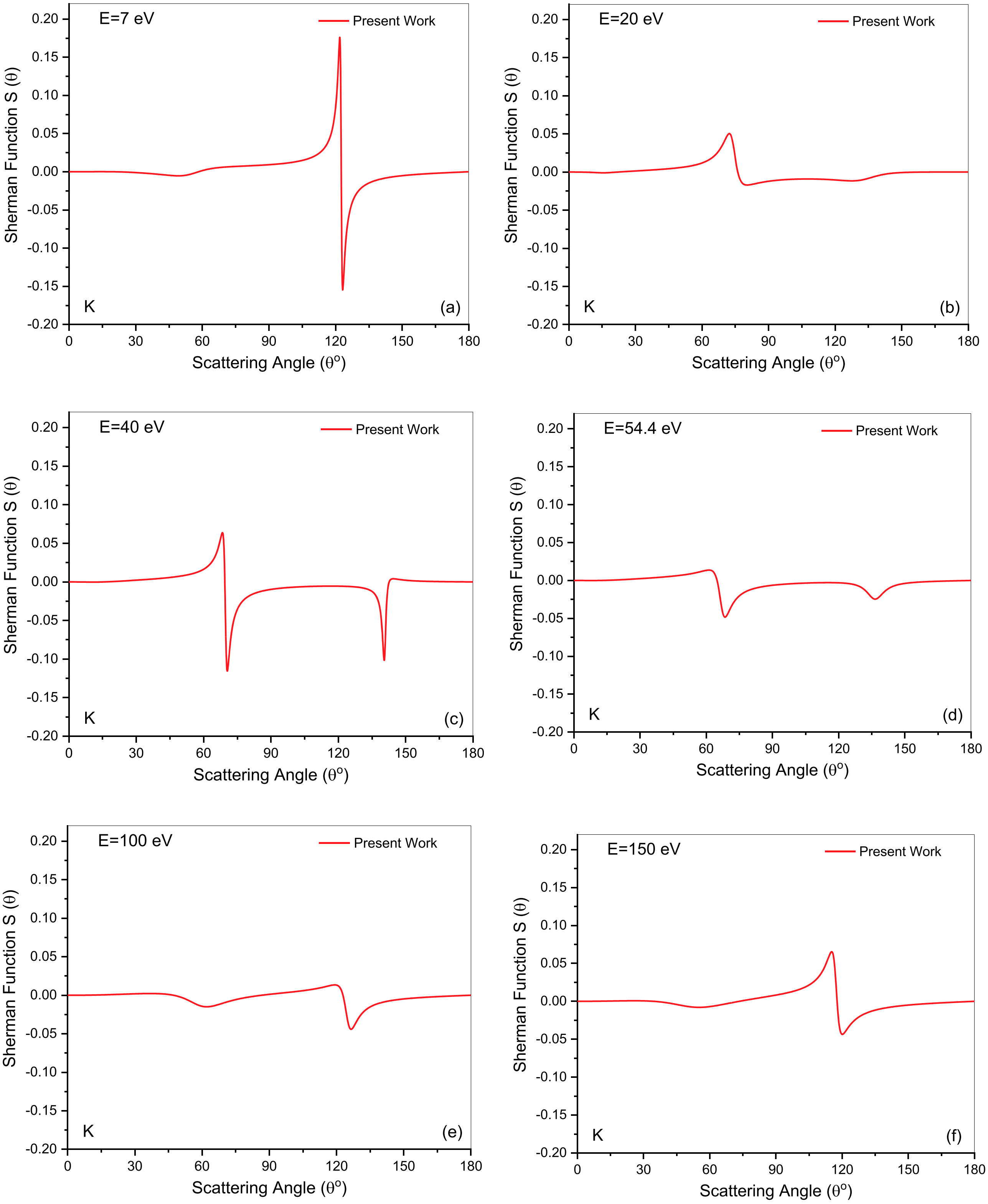

Figure 5. Angular distribution of Sherman function for electron scattering by Potassium atoms (a) 7 eV, (b) 20 eV, (c) 40 eV, (d) 54.4 eV, (e) 100 eV, (f) 150 eV.

with the results available. We got two critical points in differential cross sections at energy and angle when scattering electrons from the Potassium atom, as expected because of the destructive interference between the scattering electrons with the bound electrons of the Potassium atom. When the value of DCS is very sharp, we

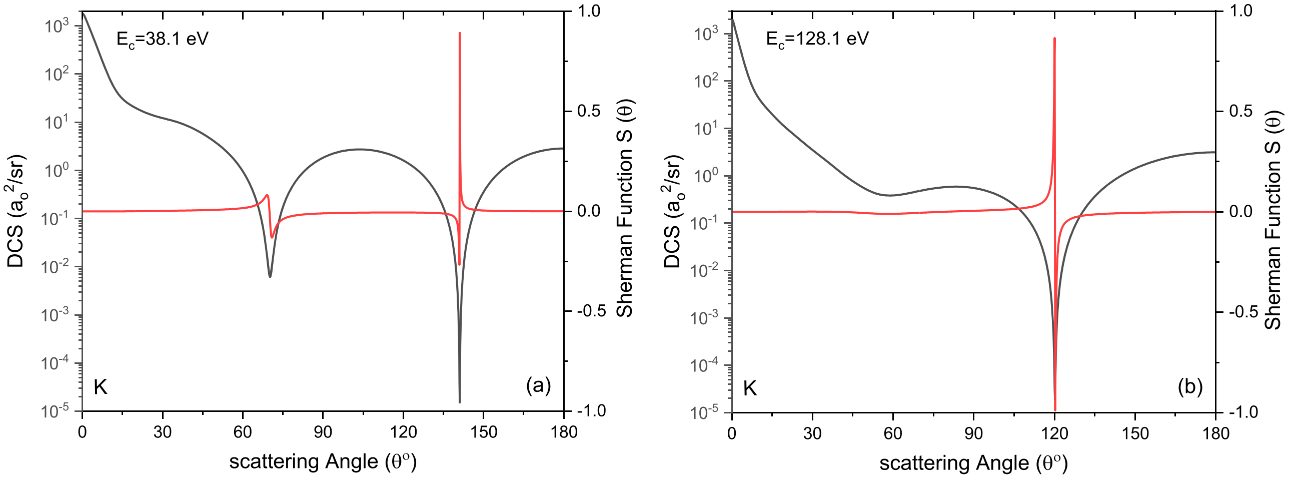

Figure 6. DCS and Sherman function at critical energy for electrons by Potassium atoms (a) 38. 1 eV and (b) 128.1 eV.

can obtain the highest polarisation of spin because the maximum value of spin polarisation is obtained near the angular distribution of critical points. We have concluded that at critical position in the differential cross section, the direct scattering amplitude is smaller than the spin–flip amplitude, this results in the total polarisation. At all energies electrons, once the scattering angle is zero the differential cross section has its highest value, and its value decreases as the scattering angle increases. Future observations and calculations for comparison may benefit from our research of critical points and other scattering observations.

Acknowledgements

I would like to thank Dr. A. H. Hussain for his contribution in adding modifications to ELSEPA code for performing calculations.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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