Z. Phys. D 30, 149–153 (1994)

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Spin polarization and cross sections of electrons elastically scattered from heavy alkaline-earth atoms

Pradeep Kumar[1], **Arvind Kumar Jain**[1], **A.N. Tripathi**[1], **Sultana N. Nahar**[2]

[1] Department of Physics, University of Roorkee, Roorkee-247667, India
[2] Department of Astronomy, Ohio State University, Columbus, OH 43210, USA

Received: 15 July 1993 / Final version: 30 August 1993

Abstract. Semi-relativistic approach is employed to compute the differential and integrated cross sections, spin polarization P and the spin polarization parameters T and U for the scattering of electrons from barium and strontium atoms in the energy range from 2.0–300 eV. The projectile-target interaction is represented both by real and complex optical potential in the solution of Dirac equation for the scattered electrons. The real optical potential includes the static, a parameter free correlation polarization and a modified semi classical exchange potentials. The complex optical potential is constructed by adding a model absorption potential as its imaginary part to the real optical potential.

PACS: 34.80.Bm; 34.80.Nz

I. Introduction

The scattering of spin polarized electron from a heavier target atom provides detailed information about the spin-dependent interaction in the electron atom collisions [1]. Recent measurements [2–3] of the polarization of scattered electrons have prompted many workers to carry out detailed calculation of these processes. In the elastic scattering of symmetric s-orbit configuration, the polarization effects are caused by spin-orbit interaction of the scattered electron in the atomic field, referred as Mott scattering [4].

In the present study we have calculated spin polarization P, polarization parameters T and U, differential cross section (DCS), integrated elastic, momentum transfer and total cross sections for the scattering of electron from barium and strontium atoms using both real and complex potential in relativistic Dirac equation [5].

II. Theory

A. Theoretical methodology

The Dirac equation for a projectile of rest mass m_0 travelling in a central field $V(r)$ at a velocity v is given by

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

For a central potential, the Dirac equation can be reduced to a set of two equations similar to the form of the Schrödinger equation such as [6–9]

$$g_\ell^{\pm\,\prime\prime}+[K^2-\ell(\ell+1)/r^2-U_\ell^{\pm}(r)]\,g_\ell^{\pm}(r)=0\,. \tag{2}$$

The effective Dirac potential terms $U_\ell^{\pm}$ expressed in atomic units are given by

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

and

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

where α is the fine structure constant (not to be confused with the Dirac matrix α of (1)). In (3–4) single and double prime corresponds to first-order and second-order derivatives with respect to r respectively. The solution of (2) behaves asymptotically as

$$g_\ell^{\pm}(K,r)\underset{r\to\infty}{\simeq}Kr[j_\ell(Kr)-\tan\delta_\ell^{\pm}\,\eta_\ell(Kr)] \tag{5}$$

where j_ℓ and η_ℓ are the spherical Bessel function of the first and second kind, respectively. The plus and minus sign to the phase shifts $\delta_\ell^{\pm}$ correspond to the $U_\ell^{\pm}(r)$ interaction i.e. δ_ℓ^{+} corresponds to the incident particle with spin up and δ_ℓ^{-} to those with spin down. The phase shifts $\delta_\ell^{\pm}$ can be obtained from the values of the radial wave function $g_\ell^{\pm}$ at the two adjacent points r and $(r+h)$ $(h\ll r)$ at very large r as

$$\tan\delta_\ell^{\pm}=-\frac{(r+h)\,g_\ell^{\pm}(r)\,j_\ell(K(r+h))-r\,g_\ell^{\pm}(r+h)\,j_\ell(Kr)}{r\,g_\ell^{\pm}(r+h)\,\eta_\ell(Kr)-(r+h)\,g_\ell^{\pm}(r)\,\eta_\ell(K(r+h))}\,. \tag{6}$$

In the present calculation, the wave function $g_\ell^{\pm}$ are obtained by numerical integration of (2) using Numerov method. In the present work, a large number of exact phase shifts, depending upon the impact energy were evaluated before using the Born approximation (for details see [9]). For example, the typical values of exact partial waves corresponding to the impact energies 2.0 and 300 eV are 20 and 150 respectively. All cross sections are converged with respect to the number of partial waves up to the value of 10^{-3} radians only.

B. Cross section and spin polarization parameters

The generalized scattering amplitude for the collision process is given as [10]

$$A = f(K,\vartheta) + g(K,\vartheta)\,\boldsymbol{\sigma}\cdot\hat{n}. \tag{7}$$

The elastic differential cross section for the scattering of the unpolarized incident beam is given by

$$d\sigma/d\Omega = |f|^2 + |g|^2 \tag{8}$$

and the amount of polarization produced in the unpolarized incident beam due to scattering is given by

$$P(\vartheta) = \frac{(fg^* + gf^*)\hat{n}}{|f|^2 + |g|^2} = P(\vartheta)\hat{n} \tag{9}$$

where $P(\vartheta)$ is called the Sherman function. The other two polarization parameters T and U describe the rotation of the polarization vector during the scattering processes. They are given as [9]

$$T(\vartheta) = \frac{|f|^2 - |g|^2}{|f|^2 + |g|^2} \tag{10}$$

$$U(\vartheta) = i\frac{fg^* - gf^*}{|f|^2 + |g|^2}. \tag{11}$$

The angle of rotation of the component of the polarization vector in the scattering plane is given by $\tan^{-1}(U/T)$. It should be noted that these three polarization parameters are interrelated through the condition $P^2 + T^2 + U^2 = 1$.

C. The interaction potential

The total interaction between the projectile and target atom is represented by a model potential. At the impact energies above the first ionization threshold, this potential is complex and is written as

$$V(r) = V_R(r) + iV_{\text{abs}}(r) \tag{12}$$

where $V_R(r)$ the real part of the total interaction potential $V(r)$, is represented by three local and real terms, namely, the static (due to direct Coulomb interaction of all the charged particles involved), exchange (arising due to the Pauli exclusion principal) and polarization potential (taking into account the distortion of the target charge cloud in the presence of incoming electron field). $V_{\text{abs}}(r)$ is the absorption potential. The inclusion of absorption potential gives the total scattering that includes both elastic and inelastic scattering such as excitation, ionization, etc. causing the absorption of the scattered beam. The static potential of the target atom is obtained by averaging over the motion of the target electrons and is given as

$$V_s(r) = \frac{Zee_p}{r} - ee_p \sum_n \sum_l \sum_m N_{nlm} \times \int |\phi_{nlm}(r')|^2 \frac{1}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}' \tag{13}$$

where Z is the nuclear charge of the target atom. e_p is the projectile charge and N_{nlm} is the occupancy number of the orbit (n,l,m). The radial part $\phi(r)$ of the spatial orbital $\phi_{nlm}(r) = \varphi_{nl}(r)\ Y_{lm}(\hat{r})$ is expanded in terms of Slater type orbital as given in the tables of Clementi and Roetti [11] and McLean and McLean [12]. Polarization potential is the parameter free polarization potential and is taken from the paper of O'Connel and Lane [13]. It has two components, the short range $[V_{\text{SR}}(r)]$ part and the long range $[V_{\text{LR}}(r)]$ part and is given by

$$V_p(r) = \begin{cases} V_{\text{SR}}(r) & \text{for } r < r_c \\ V_{\text{LR}}(r) & \text{for } r \geqq r_c \end{cases}. \tag{14}$$

Here r_c is the point where two forms cross each other for the first time. The crossing point i.e. r_c for barium and strontium atoms occur at 18.85 au and 20.05 au respectively. For the present calculations, the static dipole polarizability α_d is taken 267.93 au for barium and 186.27 au for strontium (see [14]). The exchange potential is taken to be modified semi-classical as given by Gianturco and Scialla [15] and the absorption potential is included via the semiempirical model absorption potential of Staszewska et al. [16]. We avoid repeating their expression here. The first inelastic threshold [17] for barium and strontium is at 1.90 eV and 3.03 eV while their ionization threshold is at 5.21 eV and 5.69 eV respectively.

III. Results and discussion

A. Electron scattering from barium and strontium atoms

The calculated differential cross section (DCS) for the elastically scattered electrons by barium and strontium atoms are shown in Fig. 1. In these figures the solid curve correspond to the DCS value obtained by using real potential (RP) as the total projectile-target interaction and the dashed curve corresponding to those obtained with complex potential (CP) as the interaction. At low energies, there is no difference between the results obtained using either real or complex potential but at higher impact energies there is a small difference between the two calculated values especially at those scattering angles where DCS exhibit minima and maxima in the curve. This feature is expected since at low energies the scattering is mainly elastic and there is almost no effect of the absorption on the DCS values, whereas at higher impact

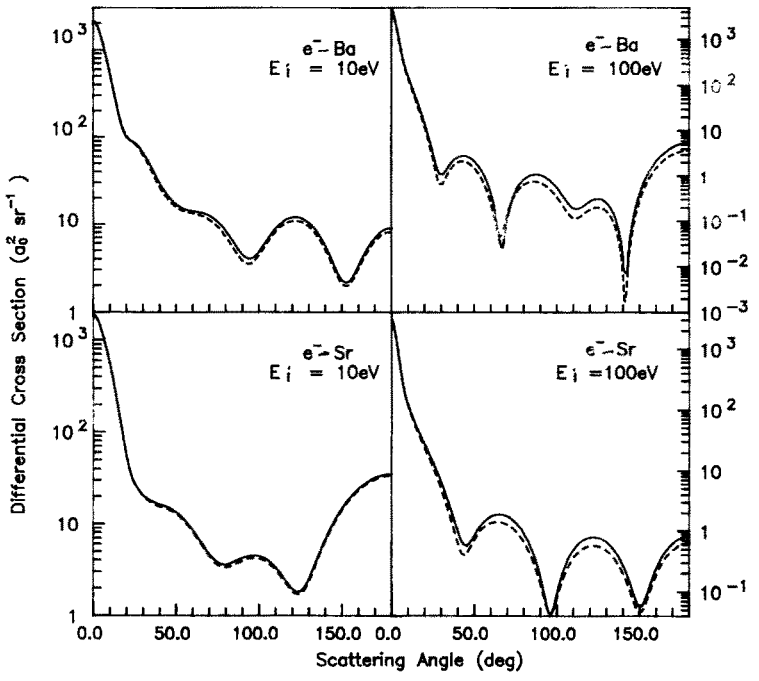

Fig. 1. Differential cross section in $(a_0^2 sr^{-1})$ for elastic scattering of electrons from barium and strontium at 10.0 eV and 100.0 eV. *Solid curves* correspond to DCS values obtained by using real potential (RP) in Dirac equation; *dashed curves* are those obtained using the complex potential (CP) in the Dirac equation

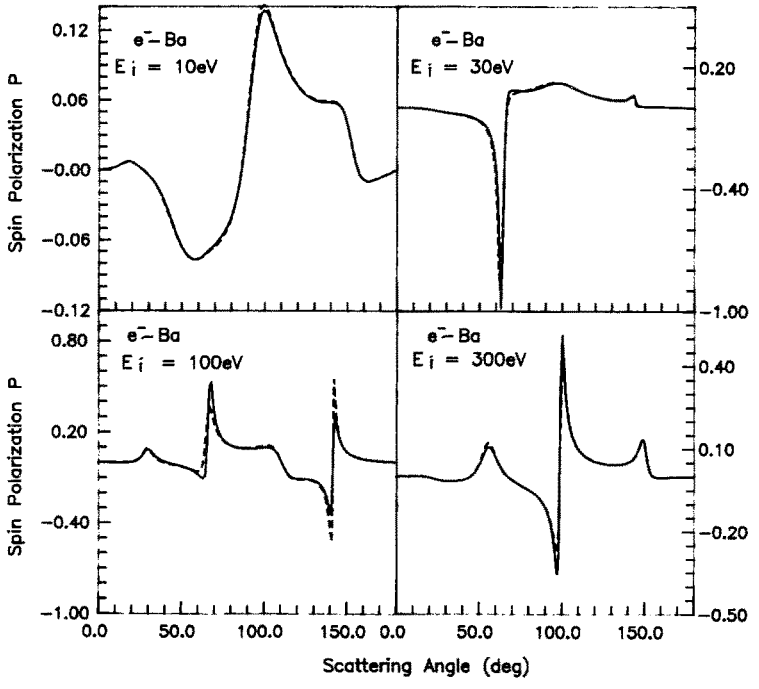

Fig. 2. Spin polarization P for electrons scattered from barium at; 10.0 eV, 30.0 eV, 100.0 eV, and 300.0 eV *solid* and *dashed curves* are same as in Fig. 1

energies there is reduction in the DCS values, in particular the structure of dips and humps (both in magnitude and width) change when the absorption effects are switched on.

The calculated values of the spin polarization P for the elastic scattering of electrons from barium and strontium atoms at various impact energies are shown in Figs. 2, 3. Like all DCS curves the solid curves correspond to the values obtained using the pure real potential and dashed curves to those obtained using complex potential in the Dirac equation. At all energies both these curves show a little difference between them, except at some minima and maxima where inclusion of absorption potential causes the minima to go deeper and the maxima to peak higher in general. Figures 2, 3 show a significant amount of spin polarization in the scattered beam at various scattering angles. This indicates that it will be of much interest to carry out the measurements of the spin polarization of the electron beam scattered by barium and strontium atoms.

The measurements of the polarization parameter T and U are difficult to carry out. The polarization parameter T and U for electrons scattered from barium atom is shown in Fig. 4 which show a similar features to spin polarization curves.

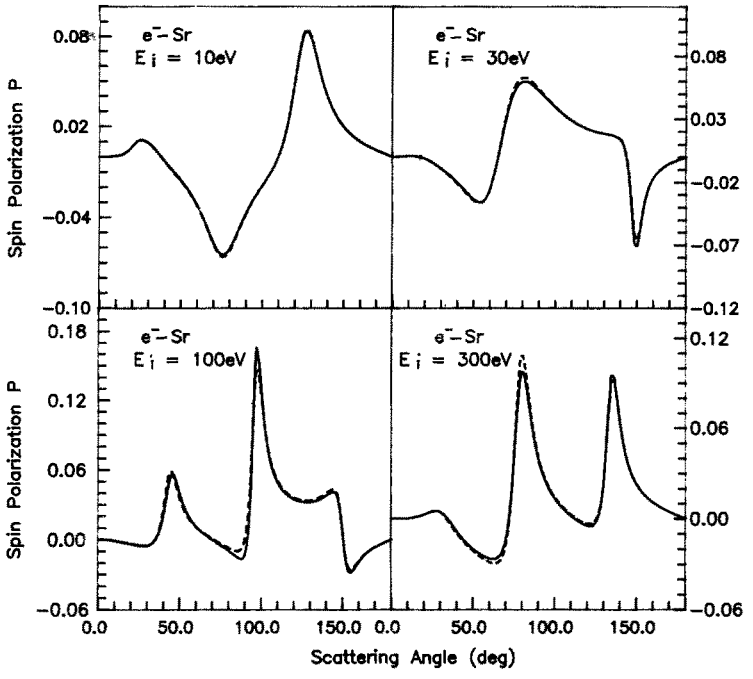

Fig. 3. Spin polarization P for electrons scattered from strontium at; 10.0 eV, 30.0 eV, 100.0 eV, and 300.0 eV *solid* and *dashed curves* are same as in Fig. 1

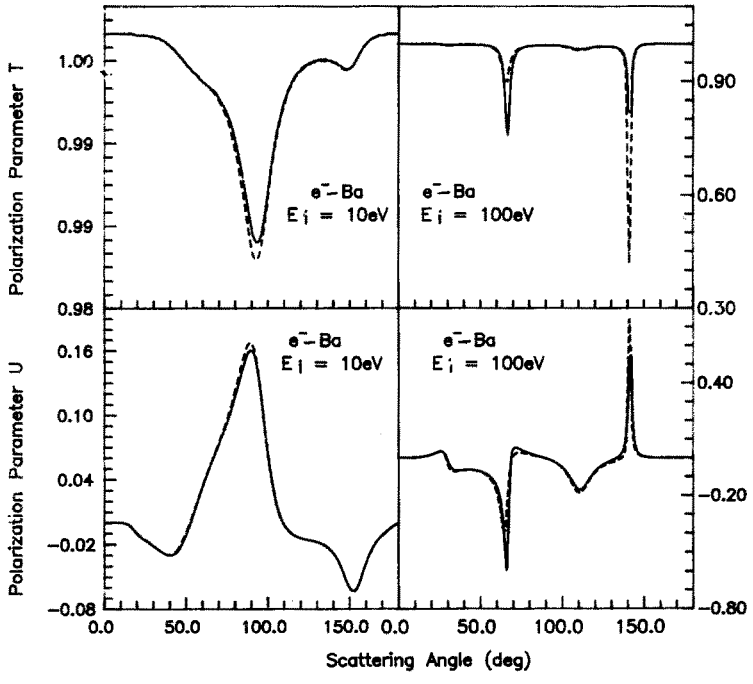

Fig. 4. Polarization parameters T and U for electrons scattered from barium at; 10.0 eV, and 100.0 eV *solid* and *dashed curves* are same as in Fig. 1

B. Elastic and total scattering cross sections

The value of the calculated integrated elastic, total and momentum transfer cross sections for barium and strontium atoms are compiled in Tables 1 and 2 respectively. The elastic cross sections are obtained using both the real and complex potentials. It is seen that the elastic cross sections with real potentials 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 the same tables. It is observed that total cross section descends rapidly at low energies and thereafter it decreases slowly with increasing impact energies. The momentum transfer cross sections are obtained using both real and complex potential. The calculated values with real potentials are higher than those obtained with complex potential. Again, the reduction in the momentum transfer cross sections is due to the inclusion of absorption effect.

Table 1. Calculated values of the integrated elastic, total cross sections and momentum transfer cross sections (in units of a_0^2) for the elastic scattering of electron from barium atom. RP corresponds to the use of real potential, CP to the use of complex potential

E (eV)	σ_{el}		σ_{tot}	Momentum transfer cross sections	
	RP	CP		RP	CP
2.0	763.09	763.09	763.09	407.85	407.85
4.0	546.22	544.03	547.42	259.61	257.42
6.0	445.03	438.20	448.39	187.62	181.30
10.0	339.54	326.26	345.96	111.09	100.93
20.0	218.17	202.10	228.02	46.56	38.17
30.0	202.93	184.96	209.39	30.14	23.77
50.0	160.06	143.49	164.33	16.06	11.95
100.0	100.12	89.09	104.24	9.69	6.82
150.0	74.52	66.46	78.49	8.64	6.17
200.0	61.05	54.77	64.75	7.87	5.77
300.0	47.00	42.74	50.14	6.48	4.98

Table 2. Calculated values of the integrated elastic, total cross sections and momentum transfer cross sections (in units of a_0^2) for the elastic scattering of electron from strontium atom. RP corresponds to the use of real potential, CP to the use of complex potential

E (eV)	σ_{el}		σ_{tot}	Momentum transfer cross sections	
	RP	CP		RP	CP
2.0	771.55	771.55	771.55	374.60	374.60
4.0	468.60	468.54	468.69	243.22	243.15
10.0	260.52	254.95	264.00	96.66	92.15
20.0	195.18	184.75	200.14	43.50	38.05
30.0	165.78	155.09	170.41	25.93	21.85
50.0	127.80	118.34	131.75	13.50	10.96
100.0	80.91	73.78	84.06	8.53	6.48
150.0	60.29	54.68	63.12	7.40	5.57
200.0	48.90	44.40	51.52	6.50	4.94
300.0	36.65	33.59	38.94	5.05	3.97

IV. Conclusions

We have presented the results of our semi-relativistic, total scattering, momentum transfer cross sections, DCS and the angular distribution of spin polarization P, and polarization parameters T and U for electrons scattered from barium and strontium atoms. In the present semi-relativistic calculations direct relativistic effect is taken into account by transforming the Dirac equation into two component Schrödinger equation. This Schrödinger equivalent of the Dirac equation for the scattered electrons was solved by Numerov method and the phase shifts extracted. In the present equation the projectile-target interaction was represented both by the real and the complex model potentials. A significant amount of spin polarization is noticed in the scattered beam at various scattering angles. This indicates that it will be of much interest to carry out the experiments to measure the spin polarization of electron beam scattered by barium and strontium atoms.

One of the authors (AKJ) gratefully acknowledges financial support from Department of Science and Technology (DST), New Delhi, India.

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