CHAPTER II

SPIN POLARIZATION PARAMETERS AND CROSS-SECTIONS FOR ELECTRON ELASTICALLY SCATTERED FROM RHENIUM AND GOLD ATOMS

2.1 INTRODUCTION

Theoretical studies of spin dependent phenomena in collisions between electrons and atoms have progressed significantly since the classic review of Kessler [1, 2]. Indeed these effects are so large that, even manifest themselves in the integral cross-sections in the elastic scattering from many heavier systems. It is well known that the relativistic interaction plays an important role in understanding this phenomenon in the scattering of electrons from heavy atomic targets. Due to enormous progress, which has recently been achieved in the development of efficient polarized electrons sources and accurate polarimeters, it is now possible to explore the spin effects through the complete scattering experiments. Within the framework of the density-matrix approach it is possible to define the set of all independent parameters which describe the dynamics of the collisions process. For example, in the case of elastic scattering process, the unpolarized differential cross-section (DCS) and the spin polarization parameters $S$, $T$ and $U$ describe the dynamics of the collision process. The $S$ parameter also known as Sherman function describes the change of polarization produced in the scattered beam due to the collision whereas the other two polarization parameters $T$ and $U$ give the angle of rotation of the component of the polarization vector in scattering plane. In recent past, a large number of studies relating to the determination of DCS and $S$, $T$ and $U$ parameters for the elastic scattering from heavy atomic systems have been carried out both theoretically and experimentally. It is worth mentioning here that recently Andersen and Bartschat [3] have published an excellent critical review with selected examples.
both from theory and experiment. Some of the older work on this subject can also be traced through the review of Hanne [4, 5] and Bartschat [6-9].

On experimental side, the measurements for the spin polarization parameters have been performed only for a few heavy atoms like inert atoms given by few groups [10-12], mercury (Hg), tellurium (Te), lead (Pb), bismuth (Bi) [13-16], thallium (Tl) [17], zinc (Zn), cadmium (Cd), indium (In) [18], and a few alkali atoms [19,20]. In turn, the theoretical side has a long history starting from the work of Walker [21, 22] and Sin Fai Lam [23] based on relativistic form of the Schrödinger equation and of Haberland and Fritsche [24] and Bartschat et al. [25] on generalized Kohn-Sham type equation and static exchange R-matrix theory respectively. Further, McEachran and Stauffer [26], Nahar and Wadehra [27] both solved the relativistic form of the Schrödinger equation within the framework of model potential approach. In the former case, the scattering potential was calculated in a hybrid way, i.e., its static part was obtained relativistically while the polarization potential was obtained in a non-relativistic manner. The exchange was exactly included through large component of the scattered wavefunction. In the latter case, a real- and complex- model potential represents the projectile target interaction. The real potential is represented by a static, exchange and a parameter-free correlation polarization potential and the complex potential is included via phenomenological absorption potential. This approach has been successfully applied to study spin polarization in elastic scattering of electrons from a number of atoms by Kumar et al. [28]. Yuan and Zhang [29, 30] have also reported their model calculations for alkaline earth atoms. In an attempt to improve upon the hybrid relativistic model of McEachran and Stauffer [31], and Szmytkowski [32] developed a fully relativistic version of the polarized orbital approximation. Szmytkowski and Sienkiewicz [33] used this approach to calculate the
spin polarization from zinc, cadmium, mercury, and inert atoms and observed that the calculated values moved in the right direction when compared to the hybrid approach. Sienkiewicz and Baylis [34] have further improved the target polarization in the relativistic version by a configuration interaction procedure.

A phenomenological model potential has also been used to examine this aspect along with the spin polarization of low energy electrons scattering from these alkaline earth atoms around the low-lying d-wave shape resonance by Kelemen et.al [35] and Yuan [36] and Dorn et.al [37] carried out theoretical calculations for spin polarization for xenon atoms based on the relativistic Schrodinger equation together with an optical potential, which included both polarization and absorption effects. The comparison of their calculations with experimental data suggests that the absorption potential must be included in the relativistic description for accurate prediction of the S, T, and U parameters.

In elastic scattering from closed-shell atoms, the polarization effects are caused by the spin-orbit interaction of the scattered electrons in the atomic field whereas from open-shell atoms that have a fine-structure splitting of their ground state, the polarization phenomenon may also be generated by the exchange interaction between the scattered and the atomic electrons along with the internal spin-orbit coupling of the atom. The present model is certainly a less good approximation for a closed shell and open-shell configuration like Rhenium (Re) and Gold (Au) atoms. However, as it is well known through the studies in atomic structure that within the framework of Hartree-Fock approximation, even a half complete shell leads to a spherically symmetric equivalent potential given by Bethe and Jackiw [38], as required here. In view of this, the present model can also be easily applied to study the elastic scattering from systems fulfilling this requirement.
We have calculated spin polarization parameters, differential cross-section (DCS), integrated elastic, momentum transfer and total cross-section for scattering of electrons from Rhenium and Gold atom, using both real and complex potential within the frame work of relativistic Dirac equations. In the following section 2.2 we review briefly the theoretical methodology and the details of our approach.

2.2 THEORETICAL METHODOLOGY

The motion of the projectile electrons in a central field \(V(r)\) is described by the Dirac equation

\[
[c \bar{a}.\bar{p} + \beta m_o c^2 - V(r) ] \psi = E \psi
\]  

(2.1)

For central potential, Dirac equation can be reduced to a set of two equations

\[
g_i^{1+} + \left[ K^2 - \frac{\ell(\ell + 1)}{r^2} - U_i (r) \right] g_i^{1-} (r) = 0
\]

(2.2)

Where \(g_i^{1+}\) is related to the radial part \(G_i^r\) of the large component of \(\psi\) as

\[
G_i = \sqrt{\eta} \frac{g_i^{1+}}{r}, \quad \eta = \frac{[E - V(r) + m_o c^2]}{\epsilon}, \quad K^2 = \frac{E^2 - m_o^2 c^4}{c^2 \hbar^2}
\]

Here, we take the total energy of the incident particle as \(E = m_o c^2 = E_i + m_o c^2\),

\[
\gamma = \sqrt{1 - \frac{v^2}{c^2}}
\]

where \(E_i\) as the kinetic energy of the incident particle of rest mass \(m_o\) and velocity \(v\). \(\alpha\) and \(\beta\) are the usual \(4 \times 4\) Dirac matrices. They \(U_i\) are the effective Dirac potential and are given in atomic units \((m_o = e = \hbar = 1, \ 1/c = \alpha)\),

where \(\alpha\) is fine structure constant) as

\[
- U_i (r) = -2 \gamma V(r) + \alpha^2 V^2(r) - \frac{3}{4} \left( \frac{\eta}{r} \right)^2 + \frac{1}{2} \frac{\eta}{\eta} \pm \left( \frac{\ell + 1}{\ell} \right) \frac{1}{r} \frac{\eta}{\eta}
\]

(2.3)

Here single and double primes denote the first and second derivatives with respect to \(r\), respectively. It should be noted that the last term of \(U_i\) in equation (2.3) corresponds to the two eigenvalues of the well-known spin-orbit interaction, one due to spin up and the other due to spin down.
\[
\frac{1}{4 m c^2} \frac{1}{r} \cdot \frac{d V(r)}{d r} \cdot \vec{\sigma} \cdot \vec{L} \tag{2.4}
\]

In the non-relativistic treatment of the Schrodinger equation, the above term is treated as a small perturbation along with the projectile-target interaction. Here \( \vec{\sigma} \) is related to the spin \( S \) as \( \vec{\sigma} = 2S \) and the value of \( \langle \vec{\sigma}, \vec{L} \rangle \) equals \( \ell \) for \( \ell = (\ell + 1/2) \) and \( -(\ell + 1) \) for \( \ell = (\ell - 1/2) \). The proper solution of equation (2.2) behaves asymptotically as

\[
g^{+}_{\ell} (K, r) = K r \left[ j_{\ell} (K r) - \tan \delta^{+}_{\ell} \eta_{\ell} (K r) \right], \quad r \to \infty \tag{2.5}
\]

where, \( j_{\ell} \) and \( \eta_{\ell} \) are spherical Bessel functions of the first and second kind respectively and \( \delta^{+}_{\ell} \) are the phase shifts due to collision interaction. The plus sign corresponds to the incident particles with spin-up and the minus sign in \( \delta \) to those with spin-down. The phase shift \( \delta^{+}_{\ell} \) can be obtained from the values of the radial wave function \( g^{+}_{\ell} \) at the two adjacent points \( r \) and \( (r + h) \) \((h << r)\) at very large \( r \) as

\[
\tan \delta^{+}_{\ell} \approx - \frac{(r + h) g^{+}_{\ell}(r) j_{\ell}(Kr) + rg^{+}_{\ell}(r + h) j_{\ell}(Kr)}{rg^{+}_{\ell}(r + h) \eta_{\ell}(Kr) - (r + h) g^{+}_{\ell}(r) \eta_{\ell}(Kr)} \tag{2.6}
\]

In the present calculation, the wave functions \( g^{+}_{\ell} \) are obtained by numerical integration of equation (2.2) using Numerov's method. The two complex scattering amplitudes \( f(K, \theta) \) (the direct amplitude) and \( g(K, \theta) \) (the 'spin-flip' amplitude) are defined as

\[
f(K, \theta) = \frac{1}{2iK} \sum_{\ell = 0}^{\infty} \left[ (\ell + 1)[\exp(2i\delta^{+}_{\ell}) - 1] + i[\exp(2i\delta^{-}_{\ell}) - 1] \right] P_{\ell} (\cos \theta) \tag{2.7}
\]

\[
g(K, \theta) = \frac{1}{2iK} \sum_{\ell = 1}^{\infty} \left[ \exp(2i\delta^{+}_{\ell}) - \exp(2i\delta^{-}_{\ell}) \right] P_{\ell} (\cos \theta) \tag{2.8}
\]
where, $\theta$ is the scattering angle and $P_i(\cos \theta)$ and $P_i^j(\cos \theta)$ are the Legendre polynomial and the Legendre associated functions, respectively. The elastic differential cross-section for scattering of the unpolarized incident electrons beam is given by

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

(2.9)

and the spin polarization parameters $S (\theta), T (\theta)$ and $U (\theta)$ have the forms by Joachain [39]

$$S(\theta) = \frac{i(f^* g - f g)}{\sigma(\theta)}, \quad T(\theta) = \frac{|f|^2 - |g|^2}{\sigma(\theta)}, \quad U(\theta) = \frac{f^* g + g^* f}{\sigma(\theta)}$$

(2.10)

The Sherman function $S$ describes the spin polarization of the scattered electrons if the incident electrons beam is unpolarized.

In the present work, a large number of phase shifts depending on the impact energy were evaluated before using the Born-Approximation. For example, the typical value of exact partial waves corresponding to the impact energies 2.0 eV and 500.0 eV is 20.0 and 100.0 respectively. Since at large distance, the interaction is dominated by the long-range part of the polarization potential $= -\alpha_{\alpha} / 2r^4$, the Born phase shift and related scattering parameters are obtained using this term only Burke [40], Nahar [41].

2.3 CHOICE OF POTENTIALS

The total interaction between an electrons and target atom is approximately represented by an effective potential and can be written as

$$V(r) = V_R (r) + i V_A (r)$$

(2.11)

where $V_R (r)$, the real part of the potential is written as the sum of three local terms, namely the static $(V_{st})$ (due to direct Coulomb interaction of all the charged particles.
involved), the exchange ($V_{ex}$) (arising due to the Pauli exclusion principle) and the polarization ($V_{pol}$) (taking into account the distortion of the target charge cloud in the presence of an incoming electrons field). All three potentials terms i.e. $V_{st}(r)$, $V_{ex}(r)$, and $V_{pol}(r)$ are functions of electronic density of the target. $V_{A}(r)$ is the absorption potential. Its inclusion parameterizes inelastic processes such as excitation, ionization, recombination etc. We will now describe the individual components of interaction in the following section.

### 2.3.1 Static Potential

The static potential $V_{st}(r)$ of the target atom is obtained by averaging over the motion of the target electrons and is given as

$$V_{st}(r) = \frac{Ze_e}{r} - e_e \sum_n \sum_{\ell} \sum_m N_{n\ell m} \int \left| \phi_{n\ell m}(r') \right|^2 \frac{1}{|\vec{r} - \vec{r}'|} d\vec{r}'$$  \hspace{1cm} (2.12)

where, $Z$ is the nuclear charge of the target atom, $e_e$ is the projectile charge and $N_{n\ell m}$ is the occupancy number of the orbit $(n, \ell, m)$. The radial part $\phi(r)$ of the spatial orbital $\phi_{n\ell m}(r) = \phi_{n\ell m}(r) y_i m(\hat{r})$ and the charge density are obtained using non-relativistic Slater-type orbitals of Roothaan and Hartree-Fock wave functions as given by McLean and McLean [42]. In addition we have also used the compilation of the analytical function as given by Salvat et al [43] which is determined by an analytical fitting procedure to Dirac-Hartree-Fock-Slater (DHFS) self consistent data. Their potential in atomic units is given by

$$V_{st}(r) = -\frac{Z}{r} \phi(r)$$  \hspace{1cm} (2.13)

where $\phi(r)$, the screening function is of the form

$$\phi(r) = \sum_{j=1}^{3} A_j \exp(-\alpha_j r)$$  \hspace{1cm} (2.14)
and similarly, the charge density of the atom is given by

\[ \rho(r) = \frac{Z}{4\pi r^3} \sum_{i=1}^{3} A_i \alpha_i^2 \exp(-\alpha_i r) \]  

(2.15)

with the condition that \( A_1 + A_2 + A_3 = 1 \).

The reliability for these parameters is demonstrated by Salvat et al. [43], firstly by showing that the Born cross-sections for elastic scattering of fast charged particle employing these analytical forms to practically coincide with those computed from the DHFS self consistent method and secondly by showing the one electron binding energy computed from the Independent Particle Model (IPM) with their analytical function agreeing closely with those of DHFS energy eigenvalues.

### 2.3.2 Polarization Potential

During last few years various authors [44-46] have proposed an approximate parameter-free polarization potential \( V_{pol} \), which is based on the correlation energy of the target atoms. The philosophy of the correlation polarization potential (COP) is quite simple. According to O'Connell and Lane [45], the correlation polarization potential is obtained in the whole \( r \) region by smoothly joining the correlation energy function and the asymptotic form \(-\alpha_d / 2r^4\), where they cross each other for the first time. The functional form of the correlation polarization potential in the inner region of the interaction is derived from an approximate local correlation energy that is obtained in terms of charge density \( \rho (r) \). Following them, it is expressed in terms of two components, the short range \( V_{SR}(r) \) and the long range \( V_{LR}(r) \) parts, and is given by

\[ V_{pol}(r) = \begin{cases} 
V_{SR}(r) & r < r_c \\
V_{LR}(r) & r \geq r_c
\end{cases} \]  

(2.16)

Here \( r_c \) is the point where two forms cross each other for the first time. The short range form for the electrons scattering with atoms is based on the free-electrons gas exchange potential and is given by
$$V_{SR}(r) = \begin{cases} 
0.0622 \ln r_s - 0.096 + 0.018 r_s \ln r_s - 0.02 r_s, & r_s \leq 0.7 \\
-0.1231 + 0.03796 \ln r_s, & 0.7 < r_s \leq 10 \\
-0.876 r_s^{-1} - 2.65 r_s^{-3/2} - 2.8 r_s^{2} - 0.8 r_s^{-5/2}, & 10 \leq r_s 
\end{cases} \quad (2.17)$$

where, $r_s = [3/4 \pi \rho(r)]^{1/3}$ and $\rho(r)$ is the electron charge density of the target system, which for spherically symmetric atom is given by

$$4 \pi \rho(r) = \sum_n \sum_i N_{ni} |\psi_{ni}(r)|^2,$$

where $N_{ni}$ is the occupancy number of the orbital $(n,i)$. All the terms of the total interaction potential can be generated using the target charge density $\rho(r)$. The long-range form of the polarization potential is given by $V_{LR}(r) = -\alpha_d / 2r^4$ where $\alpha_d$ is the static electric dipole polarizability. The crossing point for Re and Au atoms along with their dipole polarizability, ionization potential and first excitation thresholds are listed in table 2.3.

### 2.3.3 Exchange Potential

The semi classical exchange (SCE) potential, is given by Riley and Truhlar [47]

$$V^{SCE}_{ex} = -\frac{1}{2} \left[ (E - V_{st}(r)) - \left\{ [E - V_{st}(r)]^2 + 4 \pi \rho(r) \right\}^{1/2} \right] \quad (2.18)$$

The main assumption in the SCE approach is that the local momentum of the bound electrons can be disregarded with respect to that of the projectile electron. This make SCE model, a high-energy approximation. In the recent years, Gianturco and Sciaila [48] have introduced correction in the SCE theory by including local momentum of the bound electrons, which can play a significant role for lower collision energies. Thus accounting for the modification of the local momentum of the impinging electrons within the atomic charge cloud and then treating it within the framework of Fermi electrons gas model, the MSCE potential is given as:
\[ V_{MSCE}^{st} = \frac{1}{2} \left[ E - V_{st}(r) + \frac{3}{10} (3\pi^2 \rho(r))^{2/3} \right] - \frac{1}{2} \left[ \left( E - V_{st}(r) + \frac{3}{10} (3\pi^2 \rho(r))^{2/3} \right)^2 + 4\pi \rho(r) \right]^{1/2} \] (2.19)

In the present calculation, we are using the modified semi-classical exchange (MSCE) potential given by Gianturco and Scialla [48]. Realizing that the impinging electrons distort the electron charge density of target can further modify the MSCE potential. We have therefore replaced \( V_{st} \) in equation (2.19) by \( V_D = V_{st} + V_{pol} \). \( \rho(r) \) is the radial charge density of the target wave function. This modified version is used all through in the present calculations.

### 2.3.4 Absorption Potential

The impact-energy range considered in the present calculation exceeds the threshold energy of the inelastic electrons scattering from the target systems under the investigation and hence causes an absorption in the scattered beam. There exist various versions of the absorption potential describing all the inelastic processes during the scattering. To include the absorption effect in the scattered beam, we have therefore employed a modified version 3 of the semi-empirical model absorption potential of Staszewska et al. [49]. It is given by

\[ V_A = -\frac{1}{2} V_{loc} \rho(r) \overline{\sigma_b} \] (2.20)

Where

\[ V_{loc} = [2(E - V_R)]^{1/2} \] (2.21)

In equations (2.20) and (2.21) \( V_{loc} \) is the local velocity of the incident electrons for \( E - V_R \geq 0 \), \( V_R \) is the real part of the total interaction potential, i.e. \( V_R = V_{st} + V_{ex} + V_{pol} \). The factor \( \frac{1}{2} \) in equation (2.20) is introduced to account for the exchange of the incident electrons and bound electrons of the target during the scattering process. \( \overline{\sigma_b} \) is the average quasi free binary collision cross-section.
obtained non-empirically by using the free-electrons gas model for the target. The functional form of the \( \sigma_b \) is given as

\[
\sigma_b = \begin{cases} 
\frac{8\pi}{10k_F^2E} (f_1 + f_2) & ; \quad p^2 \geq \alpha + \beta - k_F^2 \\
0 & ; \quad p^2 < \alpha + \beta - k_F^2 
\end{cases}
\tag{2.22}
\]

Where,

\[
p(E) = (2E)^{1/2}
\tag{2.23}
\]

\[
f_1 = \frac{5k_F^2}{(\alpha - k_F^2)} - \frac{k_F^2[5(p^2 - \beta) + 2k_F^2]}{(p^2 - \beta)^2}
\tag{2.24}
\]

\[
f_2 = \begin{cases} 
0 & ; \quad p^2 > \alpha + \beta \\
\frac{2(\alpha + \beta - p^2)^{5/2}}{(p^2 - \beta)^2} & ; \quad p^2 \leq \alpha + \beta 
\end{cases}
\tag{2.25}
\]

\[
k_F = (3\pi^2 \rho(r))^{1/3}
\tag{2.26}
\]

In equations (2.22) to (2.26), \( p(E) \) is the incident momentum of the scattering electrons and \( k_F \) is the target Fermi momentum. The form of the two parameters \( \alpha \) and \( \beta \) introduced in \( \sigma_b \) depend on, the lowest excitation threshold energy \( (E_{th}) \) of the target and the ionization potential energy \( (I_p) \) of the target and are obtained empirically given by Stasiewska et al [49].

\[
\alpha = k_F^2 + 2[E_{th} - (I_p - E_{th})] - V_R
\tag{2.27a}
\]

\[
\beta = k_F^2 + 2(I_p - E_{th}) - V_R
\tag{2.27b}
\]

There exists number of semi-empirical forms for the absorption potential in the literature. Various versions of the absorption potential differ by varying \( \nu_{\infty} \) and modifying the parameters \( \alpha \) and \( \beta \) as given in 2.27 (a-b). In our present work, we report our results using these two versions of absorption potential. First one in which we are using \( V_R \) as defined earlier referred as version 3 and in second one we use \( V_R = V_{st} + V_{ex} \) for calculating \( \nu_{\infty} \) referred here as version 2 (as given by few group
In version 2 parameters $\alpha$ and $\beta$ become energy independent i.e.

$$V_{e\nu} = [2(E - V_{SE})]^{1/2}$$  \hspace{1cm} (2.28)

$$\alpha = k_F^2 + 2E_{th}$$  \hspace{1cm} (2.29)

$$\beta = k_F^2$$  \hspace{1cm} (2.30)

In our present calculations $V_R$ is constructed with static plus $V_{ex}^{MSCE}$ and parameter free correlation polarization potential outlined earlier.

2.4 RESULTS AND DISCUSSIONS

We have performed a relativistic calculation of the partial cross-section, differential cross-sections (DCS), spin polarization parameters, integral elastic, momentum transfer and total cross-sections in the energy region of 2.0 – 500 eV employing a parameter-free-model potential for polarization.

2.4.1 Electrons Scattering from Rhenium Atom

2.4.1.1 Radial Shapes

The various components of the interaction terms and charge density as obtained using the non-relativistic HF wave function of McLean and McLean as given by [42] are displayed in Figure 2.1 (a) for e$^-$ - Re atoms. In general, it is found that the static interaction dominates all other interactions i.e. exchange and polarization for e$^-$ - Re in Figure 2.1 (a) at small values of $r \sim 3.5$ a.u., and thereafter the correlation polarization takes over all other interactions. In e$^-$ - Re, the energy dependent exchange interaction $V_{ex}^{MSCE}$ at $E = 100$ eV remains weaker than the static interaction up to very large values of $r$. Figure 2.1(b) shows the radial electron charge density for Re atom using both HF and DHFS wave function respectively. The number of small peaks exhibited by the charge density curve indicates various shell contributions associated with the atom. The calculated density obtained by the
analytical fitting procedure to DHFS wave function as given by Salvat et al. [43] shows a reasonable agreement with the HF wave function. It is noted that the analytical density curve only partially reproduces the small peaks of the non-relativistic density associated with different shell contributions. Theoretical shapes of various terms of the potential and density for Re, with both Wave-functions are quite similar in nature.

Figure 2.1 (a) Negative of Various interacting potentials $V_s$ (static), $V_p$ (pol), $V_{ex}$ (exchange), and $V_{ab}$ (absorption) in log₁₀ for electrons scattering from Re atoms at energy 100 eV. The curves represent the absolute values of the potentials which are all negative except $V_s$ of positive. (b) Spherical charge density of the Re atom.
2.4.1.2 Angle-Integrated Elastic Cross-Sections and Contribution of Partial Waves at low Energy (E<10eV).

We have performed calculations in different models potential, which are described as follows. For electrons scattering, we consider SEP (Static + Exchange + Polarization) and SEPa (SEP + absorption) model potential. In the present study, we have reported the calculation in these models using McLean and McLean [42] HF wave functions. In Figure 2.2 we are presenting the results for the first four partial cross-sections of s, p, d and f waves in SEPa model for e⁻ - Re scattering. It is observed from Figure that first inelastic threshold energy $E_{th}$, s and p wave partial cross-sections contributes maximum to $\sigma_{el}$ and near and above to $E_{th}$, d wave dominates. The maximum in the d-wave cross-sections arises from shape resonance at energies $E_r = 2.99$ eV for e⁻ - Re. The total cross-sections are also plotted in the Figure under this model. Each curve shows a narrow low-energy peak followed by sharp fall of the cross-sections up to the first inelastic threshold.

![Graph](image)

*Figure 2.2* Partial cross-sections in unit of $10^{-16}$ cm² for scattering of e⁻ - Re. Present calculation s, p, d, and f waves, integral cross-section
2.4.1.3 Differential Cross-Sections and Asymmetry Parameter

We present elastic DCS and S-parameter, T-parameter and U-parameter for e⁻-Re for both the real and the complex potentials. Figures 2.3 to 2.8 correspond to the DCS and S, T and U parameter at incident electrons energies 5.0, 10.0, 20.0, 50.0, 100.0, 200.0 and 500.0 eV respectively. It is seen that the present theory predicts the forward peak, minima and maxima at middle angles and enhanced backward slopes of the DCS. To illustrate the importance of the absorption effect we have displayed the DCS in the SEPa model. The calculated angular variation in DCS exhibits deeper minima, which occur at slightly lower scattering angles for SEPa model compared to SEP model with real potentials. These Figures also show the spin-polarization parameter at the same energies. At lower energy, the present phenomenological absorption potentials does not make any change in the calculated values, however, at higher energy DCS and S-parameter exhibit a rapid variation with scattering angles.
Figure 2.3 DCS and asymmetry parameter S for elastic $e^-\text{-Re}$ scattering at energies (a, c) 5 eV; (b, d) 10 eV; (e, g) 20 eV; (f, h) 50 eV. Present calculation: --- with complex potential (SEPa); -- with real potential (SEP).
Figure 2.4 DCS and asymmetry parameter S for elastic $e^-$-Re scattering at energies (i, k) 100 eV; (j, l) 200 eV. Present calculation: — with complex potential (SEPa); - - - - with real potential (SEP).
Figure 2.4 DCS and asymmetry parameter $S$ for elastic $e^{-}\text{Re}$ scattering at energies (i, k) 100 eV; (j, l) 200 eV. Present calculation: — with complex potential (SEPa); --- with real potential (SEP).
Figure 2.7 T and U parameters at energy (c, d) 10 eV; (e, f) 20 eV; (g, h) 50 eV; (i, j) 100 eV. Present calculation: —— with complex potential (SEPa); ——— with real potential (SEP).
Figure 2.5 DCS and asymmetry parameter S for elastic $e^- - Re$ scattering at energies (m, n) 500 eV. Present calculation: — with complex potential (SEPa); - - - with real potential (SEP).

Figure 2.6 T and U parameters at energy (a, b) 5 eV for elastic scattering of $e^- - Re$. Present calculation: — with complex potential (SEPa); - - - with real potential (SEP)
Figure 2.8 T and U parameters at energy (k, l) 200 eV; (m, n) 500 eV. Present calculation: —— with complex potential (SEPc). ----- with real potential (SEP).

2.4.1.4 Elastic, Total and Momentum-Transfer Cross-Sections

The results of our present integrated elastic, total and momentum-transfer cross-sections for Re atoms are presented in tables 2.1 and 2.2. The elastic cross-sections are obtained using both the real and complex potentials. It is noted that at all energies the elastic cross-sections ($\sigma'$) obtained with only real potential are larger than those obtained with the complex potential, i.e. $\sigma$. This feature is similar to the earlier observations with several other heavier atoms is given by few groups [50-58]. This is not unexpected as we have seen that the inclusion of absorption reduces the DCS and consequently, the angle-integrated cross-section. The momentum-transfer
cross-sections ($\sigma_m$) using both real and complex potentials exhibit a minimum around 20 eV for Re atom. Such a feature is absent in the results of $e^{-}$ - Re scattering where cross-sections fall off with the increase of energy. Again, the calculated values of ($\sigma_m$) are higher for the real potential than for the complex potential. We have also shown in the table the cross-section with only absorption potential ($\sigma_{abs}$) as well as the total cross-section ($\sigma_t$) which includes all the elastic and inelastic cross-sections. The total cross-section descends rapidly at lower energies and thereafter varies slowly with increasing impact energies.

2.4.2 Electrons Scattering From Gold Atom

2.4.2.1 Radial Shapes

The various components of the interaction terms and charge density as obtained using the non-relativistic HF wave function of McLean and Mclean [42] are displayed in Figure 2.9 (a) for $e^{-}$ - Au atoms. In general, it is found that the static interaction dominates all other interactions i.e: exchange and polarization for $e^{-}$ - Au in Figure 2.9 (a) at small values of $r \sim 3.5$ a.u., and thereafter the correlation polarization takes over all other interactions. In $e^{-}$ - Au, the energy dependent exchange interaction $V_{ex}^{MSCE}$ at $E = 100$ eV remains weaker than the static interaction up to very large values of $r$. Figure 2.9 (b) shows the radial electronic charge density for Au atom using both HF and DHFS wave function respectively. The number of small peaks exhibited by the charge density curve indicates various shell contributions associated with the atom. The calculated density obtained by the analytical fitting procedure to DHFS wave function as given by Salvat [43] shows a reasonable agreement with the HF wave function. It is noted that the analytical density curve only partially reproduces the small peaks of the non-relativistic density associated with different shell contributions. Theoretical shapes of various terms of the potential and density for Au, with both wave-functions are quite similar in nature.
Figure 2.9 (a) Negative of Various interacting potentials $V_s$ (static), $V_p$ (polarised), $V_{ex}$ (exchange), and $V_{ab}$ (absorption) in $\log_{10}$ for electrons Scattering from Au atoms at energy 100 eV. The curves represent the absolute values of the potentials which are all negative except $V_s$ of positive. (b) Spherical charge density of the Au atom.
2.4.2.2 Angle-Integrated Elastic Cross-Sections and Contribution of Partial Waves at low Energy (E<10 eV).

We have performed calculations in different models potential, which are described as follows. For electrons scattering, we consider SEP (Static + Exchange + Polarization) and SEPa (SEP + absorption) model potential. In the present study, we have reported the calculation in these models using McLean and McLean [42] HF wave functions. Let us discuss first our partial cross-section for s, p, d and f waves in SEPa approximation for Au as shown in Figure 2.10. For Au as can be seen from the Figure in low energy region < 4 eV, the main contribution to the $\sigma_{pl}$ comes from s and p waves. In the elastic region, the maximum of cross-section comes from s waves whereas near and beyond the inelastic threshold p wave makes the maximum contribution. The maximum in the p wave cross-section arise from shape resonance at energy $E_r$ equal to 0.78 eV for Au. The total cross-sections are also plotted in Figure in this model. Each curve shows a narrow low energy maximum followed by sharp fall of the cross-sections up to the first inelastic threshold. It is seen that the total cross-section shows broad maxima at low energies. The broad structure is due to the maximum in each of s-, p- and d-wave partial cross-sections. Further it is noted that for this case, the f wave also contribution significantly to the total Cross-sections beyond the first inelastic threshold.
Figure 2.10 Partial cross-sections in unit of $10^{-16}$ cm$^2$ for elastic scattering of $e^-\cdot$Au. Present calculation s, p, d, and f waves, integral cross-sections.

2.4.2.3 Differential Cross-Sections and Asymmetric Parameter

The calculated differential cross-section in the range from 5.0 eV to 500.0 eV is shown in Figures 2.11 to 2.15. In these Figures the solid curve corresponds to the DCS value obtained by using the real potential as the total projectile-target interaction and the dash curved correspond to those obtained with complex potential as the interaction. At low energy, there is no difference between the results obtained using either the real or complex potential, but at higher impact energies there is small difference between to calculated values, especially at those scattering angles where the DCS exhibit minima and maxima in the curve. This feature is expected since at low energies the scattering is mainly is elastic and there is almost no effect.

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of absorption on the DCS values, the structure of dips and hump (both in magnitude and width) changes when the absorption effects switched on. Like DCS Figs, here also, all the solid curves correspond to values obtained using the real potential and dash curves to values obtained using complex potential in the Dirac equation. It is noticeable that the inclusion of the absorption potential in the interaction causes the minima to go deeper and maxima to peak in general, but this feature is more clearly at high impact energies. This difference indicates that the cross-section and consequently, the polarization parameters are sensitive to the choice of the interaction potential. Since the values of $S$ are measured more often than those of the parameters $T$ and $U$ which are observed only in a triple scattering experiment.
Figure 2.11 DCS and asymmetry parameter S for elastic e-Re scattering at energies (a, c) 5 eV; (b, d) 10 eV; (e, g) 20 eV; (f, h) 50 eV. Present calculation. — with complex potential (SEPa); - - - - with real potential (SEP).
Figure 2.12 DCS and asymmetry parameter $S$ for elastic $e^-$-Re scattering at energies (i, k) $100$ eV; (j, l) $200$ eV. Present calculation: — with complex potential (SEPa); - - - - with real potential (SEP).
Figure 2.13 DCS and asymmetry parameter $S$ for elastic $e^-$-Re scattering at energies $(m, n)$ 500 eV. Present calculation: — with complex potential (SEP$a$); - - - - with real potential (SEP).

Figure 2.14 $U$-parameters at energy (a) 5 eV (b) 10 eV for elastic scattering of $e^-$-Au. Present calculation: — with complex potential (SEP$a$); - - - - with real potential (SEP).
Figure 2.15 U-parameter for elastic $e^-$ - Au scattering at energies (c) 20 eV; (d) 50 eV; (e) 100 eV; (f) 200 eV (g) 500 eV. Present calculation: — with complex potential (SEP); - - - - with real potential (SEP).
2.4.2.4 Elastic, Total and Momentum-Transfer Cross-Sections

The value of calculated integrated elastic, total and momentum – transfer cross-sections for Gold atoms are complied in table 2.1 and 2.2 respectively. The elastic cross-sections are obtained using both real and complex potentials. It is seen that the elastic cross-section with real potential are larger than those obtained with the complex potentials at all energies. This is not unexpected because the inclusion of absorption interaction reduces the DCS and consequently the elastic cross-sections. The total cross-sections and momentum – transfer cross-sections are also presented in some tables. It is observed that total cross section decreased rapidly at low energies and there after it decrease slowly with increase- impact emerges. The momentum transfer cross-sections obtained using both real and complex potentials. The calculated values with real potentials are higher than those obtained with complex potentials. Again the reduction in the momentum transfer cross-sections is due to the inclusion of absorption effect.
<table>
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<th>(\sigma^-) - Au</th>
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<td>(\sigma^\prime_{el})</td>
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Table 2.3 Electronic configuration, term symbols, dipole polarizability, ionization potential (I.P), and crossing points ($r_c$) for Re and Au atoms.

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<th>Z (atomic number)</th>
<th>Element</th>
<th>Electronic Configuration</th>
<th>Term</th>
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<th>Ionization potential (eV)</th>
<th>Crossing point (a.u.)</th>
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2.5 CONCLUSION

We have presented the result of our relativistic, total scattering, momentum transfer cross-sections, DCS and the angular distribution of the spin polarization parameter $S$, $T$ and $U$ for electrons scattered from Rhenium and Gold atoms. We showed that the present relativistic model is capable of explaining the features of the electrons spin polarization parameter. The agreement seems to be better at higher impact energies. For rhenium, the complex part (absorption potential) of the optical potential has no effect on the polarization parameter & except that only its addition above the inelastic threshold has a discernable effect, but the same is more significant for gold atoms. Thus, a better representation of absorption potential which accounts the combined effect of all the inelastic channels is desirable. The electrons scattering from heavier species Rhenium and Gold atoms, shows significant amount of spin polarization compared to lighter ones. The difference between present model calculations of our and that of others can be said to be due, basically to the different to the different choices of both and correction potential and the charge density which correctly simulate the required dynamical effect of the scattering process.
REFERENCES


