Electron Scattering By Potassium Atoms

Ahlam K. Yassir[1] Doha Al-Feadh[2]
[1,2]Department of Physics, College of Science, University of Basrh, Basrah, Iraq
[1]Corresponding author. E-mail ahlam.ashour.sci@uobasrah.edu.iq
[2]Corresponding author: E-mail doha.mansoor@uobasrah.edu.iq

Abstract:

This work will determine cross sections for momentum transfer, total cross sections, and differential cross sections (abbreviated as DCSs, TCSs, and MTCSs, respectively) of electron scattering interactions with potassium atoms. Moreover, the spin polarization parameter S(θ) will be established. The calculations encompass an energy spectrum ranging from 5 to 500 electron volts (eV). The Perdew-Zunger correlation potential is included for short-range distances, while the static and polarization potentials are integrated for long-range distances. The results demonstrate a notable agreement with empirical data and the conclusions from earlier theoretical investigations.

Keywords: Dirac equation , Spin Polarization ,K-atoms

استطارة الالكترون بواسطة ذرات البوتاسيوم

احلام خضير ياسر[1] ضحى محمود منصور[2]
جامعة البصرة /كلية العلوم / قسم الفيزياء[1،2]

المستخلص

سوف يحدد هذا الشغل المقاطع العرضية للزخم الانتقالي ، المقاطع العرضية الكلية (DCSs,TCSs,MCSs) على التوالي للالكترونات المستطارة والمتفاعله مع ذرات البوتاسيوم بالاضافه الى ذلك ايجاد معامل استقطاب البرم($\boldsymbol{\theta}$) S، وشملت حسابات طيف الطاقة عند المدى (5-500) الكترون فولت وتضمنت الجهود ، جهد ترابط P-Z لمدى المسافات القصيرة، بينما جهد الاستقطاب والجهد المستقر لمدى المسافات الطويلة.بينت النتائج توافق معقول مع القراءات التجريبية والدراسات النظريةالحديثة.

الكلمات المفتاحية / معادلة ديراك ، ذرات البوتاسيوم ، استقطاب البرم

Introduction:

The mechanism by which electrons are scattered from atoms is a significant occurrence that provides essential insights into the structure and behavior of cosmic entities [1]. The capacity to calculate the cross-sections resulting from electron atomic scattering is crucial in various academic disciplines, including astronomy, meteorology, plasma physics, and biology [2]. Based on Kessler's evaluation, much progress has been made in the theoretical exploration of relativistic phenomena and spin-related occurrences during electron-atom collisions. Specifically, these developments have resulted in significant breakthroughs [1]. The scientific community is aware of and agrees with electron scattering. The interaction between the magnetic moments of electrons and the magnetic field generated by their orbital motion concerning the target atom gives rise to spin-orbit interactions in electron scattering. This interaction is what gives origin to the spin-orbit interaction. As a result, it is seen that the

spin-orbit interaction can exert an impact on the spins of scattering particles, even in cases where the incoming beam of projectiles does not possess polarization. This phenomenon ultimately gives rise to a desirable net spin polarisation. The significance of relativistic interactions in comprehending and interpreting electron scattering by heavy atomic objects has been underscored by recent advancements in polarised electronic resource efficiency and accurate polarisation measurements. In this particular context, a comprehensive investigation has been conducted on various key parameters, namely the spin polarisation parameter S (θ), the differential cross sections (DCS), the total cross sections (TCS), and the momentum transfer cross sections (MTCS), within the framework of the gravimetric elastic-dispersion process in atomic systems. Researchers like Ratnavelu [3], Madison [1995], and Bray et al.[4] have conducted an in-depth investigation of electron scattering from atomic structures. The study conducted by Bray et al. involved the computation of the Differential Cross Section (DCS), Total Cross Section (TCS), and Momentum Transfer Cross Section (MTCS) about the phenomenon of electron scattering by potassium (K) atoms. In the course of this research, an incident energy spectrum spanning from 7 to 500 electron volts was analyzed. For the phenomena of electron scattering by potassium (K) atoms throughout a spectrum of incoming energies ranging from 7 to 500 electron volts (eV), the values of Differential Cross Section (DCS), Total Cross Section (TCS), and Momentum Transfer Cross Section (MTCS) were computed. The crucial elements are the static potential V(r) and the semi-classical exchange potential V(r)ex. The absorption potential V(r)abs, the second component of the complex term, is generated [5]. The computations in this study were initiated by utilizing the Dirac equation as the foundational framework for analyzing the scattering and computational aspects of the system. The study focused on analyzing cross-sectional data, and Sherman functions about the scattering behavior of potassium atoms at different input energy levels. Calculating the Sherman function, often called the spin polarisation function, involves the manipulation of electron collisions within a relativistic framework. This study aims to understand further the discrepancies in spin-up and spin-down asymmetries within the context of electron scattering. This study will thoroughly analyze the theoretical underpinnings employed in this research in Section 2. This section offers new understandings of the kinetics of the electron-target atom interaction and the computation of the spin polarisation coefficient. The presentation of results and the analysis that follows will be covered in Section 3 of this article. The last portion of this study will provide a comprehensive overview of the research's findings, including the notable results and contributions that have enhanced our comprehension of electron scattering phenomena involving potassium atoms." According to the Dirac field theory principles, the following equation represents the path a projectile takes with a rest mass (m_o) and velocity (v) as it passes through a central field. [6].

$$\left[C\alpha.P+\beta m_{\circ}C^{2}+V_{(r)}\right]\psi=E\psi \qquad (1)$$

Where

$E=m_o\,\gamma c^2=\ E_i+\ m_{\circ}\ c^2$ Is the total energy, $\gamma=\left(1-{v^2}/{c^2}\right)^{-1/2}$

Within the Dirac field theory framework, the governing equation can be split into two different equations when dealing with a central potential and considering the kinetic energy of the incident particle, denoted as Ei. These equations involve the conventional 4x4 Dirac matrices, α and β, and describe the behavior of the spinor Ψ, which is composed of four components: Ψ = (ψ1, ψ2, ψ3, ψ4). Among these components, (ψ1, ψ2) are the significant components, while (ψ3, ψ4) represent the minor components of ψ.

$$(g_i^{\pm})''+\left[k^2-I(l+1)r^2-U_l^{\pm}(r)\right]g_l^{\pm}(r)=0 \qquad (2)$$

In this context, $g_i^{\pm}$ corresponds to the radial component of the equation$G_i^{\pm}$, which specifically pertains to the behavior of the significant component of the spinor Ψ, as described in reference [7].

$$G_l=\sqrt{\eta}\frac{g_l}{r}.\eta=\frac{[E-V(r)+m_{\circ}c^2]}{\hbar c}\ .\qquad k^2=\frac{(E^2-m_{\circ}^2c^4)}{\hbar^2c^2}$$

The effective Dirac potentials, denoted as $U_l^{\pm}$ are commonly used in atomic units to describe their properties.$\alpha=\frac{1}{c}$,(m_o = e =ħ =1 ,where α is the fine structure constant)by [8]

$$-U_l^{+}(r)=-2\gamma V+\alpha^2V^2-\frac{3}{4}\frac{(\eta')^2}{\eta^2}+\frac{1}{2}\frac{\eta''}{\eta}+\frac{(l+1)}{r}\frac{\eta'}{\eta} \qquad (3)$$

And

$$-U_l^{-}(r)=-2\gamma V+\alpha^2V^2-\frac{3}{4}\frac{(\eta')^2}{\eta^2}+\frac{1}{2}\frac{\eta''}{\eta}+\frac{1}{r}\frac{\eta'}{\eta} \qquad (4)$$

The variable "r" is represented by a prime (') and a double prime (") to signify its first and second-order differentiation, correspondingly. It is essential to highlight that the ultimate component of Ul +- in Equations (3) and (4) corresponds to the pair of eigenvalues associated with the well-established spin-orbit interaction. In this interaction, one eigenvalue signifies spin up, while the other signifies spin down [7].

$$\frac{\mathbf{1}}{\mathbf{4}m_{\circ}^{2}c^{2}}\frac{\mathbf{1}}{r}\frac{\partial V(r)}{\partial r}\boldsymbol{\sigma}\cdot\boldsymbol{L} \qquad (\mathbf{5})$$

The relationship between the value of l and spin S can be observed by considering the equation j = l + 1/2 for one case and j = l - 1/2 for another case, where j represents the total angular momentum. Additionally, it is worth noting that the value of l is associated with the abovementioned relationship. The solution to equation (2) exhibits asymptotic behavior [9].

$$g^{\pm(k_9 r)=k_r}[j_l\,(kr)-tan(\delta_l^{\pm})\eta_l(kr)] \qquad (\mathbf{6})$$

jl when r and where are the spherical Bessel functions of the first and second classes. The phase shifts in question correlate with incoming particles exhibiting spin up and spin down, denoted by the positive and negative signs. Determining phase shifts may be achieved by evaluating the radial wave function at two adjacent positions, r, and r + h (h), where h represents an infinitesimally small increment. These positions are chosen because of their ability to provide substantial results.

$$tan\,\delta_l^{\pm} = -\frac{(r+h)g_l^{\pm}(r)j_l[k(r+h)] - rg_l^{\pm}(r+h)j_l(k_r)}{rg_l^{\pm}(r+h)\eta_l(kr) - (r+h)g_l^{\pm}(r)\eta_l[k(r+h)]} \qquad (\mathbf{7})$$

The methods in the cited work are used to figure out how much energy is transferred between the bullet and the atom of the target [10].

$$v_{st}(r) = Z_o\ e\emptyset(r)\ =\ Z_o e\,[\emptyset_n\,(r) + \emptyset_e(r)] \qquad (\mathbf{8})$$

The electrostatic potential (E) and charge (Zo e) of the projectile and the target atom, respectively, can be used to calculate the kinetic energy of the hit. It is possible to think of the electrostatic potential (E) as the total of the charges attached to the electron cloud and the atomic nucleus [10].

$$\varphi_n(r) = e\left(\frac{1}{r}\int_0^r \rho_n(r')4\pi r'^2\,dr' + \int_r^{\infty}\rho_n\,(r')4\pi r'\,dr'\right) \qquad (\mathbf{9})$$

And

$$\boldsymbol{\varphi_e(r) = -e\left(\frac{1}{r}\int_0^r \rho_e(r')4\pi r'^2\, dr' + \int_r^\infty \rho_e(r')4\pi r'\, dr'\right)} \qquad (10)$$

$$\boldsymbol{\chi(r) = \frac{r}{Z_e}\emptyset_r} \qquad (11)$$

For spherically symmetric systems with r > 0, the equation can be written as [11].

$$\boldsymbol{\rho_n(r) - \rho_c(r) = \frac{1}{4\pi e r}\frac{d^2}{dr^2}[r\varphi(r)] = -\frac{z}{4\pi r}\frac{d^2x(r)}{dr^2}} \qquad (12)$$

Where $\rho_n(r)$ It is calculated using the Fermi distribution as [11]:

$$\boldsymbol{\rho_n(r) = \frac{\rho_o}{\exp\left[\frac{r - R_n}{Z}\right] + 1}} \qquad (13)$$

In the present investigation, several vital parameters are utilized. Notably, Z is defined as t / (4ln 3), which equates to 0.546 x 10^-13 cm, with t representing the thickness of the skin, measured at 2.4 x 10^-13 cm. The precise definition of thickness is the measurement between 0.9 and 0.1 times the central value of density. In addition, the sign Rn is commonly used to denote the numerical value of 1.07 x 10-13 A (1/3) cm, which is well recognized as the average or half-density radius. In order to achieve normalization, a constant is computed, denoted as twice the proton density at the radial position r = Rn. Determining the electrostatic potential (r) represented by the Fermi distribution necessitates using numerical techniques. In this study, self-consistent relativistic Dirac-Fock (DF) calculations were employed to ascertain the electron densities of unbound atoms with the highest level of precision [11]. The same density function, which is written as r, is used to figure out the electron exchange potential. Furthermore, the simulations conducted in this study integrate the exchange potential model proposed by Furness and McCarthy[12].Regarding the reference's description of the exchange interaction's local approximation [11].

$$\boldsymbol{v_{ex}(r) = \frac{1}{2}[E - v_{st}(r)] - \frac{1}{2}\{[E - v_{st}(r)]^2 + 4\pi a_o e^4 \rho_e(r)\}^{\frac{1}{2}}} \qquad (14)$$

In the context of the projectile's total energy, denoted as E, the correlation-polarization potential Vcpol(r) is introduced. This parameter-free polarisation potential was created based on the correlation energy connected to the target atom. The idea is that the correlation energy of a projectile at point r is similar to that of a projectile moving through a free-electron gas with a density equal to the density of atomic electrons in the area around point r. By using the local density approximation, as described in the mentioned literature, it is possible to

determine the short-range (V_SR(r)) and long-range (V_LR(r)) components of the potential[1,13].

$$\boldsymbol{V_{CpoI}(r) = \begin{Bmatrix} V_{cor}^{SR}(r), & r < r_c \\ V_{POl}^{LR}(r), & r \geq r_c \end{Bmatrix}} \quad (15)$$

In the present context, the initial point of intersection between the two forms occurs at a distinct radius referred to as RC Perdew and Zunger [14]. The present discussion aims to elucidate the behavior of atomic electron scattering at small distances, emphasizing the correlation potential, as expounded in the provided reference [15].

$$\boldsymbol{v_{COR}^{SR}(r) =} \begin{bmatrix} \frac{e^2}{a_\circ}(0.0311\, In(r_s) - 0.058 + 0.0013 r_s\ ln(r_5) - 0.0084 r_s) at\ r_s < 1 \\ -\frac{e^2}{a_\circ}\left(\frac{-0.1423 - 0.1748\sqrt{r_s} - 0.0633 r_s}{(1 + 1.0529\sqrt{r_s} + 0.3334 r_s)^2}\right) at\ r_s \geq 1 \end{bmatrix} \quad (16)$$

Where r_s represents the density parameter, and $\rho_e(r)$ is the undistorted electronic density of the target. As per the Buckingham model [11], the polarization potential exhibits a long-range form:[15]

$$\boldsymbol{\sigma_i\ (\theta) = \frac{d\sigma}{d\Omega} = |f|^2 + |g|^2} \quad (17)$$

S(θ) The spin polarisation parameter, denoted as, is expressed in the following form: [10];

$$\boldsymbol{S(\theta) = \frac{i\,(f g^* - f^*)}{\sigma_i(\theta)}}$$

The utilization of Sherman function S, a parameter that characterizes spin polarisation, is utilized to elucidate the characteristics of scattered electrons in scenarios where the starting electron beam lacks polarization. A three-part effective potential with the symbol V(r) controls the complete interaction between an electron and a target atom: The three potentials being studied right now are the static potential (Vst(r)), the exchange potential $V_{ex}(r)$and the correlation-polarization potential (Vcpo(r)). The calculations described above depend on the target's electron density and provide estimates for the kinetics of collisions.

$$\boldsymbol{f(k,\theta) = \frac{1}{2ik}\sum_{i=1}\{(l+1)[\exp(2i\delta_-^+) - 1] + l[\exp(2i\,\delta_i^-) - 1]\}} \quad (18)$$

&

$$g(k,\theta) = \frac{1}{2ik}\sum_{l=1}^{\infty}[exp(2i\delta_{-}^{+})]P_1^{`}cos(\theta) \qquad (19)$$

The Legendre polynomial (P1), scattering angle (θ), and Legendre-related function (P1cos(θ)) are all covered by the definitions given. If an incoming electron beam is not polarised, the equation for the elastic differential cross-section of that beam may be written as[7]. Even when the input electron beam is not polarised, the spin polarisation defines the spin polarisation parameter (Sherman function) S(θ) (for the scattering electrons). Parameters can be computed as well[16].

$$\mathbf{T}(\boldsymbol{\theta}) = \frac{|f|^2 + |g|^2}{\rho(\theta)} \qquad (20)$$

$$\mathbf{U}(\boldsymbol{\theta}) = \frac{fg^* - f^*g}{\rho(\theta)} \qquad (21)$$

3. Result and Discussion:

In the following section, we present the results of our calculations and engage in a discussion of the findings: Using the relativistic Dirac technique and the ELSEPA software, the cross sections for electron scattering and momentum transfer for a gaseous potassium (K) atom were determined [10]. In Figure 1, the incidence energy for K-atoms is graphically shown for a range of incoming energies, including 7, 20, 54.4, 100, 200, and 300 electron volts (eV). The total cross sections (TCSs) are examined in this study, focusing on the sensitivity of the potential to the energy of the incident electron, particularly at lower energy levels. Figure (2) shows the TCSs for scattering involving K-atoms and contrasts them with the results of Ratnavelu et al.'s theoretical calculations[3]. According to our research, the static effect mainly governs the scattering mechanism. The data support these estimates. Vuskovic et al. claim in their study[17] that discrepancies emerge at low energies, where these sections are notably high. This divergence can be attributed to the substantial influence of electron beams at these energy levels. Figure 3 exhibits momentum transfer cross sections originating from K-atoms, primarily detected at elevated energy levels, lacking comparable reference data. The spin polarization (S) phenomenon is characterized by decreased cross sections for momentum transfer, which depends on electron energy and potential.

Furthermore, the outcomes of our computations regarding spin polarisation (S) in electron scattering by K-atoms are depicted in Figure 4. These calculations encompass a range of impact energies from 5 to 500 eV. It is vital to take into account the fact that the results of this research can vary depending on the quantity of energy that is being introduced, the intensity of the reaction, and the

manner in which the spin-orbit interaction (SOI) is changed in relation to other factors. We must emphasize that the outcomes of our approach are perfectly consistent with those of other researchers.

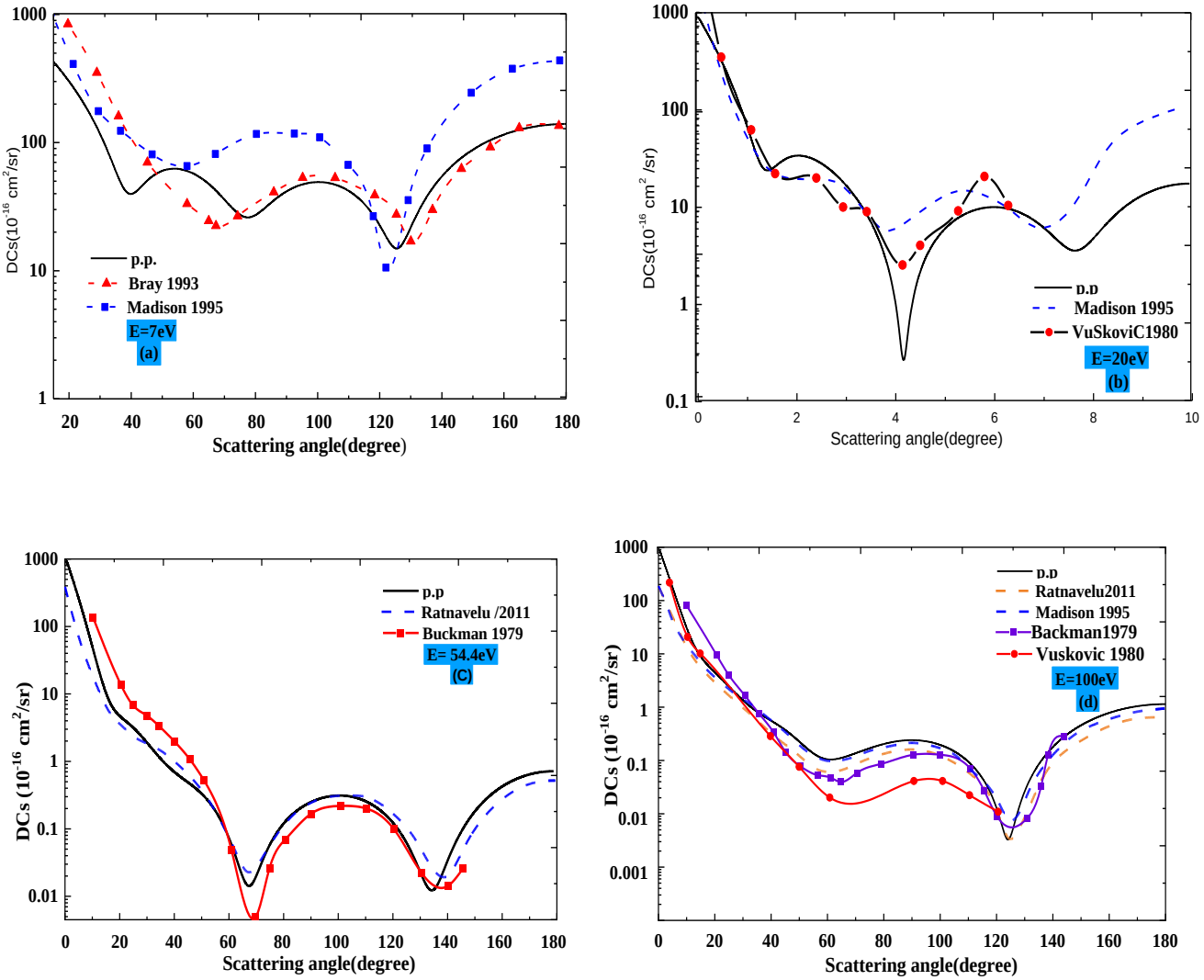


Figure 1. DCs (10^{-16} cm^2/sr) for the scattering of electrons from K-atoms at energies of 7 (a), 20 (b), 54.4 (c), and 100 (d) eV.Theoretical: Madison[18] ,Ratnavelu[3],experimental: Bray[4],Bukman[19] .and Vuskovic[17].

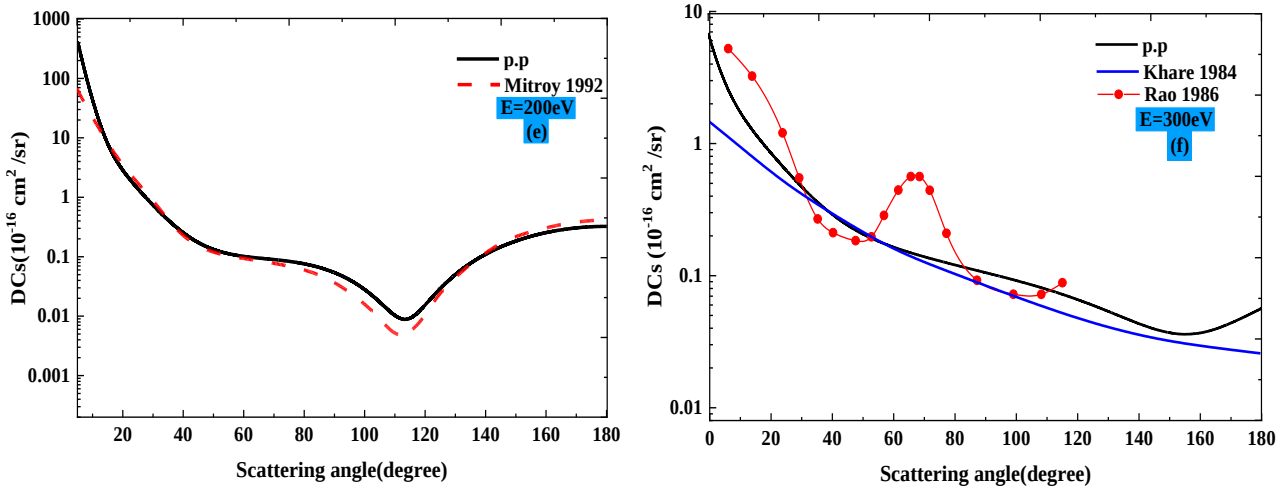
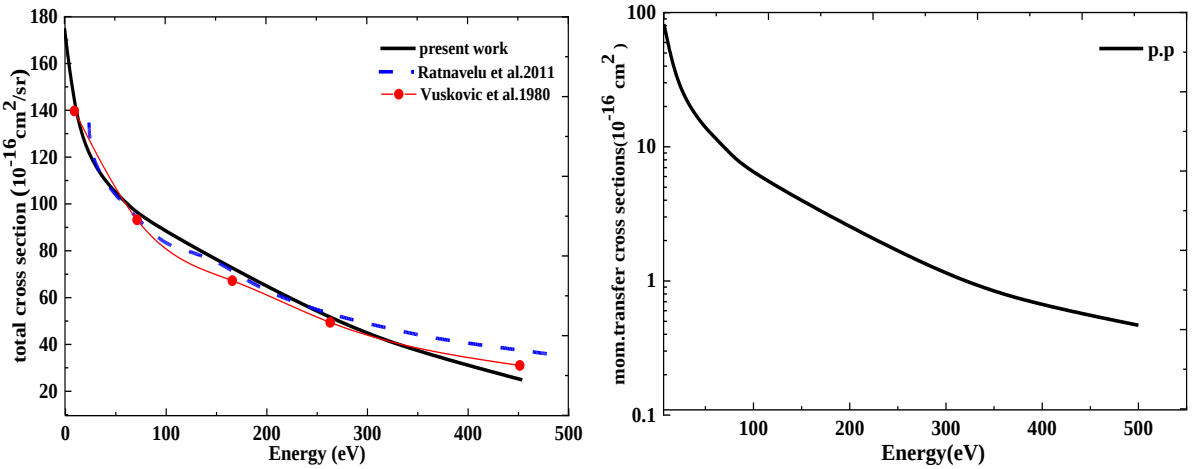


Figure 1. For the scattering of electrons from K- atoms at energies of (e)200 and (f)300, DCs (10 $^{-16}$cm^2/sr). Theoretical; Mitroy[20] ,Khare[21], experimental: Rao[22].



Figures 2&3: show The cross-sections for total and momentum transfer for the scattering of electrons from K-atoms in the energy range of the incident electrons (5-500 eV).

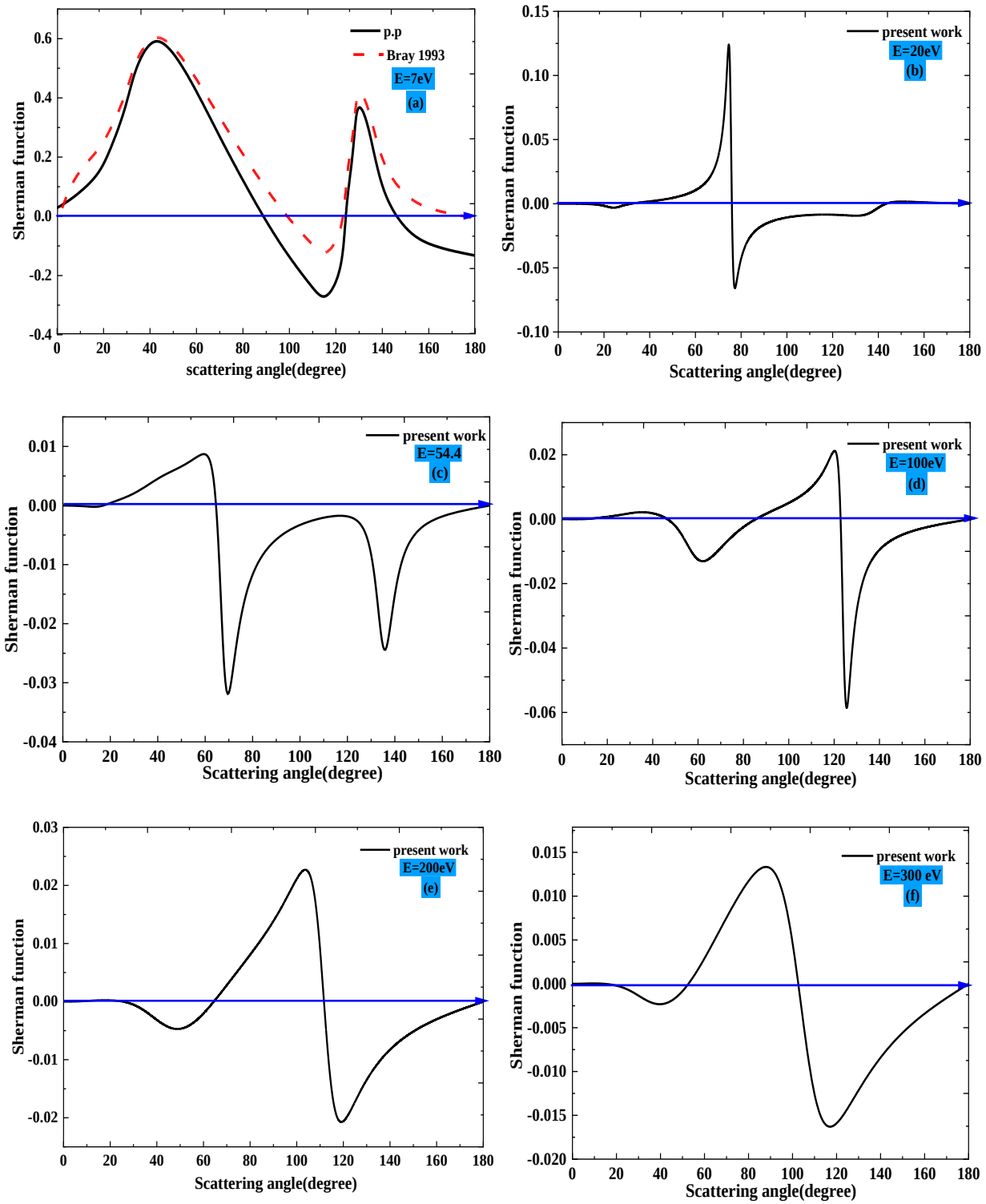


Figure 4 illustrates the spin polarisation parameter (S) fluctuation concerning the scattering angle at incident energy. Energy levels include 7, 20, 54, 4, 100, 200, and 300 eV.

Reference

1. Dummler, M., G. Hanne, and J. Kessler, *Left-right asymmetries in elastic and inelastic scattering of polarized electrons from argon, krypton and xenon atoms.* Journal of Physics B: Atomic, Molecular and Optical Physics, 1995. **28**(14): p. 2985.
2. Jain, A., *Low-energy positron-argon collisions using parameter-free positron correlation polarization potentials.* Physical Review A, 1990. **41**(5): p. 2437.
3. Ratnavelu, K. and W. Ong, *Electron and positron scattering from atomic potassium.* The European Physical Journal D, 2011. **64**(2): p. 269-285.
4. Bray, I., D.V. Fursa, and I.E. McCarthy, *Calculation of electron-potassium scattering.* Physical Review A, 1993. **47**(5): p. 3951.
5. Khalf, A., *The Elastic Scattering of Electrons from Cadmium Atom with the Model-Potential Approach.* basrah journal of science, 2008. **26**(1A english).
6. Yassir, A., A. Hussain, and F. Ali, *Relativistic Dirac Calculations for Electrons Scattering from Mg and Ca Atoms at Different Energies.* Journal of Kufa-Physics, 2018. **10**(2).
7. Nahar, S.N. and J. Wadehra, *Relativistic approach for e±scattering from argon.* Physical Review A, 1991. **43**(3): p. 1275.
8. P.Kumar, A.K.J., A.N.Tripathi and S.N.Nahar, Phys.Rev.A,49,8991994.
9. Eisberg, R.M., *Fundamentals of Modern Physics. Jonhn Wiley and Sons.* Inc., New York London Sydney, 1961.
10. F.Salvat, A.J., C.J.Powell,, Comp..Phys.Comm., 2005: p. 165,157
11. Desclaux, J.P., *A multiconfiguration relativistic Dirac-Fock program.* Computer Physics Communications, 1975. **9**(1): p. 31-45.
12. Furness, J. and I. McCarthy, *Semiphenomenological optical model for electron scattering on atoms.* Journal of Physics B: Atomic and Molecular Physics (1968-1987), 1973. **6**(11): p. 2280.
13. Beerlage, M., Z. Qing, and M. Van der Wiel, *The polarisation of electrons elastically scattered from argon and krypton at energies between 10 and 50 eV.* Journal of Physics B: Atomic and Molecular Physics (1968-1987), 1981. **14**(23): p. 4627.
14. Perdew, J., E. McMullen, and A. Zunger, *Density-functional theory of the correlation energy in atoms and ions: a simple analytic model and a challenge.* Physical Review A, 1981. **23**(6): p. 2785.
15. Walker, D., *Relativistic effects in low energy electron scattering from atoms.* Advances in Physics, 1971. **20**(85): p. 257-323.
16. Jablonski, A., F. Salvat, and C.J. Powell, *Comparison of electron elastic-scattering cross sections calculated from two commonly used atomic potentials.* Journal of physical and chemical reference data, 2004. **33**(2): p. 409-451.

17. Vuskovic, L. and S. Srivastava, *Scattering of intermediate-energy electrons by potassium.* Journal of Physics B: Atomic and Molecular Physics, 1980. **13**(24): p. 4849.
18. Madison, D.H., et al., *Elastic and inelastic scattering of electrons from potassium.* Journal of Physics B: Atomic, Molecular and Optical Physics, 1995. **28**(1): p. 105.
19. Buckman, S., C. Noble, and P. Teubner, *Intermediate energy electron scattering from potassium.* Journal of Physics B: Atomic and Molecular Physics (1968-1987), 1979. **12**(18): p. 3077.
20. Mitroy, J., *Electron scattering from potassium at intermediate energies.* Journal of Physics B: Atomic, Molecular and Optical Physics, 1993. **26**(14): p. 2201.
21. V, K.S.P.a.V., private communication, 1984.
22. MVVS, R., *Elastic scattering of intermediate-energy electrons by sodium, potassium and rubidium atoms.* 1987.