

Electron Scattering from Gold (Au) atom

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Abstract: Using Dirac equation, we have performed relativistic calculations for differential cross-sections and spin polarization parameters for scattering of electrons with Gold (Au) atoms with the energy range from 2.0 to 500.0 eV. The target-projectile interaction is represented by real and complex optical potentials. Gold is a d-block transition metal having one electron in the last s-orbit (term ^2S). Differential cross-sections and spin polarization parameters show that gold atom as a heavy atom is a favorite target for the generation of polarized beam of electrons. We expect that the importance of relativistic effects is substantial for such heavy atoms. We hope experimental results will be reported in the light of our calculations for the e^- -Au scattering.

Keywords: Relativistic calculation, Electron scattering.

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1. Introduction

Relativistic interactions play very crucial role in the spin-dependent phenomenon in collision between slow electrons and heavy atomic systems. Indeed these effects are so large that, even manifest themselves in the integral cross-sections in the elastic scattering from many heavier systems. In recent years, the scattering of electrons by such atoms has been studied extensively both experimentally and theoretically. It is worth mentioning that Anderson and Bartschat¹ have published an excellent critical review with selected examples both from experiments and theory.

The older works on this subject can be traced in the classic reviews of Kessler² and Hanne³. Due to enormous progress, which has been achieved in the development of efficient polarized electron sources and accurate polarimeters, the spin dependence of the scattering process can be readily studied through the complete scattering experiments. Within the framework of the density matrix.

Formalism²⁻⁴, it is possible to define a set of observables, which describe the elastic scattering process, namely the un-polarized differential cross-section (DCS) and the S, T and U polarization parameters. The S parameter also known as Sherman function describes the change of polarization produced in the scattered beam due to collision and the other two polarization parameters T and U give the angle of rotation of the component of the polarization vector in the scattering plane. On the theoretical side, there exists a long history for such calculations beginning with Walker⁵ based on relativistic Hartree-Fock equation, Fai Lam⁶ based on a relativistic form of the Schrodinger equation, Haberland and Fritzsche⁷ based on Kohn-Sham type equations and Bartschat *et al.*⁸ using the generalized Kohn-Sham (GKS) and static exchange R-matrix theory⁹. Further, both Mc Eachran and Staufer¹⁰ and Nahar and Wadehra¹¹ solved the relativistic Schrodinger equation within the framework of model potential approach. In the former case, a hybrid way was used to calculate the scattering potential, *i.e.* its static part was obtained relativistically while the polarization potential was obtained in a non-relativistic manner. In the latter case, a real and complex model potential represents the projectile-target interaction. This approach has been successfully applied to study spin polarization in elastic scattering of electrons from a number of atoms by Kumar *et al.*¹² and Yuan and Zhang¹³. To improve the hybrid relativistic model of Mc Eachran and Staufer¹⁰, Szmytkowski¹⁴ developed a fully relativistic version of the polarized orbital approximation. This approach was used by Szmytkowski and Sienkiewicz¹⁵ and observed that the calculated values moved in the right direction when compared to the hybrid approach. Sienkiewicz and Baylis¹⁶ have further improved the target polarization in the relativistic version by configuration interaction procedure. Dorn¹⁷ 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 STU parameters. This aspect has been further examined by Neerja¹⁸. They have computed the spin polarization parameters STU and correlation for the electrons elastically scattered from closed shell atoms like ytterbium (Yb), radon (Rn), radium (Ra), europium (Eu) and bismuth (Bi) atoms. Recently some more calculations are performed using this model²⁷⁻²⁹.

In the present paper, we have extended earlier calculations¹²⁻¹⁸ to study the electron collisions with open shell elements like gold (Au) atoms. The electronic configurations of Au is [Xe] 4f¹⁴5d¹⁰6s¹ (Spectroscopic term ²S).

It is well-known that within the framework of Hartree-Fock approximation, even a half-complete shell leads to a spherically symmetric equivalent potential (Bethe and Jackiw ¹⁹), as required here. In view of this, the present model can be easily applied to study the elastic scattering from systems with open-shell atoms fulfilling this requirement.

2. Theoretical Methodology

The total interaction between a particle and the target atom is represented by an effective potential $V(r)$, which is sum of two parts, $V_R(r)$ and $V_A(r)$. For electron scattering, real part of the potential $V_R(r)$ is expressed as sum of three local terms, $V_R(r) = V_{st}(r) + V_{ex} + V_{pol}(r)$, where $V_{st}(r)$, V_{ex} and $V_{pol}(r)$ are static, exchange and polarization potentials respectively. $V_A(r)$ is the absorption potential. Its inclusion parameterizes inelastic processes such as excitation, ionization, recombination etc. All potential terms are functions of ground state density $\rho(r)$ of the target. The static potential $V_{st}(r)$ and the charge density $\rho(r)$ are obtained using non-relativistic Slater type orbital of Roothan and Hartree-Fock wave functions as given in McLean and McLean ²⁰. In addition, we have used the compilation of analytical function given by Salvat et al. ²¹, which is determined by an analytical fitting procedure to Dirac-Hartree-Fock-Slater (DHFS) self-consistent data. In the present calculations, we are using the modified semi-classical exchange (MSCE) potential V_{ex}^{MSCE} given by Gianturco & Scialla ²².

$$(1) \quad V_{ex}^{MSCE} = \frac{1}{2} \left[E - V_{st}(r) + \frac{3}{10} \{ (3\pi^2 \rho(r))^{2/3} \} \right],$$

$$- \frac{1}{2} \left\{ \left[E - V_{st}(r) + \frac{3}{10} \{ (3\pi^2 \rho(r))^{2/3} \} \right]^2 + (4\pi \rho(r)) \right\}^{1/2},$$

It is important to note that the impinging electron distorts the electronic charge density of target which can further modify this exchange potential. This effect has been taken into account by considering the polarization of the target wave-function by replacing the term $V_{st}(r)$ in equation (1) by

$V_D = V_{st}(r) + V_{pol}(r)$. Moreover, the polarization potential $V_{pol}(r)$ is based on the correlation energy by the target atom, which has short $V_{SR}(r)$ and long range $V_{LR}(r)$ potentials given by

$$(2) \quad V_{pol}(r) = \begin{cases} V_{SR}(r) & \text{if } r < r_c \\ V_{LR}(r) & \text{if } r \geq r_c \end{cases},$$

where r_c is the point where two forms cross each other for the first time. The short range form of the electron $V_{SR}^-(r)$ scattering with atoms is based on the free-electron gas-exchange potential and is given by

$$(3) \quad V_{SR}^-(r) = \begin{cases} 0.0622 \ln r_s - 0.096 + 0.018 r_s \ln r_s - 0.02 r_s, & \text{if } r_s \leq 0.7 \\ -0.1231 + 0.03796 \ln r_s & \text{if } 0.7 < r_s \leq 10. \\ -0.876 r_s^{-1} + 2.65 r_s^{-3/2} - 2.8 r_s^{-2} - 0.8 r_s^{-5/2} & \text{if } 10 \leq r_s \end{cases}$$

where $r_s = [3/4\pi\rho(r)]^{1/3}$ and $\rho(r)$ is the electron charge density of the target system. The long-range polarization potential is given by $V_{LR}(r) = -\alpha_d / 2r^4$, where α_d is the static dipole polarizability (for Au, $\alpha_d = 36.1 a.u.$) and $r_c = 3.921$ for electron scattering. There exist various versions of the absorption potentials describing all the inelastic processes during the electron scattering. To include the absorption effect in the scattered beam potential is given by

$$(4) \quad V_A = -\frac{1}{2} v_{loc} \rho(r) \overline{\sigma_b},$$

$$(5) \quad v_{loc} = [2(E - V_R)]^{1/2},$$

In Eqn. (5) V_{loc} is the local velocity of the incident electron for $E - V_R \geq 0$. The factor $1/2$ in Eqn. (4) is introduced to account for the exchange of the incident electron 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-electron gas model for the target.

3. Results and Discussion

A. Partial Cross-Sections in the low energy region ($E < 10$ eV)

We have performed calculations in different models potential, which are described as follows. For electron 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 McLean²⁰ HF wave functions. Let us discuss first our partial cross section for s, p, d and f waves in SEP approximation for Au as shown in fig 1(a). For Au as can be seen from the figure in low energy region < 4 eV, the main contribution to the σ_{el} 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 d wave cross section arise from shape resonance at energy E_r equal to .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.

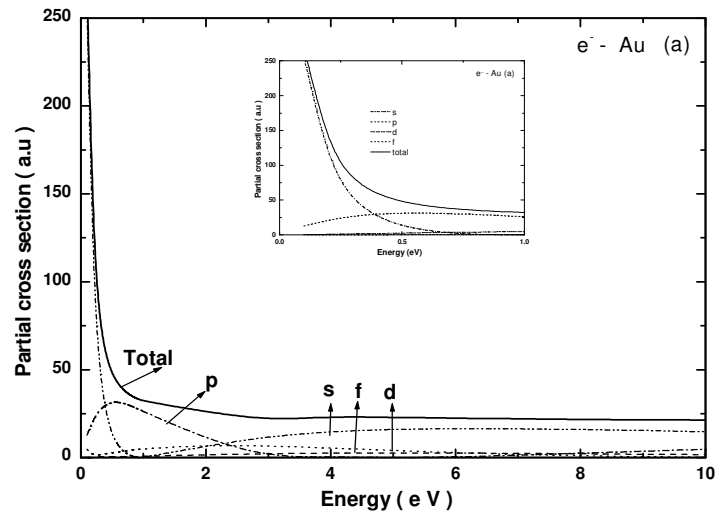
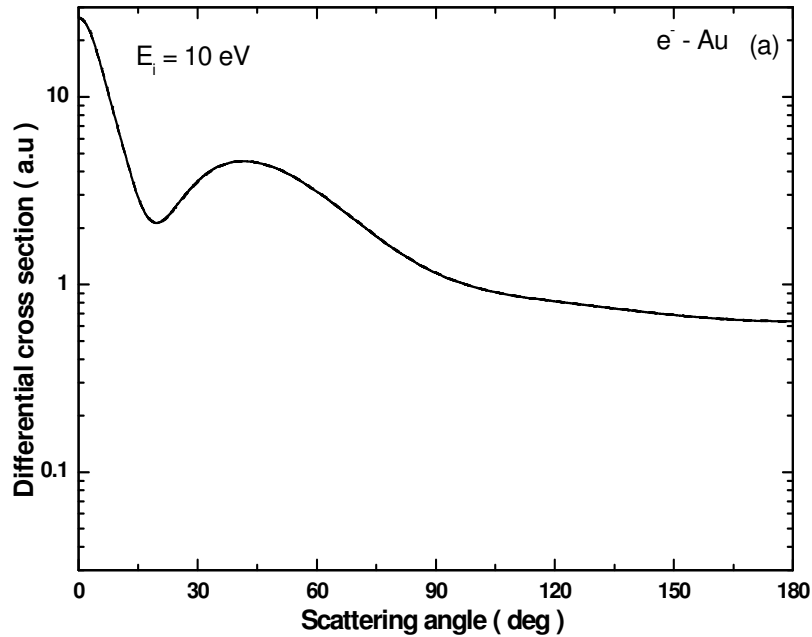


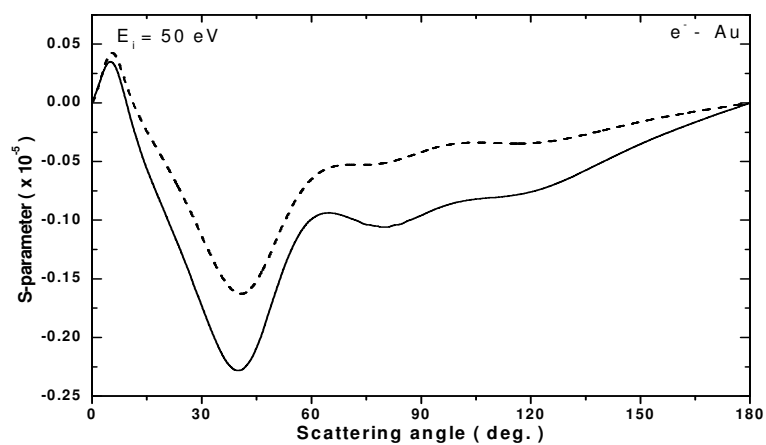
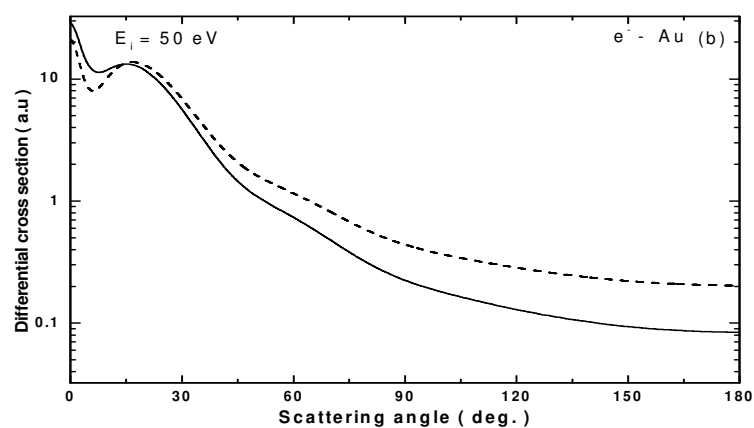
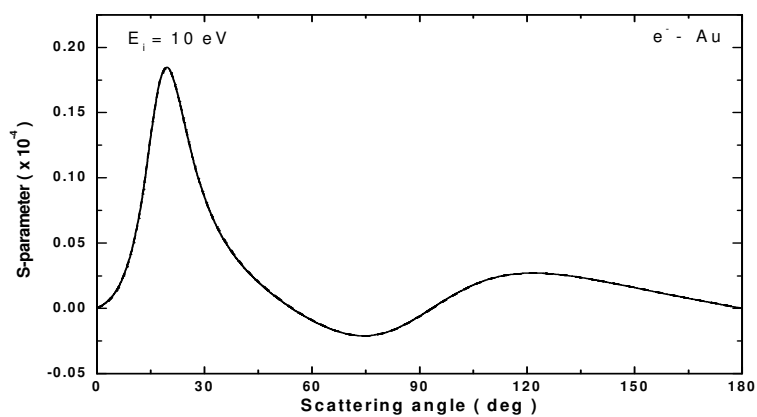
Fig.1 Partial cross-sections for e^- - Au scattering at different energy.

A. Differential cross-sections and spin polarization parameter

The calculated differential cross section in the range from 10.0 eV to 200.0 eV is shown in figure 2(a-d). 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 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 figures, 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 notice 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.





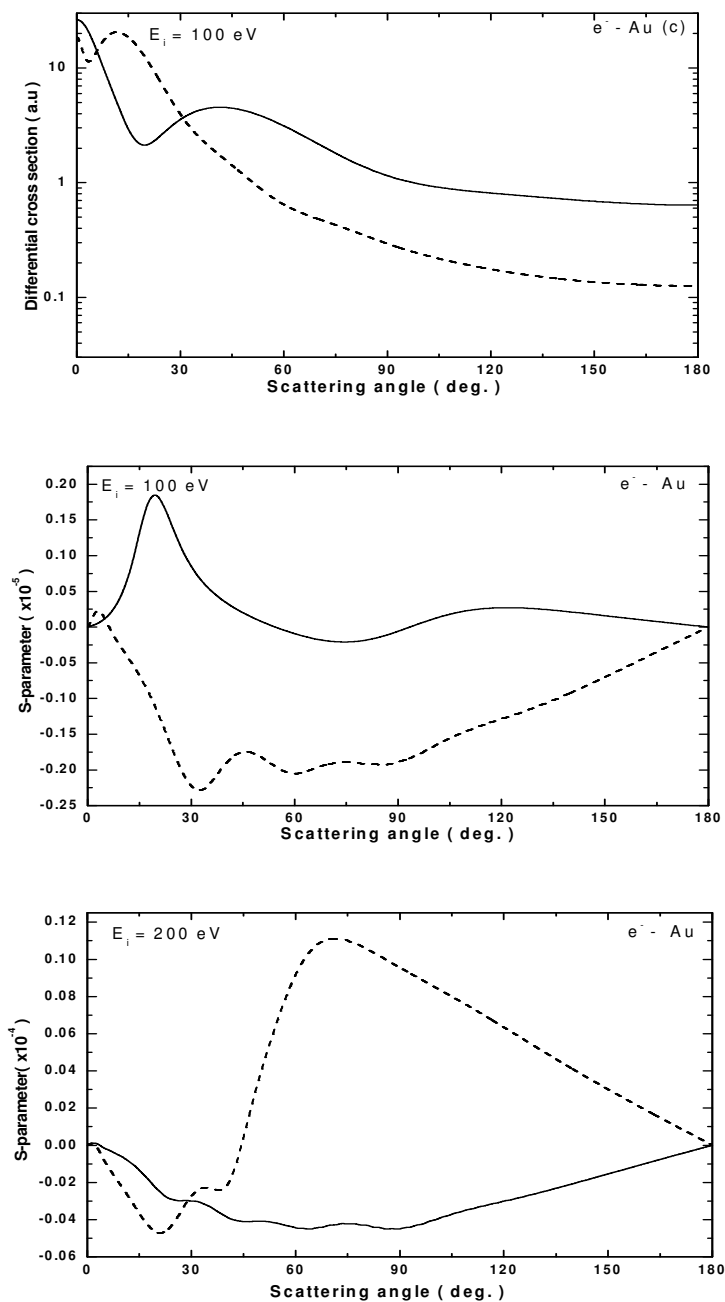


Fig. 2 (a-d) Differential Cross Section and S-parameter for e^- -Au scattering, solid line with real potential, dash line with complex potential.

4. Conclusion

We have presented our relativistic theoretical results for the elastic integral, momentum transfer, total cross section; DCS and the angular variation of spin polarization parameters for electron Au atom at energies 2.0 to 500.0 eV. We have performed the calculations in two models, the first one includes a parameter free correlation polarization potential to account for the polarization of atomic charge cloud and the other one uses a phenomenological absorption potential to account for loss of electron flux into the nonelastic channels in addition to the polarization potential. Further, the electron scattering from heavy species presented here shows significant amount of spin polarization in the scattered beam at various scattering angles. This clearly indicates that there is a need for experimental measurements and other theoretical calculations in this energy region, so that it may provide a possibility of assessing accuracy of the present optical model.

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References

1. N. Andersen and K. Bartschat, *Adv. At. Mol. Phys.*, **36** (1996) 1.
2. J. Kessler, *Adv. At. Mol. Opt. Phys.*, **27** (1991) 81.
3. G. F. hanne, *Phys rep.*, **95** 1983.
4. K. Blum, *Density matrix Theory and Application Plenum*, New York 1981.
5. D. W. Walker, *J. Phys. B: At. Mol. Opt. Phys.*, **2** (1969) 356.
6. L. Sin, Fai. *J. Lam Phys.*, **(B) 15** (1982) 119.
7. R. Haberland and L. Fritsche, *J. Phys. B: At. Mol. Phys.*, **20** (1987) 121.
8. K. Bartschat, H. J. Goerss and R. P. Nordbeck, *Z. Phys.*, **(D) 17** (1990) 25.
9. K. Bartschat, *J Phys.*, **(B) 20** (1987) 815.
10. R. P. Mc Eachran and A. D. Stauffer *J. Phys.*, **(B) 19** (1986) 3523.
11. S. N. Nahar and J. M. Wadehra, *Phys., Rev (A)* **43** (1991) 1275.
12. P. Kumar, A. K. Jain, A. N. Tripathi and S. N. Nahar *Phys., Rev. (A)* **49** (1994) 899.
13. J. Yuan, Z. Zhang, *Phys., Lett. (A)* **168** (1992) 291. *Phys., Lett., (A)* **160** (1991) 181.
14. R. Szmytkowski, *J. Phys. B: At. Mol. Opt. Phys.* **24** (1991) 3895. *J. Phys. B: At. Mol. Opt. Phys.*, **26** (1993) 535.
15. R. Szmytkowski, J. E. Sienkiewicz, *J. Phys. B: At. Mol. Opt. Phys.*, **27** (1994) 2277; *Phys. Rev. (A)* **50** (1994) 4007.
16. J. E. Sienkiewicz and W.E. Baylis, *Phys. Rev. (A)* **55** (1997) 1108.

17. A. Dorn, A. Elliot, J. Lower, S. F. Mazevet, R. P. McEachran, I .E .McCarthy, and E. Weigold, *J. Phys. B: At. Mol. Opt. Phys.*, **31** (1998) 547.
18. Neerja, A. N. Tripathi and A. K. Jain, *Phys., Rev.*, **(A) 61** (2000) 032713.
19. H. A. Bethe and R. Jackiw, *Intermediate Quantum Mechanics*, 2nd edn. (*The enjamin/Cummings publishing company, a USA*), (1968) 68.
20. A. D. McLean and R. S. McLean, *At. Data Nucl. Data Table* **26** (1981) 197.
21. F. Salvat, J. D. Martinez, R. Mayol and Parellada, *Phys. Rev.*, **(A) 36** (1987) 467.
22. F. A. Gianturco and S. Scialla, *J. Phys. B At. Mol. Opt. Phys.*, **20** (1987) 3171.
23. J. K. O'Connell, N. F. Lane, *Phys. Rev.*, **(A) 27** (1983) 1893.
24. G. Staszewska, D. Schwenke, W. Schwenkeand and D. G. Truhlar *Phys., Rev.*, **(A) 29** (1984) 3078.
25. P. G. Burke, *Potential Scattering in Atomic Physics Plenum*, New York, (1977).
26. F. Kauseen, H .Geesmann, G .F .hanne, J. Kessler, *J. Phys.B: At. Mol. Opt. Phys.*, **20** (1987) 151.
27. Harish Mohan, A .K Jain and Sunita Sharma, *Journal of Physics Conference Series*, **199** (2010) 012023.
28. R. K. Gangwar, A .N .Tripathi, Lalita Sharma, and Rajesh Srivastava, *Journal of Physics Conference Series*, **194** (2009) 042012.
29. R. P. Mc Eachran and A .D. Stauffer *Journal of Physics Conference Series* **194** (2009) 072014.
30. Kapil k. Sharma, Neerja and R. P. Vats, *European Physical Journal D*, Communicated 2010.