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Electron impact excitation of rubidium atoms

S. Saxena[a] and R. Srivastava[b]

Physics Department, Indian Institute of Technology, Roorkee-247667, India

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Abstract. We have carried out distorted wave calculations for electron impact 5 ^{2}S $\rightarrow$ 5 ^{2}P, 6 ^{2}S and 4 ^{2}D excitations of rubidium atom at incident electron energies in the range of 10–200 eV. Results are presented for differential and total cross-sections of these excitations, Stokes parameters of the excitation of the fine-structure resolved and unresolved 5 ^{2}P and 4 ^{2}D states, complete experiment parameters for the excitation of 5 ^{2}P state and the STU spin parameters of its fine structure states. Good agreement is found on comparison of our results with the available experimental data and the earlier theoretical calculations. Except for the resonance 5 ^{2}S $\rightarrow$ 5 ^{2}P transition no earlier calculations were reported for the excitation of the higher 6 ^{2}S and 4 ^{2}D states.

PACS. 34.80.Dp Atomic excitation and ionization by electron impact – 34.80.Nz Spin dependence of cross-sections; polarized electron beam experiments

1 Introduction

The resonance n ^{2}S–n ^{2}P excitations of lighter alkali atoms [viz. Li ($n = 2$), Na ($n = 3$) and K ($n = 4$)] by electron impact have been extensively studied both theoretically and experimentally and results for various collision parameters have been reported [1,2]. In recent years, the studies have focused on heavier alkali atoms to explore the relativistic effects. Consequently, electron impact 6 ^{2}S–6 ^{2}P transition in Cs has received considerable attention [2,3]. However, among alkalis, the electron impact resonance 5 ^{2}S–5 ^{2}P transition of Rb has been the least studied. This may be due to the reason that Rb (having atomic number 37) is thought not heavy enough to probably warrant the relativistic treatment of its theoretical study. It would therefore be interesting to test such aspect.

For electron impact 5 ^{2}S–5 ^{2}P transition in Rb, Vuskovic et al. [4] reported the measurements of both the differential and total cross-sections while Chen and Gallagher [5] and Zapesochnyi et al. [6] published their experimental data of total cross-sections (TCS) only. To compare with these experiments Pangantiwar and Srivastava [7] carried out distorted wave Born approximation (DWBA) calculations where they used the Mott and Massey version of the DWBA T-matrix and adopted Ochkur's approximation to simplify the exchange T-matrix. Much later Zeman et al. [8] performed relativistic distorted wave (RDW) calculations for the resonance transitions of Rb and many other alkali atoms. They compared their differential cross-section (DCS) and TCS results of Rb with the experiment [4–6] and the DWBA calculations [7]. They also reported other collision parameters viz. Stokes parameters and some spin parameters. Currently there has been renewed experimental activities for studying the resonance transition of Rb viz. for measuring the Stokes parameters using super elastic scattering technique [9] as well as the spin asymmetry using spin polarized electron beam [10]. In order to supplement the on going and expected more future experiments, we consider in the present paper electron impact excitations of Rb and report our detailed calculations for some of lower excited states.

Recently, we have used an improved version of distorted wave approximation (DWA) method [11,12] for the calculation of the resonance and non resonance excitations in lighter Li, Na and K alkali atoms which provided results in good agreement with the experiments. In the present paper, we extend the same DWA method to the calculation of the 5 ^{2}S–5 ^{2}P transition in Rb. We report our results for DCS, TCS, Stokes parameters, spin parameters and complete experiment parameters. We compare our results with the only few available experimental data [4–6,9] as well as with the RDW calculations of Zeman et al. [8] to see the influence of relativistic effects. Vuskovic et al. [4] also reported experimental DCS results for the combined excitation of the higher 6 ^{2}S and 4 ^{2}D states but there are no calculations to compare with their data. We therefore, also calculate results of DCS and TCS for the excitation of these two states and Stokes parameter results for excitation of the 4 ^{2}D state.

[a] e-mail: sasasdph@iitr.ernet.in
[b] e-mail: rajsrfph@iitr.ernet.in

In Section 2, we outline our DWA method and briefly mention calculation of the different collision parameters. In Section 3, the results are presented and finally some conclusions are drawn in Section 4.

2 Theoretical considerations

2.1 Distorted wave approximation (DWA) theory

In our present study, the rubidium atom is treated as one-electron system and the effect of the core electrons is incorporated in the form of a core potential. The T-matrices in the *distorted wave approximation* for the electron impact excitation of rubidium atom from the initial ground state i to any final excited state state f (with magnetic quantum number M) in the singlet (s) or triplet (t) mode can be expressed as [11,12]

$$T_{if}^{s(t)}(M) = T_{if}^{d}(M) \pm T_{if}^{ex}(M). \tag{1}$$

The $+(-)$ sign is associated with the scattering in the singlet (triplet) mode. Further, the spin-averaged direct (T_{if}^{d}) and exchange (T_{if}^{ex}) T-matrices are given by

$$T_{if}^{d}(M) = \left\langle F^{-}(\mathbf{k}_f, 2)\phi_f(1)\left|V(1,2) - U_f(2)\right|\phi_i(1)F^{+}(\mathbf{k}_i, 2)\right\rangle \tag{2}$$

and

$$T_{if}^{ex}(M) = \left\langle F^{-}(\mathbf{k}_f, 2)\phi_f(1)\left|V(1,2) - U_f(2)\right|\phi_i(2)F^{+}(\mathbf{k}_i, 1)\right\rangle. \tag{3}$$

Here, V is the total interaction potential between the projectile electron and target rubidium atom expressed by (atomic units are used throughout):

$$V = -\frac{1}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} + V^{core}(r_2) \tag{4}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are respectively the position co-ordinates of the target and projectile electrons with respect to the target nucleus. Further, the core potential, V^{core}, of the rubidium atom is given by

$$V^{core} = \sum_{n,l} N_{nl} \int \frac{|R_{nl}(r)|^2 r^2 dr}{r_>} \tag{5}$$

where, N_{nl} represents the occupation number of the electrons in different core orbitals of Rb referred to by n and l quantum numbers and R_{nl} is the corresponding radial wave function.

$\phi_{i(f)}$ is the bound state initial (final) wave function of the target atom. $F^{+(-)}(\mathbf{k}_{i(f)}, \mathbf{r})$ is the projectile distorted wave in the initial (final) channel with wave vector $\mathbf{k}_i(\mathbf{k}_f)$ and the associated superscript $+(-)$ indicates the usual outgoing (incoming) wave boundary conditions. These satisfy following equation:

$$\left[\nabla^2 + k_{i(f)}^2 - 2U_{i(f)}(r)\right] F^{+(-)}(\mathbf{k}_{i(f)}, \mathbf{r}) = 0 \tag{6}$$

$U_{i(f)}$ is the distortion potential in the initial (final) channel given by

$$U_{i(f)} = V_{i(f)}^{stat} + V_{i(f)}^{exch} \tag{7}$$

with static potential $V_{i(f)}^{stat} = \langle\phi_{i(f)}|V|\phi_{i(f)}\rangle$ and the exchange potential $V_{i(f)}^{ex}$ is taken to be the widely used form [13].

We expand the distorted waves F^{+} and F^{-} using the following general form of partial wave expansion

$$F^{+(-)}(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{k}} \sum_{\ell=0}^{\infty} (2\ell+1) i^{\ell}\, e^{\pm i\delta_\ell(k^2)} \frac{u_\ell^{\pm}(k,r)}{r} P_\ell\left(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}}\right) \tag{8}$$

where δ_ℓ is the phase shift of the ℓth partial wave, P_ℓ is the Legendre polynomial of order ℓ and $u_\ell^{\pm}(k,r)$ is radial part of the distorted wave. On substituting $F^{\pm}$ as given above from equation (8) into equation (6) we get

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} + 2U(r)\right] u_\ell(k,r) = 0 \tag{9}$$

which is solved numerically subject to the following usual boundary conditions

$$u_\ell(k,r) \underset{r\to 0}{=} 0 \tag{10}$$

and

$$u_\ell(k,r) \underset{r\to\infty}{=} \frac{1}{\sqrt{k}} \sin\left[kr - \frac{1}{2}\ell\pi + \delta_\ell\left(k^2\right)\right]. \tag{11}$$

There is flexibility in the choice of distortion potentials U_i and U_f in the DWA method. A traditional approach as described by Mott and Massey [14] is that the U_i is represented by initial ground state static potential of the target and U_f is represented by final excited state static potential of the target. However, a number of DWA calculations [15–17] suggest that the use of same potential in both the channels, which ensures orthogonality between the incident and scattered electron distorted waves, explains the experimental data in better manner. Also it has been almost established now that the use of excited state potential of the target in both the channels explains the experiments in the best way. The same choice will also be adopted for the present calculations.

From equation (1) the direct and exchange T-matrices are evaluated for the excitation of each magnetic state M of the final excited state. We obtain the T-matrices for the singlet (s) and triplet (t) modes separately. Further, the scattering amplitude for each magnetic sub state M of the final excited state is related to the T-matrix by

$$a_M^{s(t)} = -\frac{1}{2\pi} T_{if}^{s(t)}(M). \tag{12}$$

The differential cross-section in the singlet (triplet) mode can therefore be expressed in terms of the scattering amplitude as

$$\sigma_M^{s(t)} = \frac{k_f}{k_i} \left| a_M^{s(t)} \right|^2 \tag{13}$$

and the spin-averaged DCS as

$$\sigma_M = \frac{1}{4}\sigma_M^s + \frac{3}{4}\sigma_M^t. \tag{14}$$

Finally, the DCS summed over the different values of M is

$$\sigma = \sum_M \sigma_M. \tag{15}$$

In addition, the total cross-section after integrating over all scattering angles for different values of M are obtained in terms of the spin-averaged DCS by

$$Q_M = \int \sigma_M \, d\Omega \tag{16}$$

and the total cross-section summed over all values of M by

$$Q = \int \sigma \, d\Omega. \tag{17}$$

2.2 Stokes parameters and alignment and orientation parameters

2.2.1 Measured Stokes parameters

For the light emitted from the decay of the electron impact excited 5 ^{2}P and 4 ^{2}D states of Rb, the usual Stokes parameters P_i ($i = 1, 2, 3$) measured perpendicular to the scattering plane are [1,18,19]

$$P_1 = \frac{I(0^\circ) - I(90^\circ)}{I(0^\circ) + I(90^\circ)} \tag{18}$$

$$P_2 = \frac{I(45^\circ) - I(135^\circ)}{I(0^\circ) + I(135^\circ)} \tag{19}$$

$$P_3 = \frac{I(\mathrm{RHC}) - I(\mathrm{LHC})}{I(\mathrm{RHC}) + I(\mathrm{LHC})} \tag{20}$$

while, analogous to P_1, the Stokes parameter P_4 measured parallel to the scattering plane is given by

$$P_4 = \frac{I(0^\circ) - I(90^\circ)}{I(0^\circ) + I(90^\circ)} \tag{21}$$

here $I(\phi)$ is the intensity of light with polarization detector in the ϕ-direction with respect to incident electron direction and I(RHC) and I(LHC) are respectively the intensities of the right and left circularly polarized light components, respectively.

2.2.2 Calculation of Stokes parameters

Further, the Stokes parameters P_i ($i = 1, 4$) can be expressed as below in terms of the state multipoles of the electron impact excited state (i.e. 5 ^{2}P and 4 ^{2}D states of Rb atom) which are related to the scattering amplitude or the T-matrix. In general, for the photon decay for the transition $L_f \to L_d$, we can write [18]

$$P_1 = \frac{1}{I^Y} \begin{Bmatrix} 1 & 1 & 2 \\ L_f & L_f & L_d \end{Bmatrix} \left[\sqrt{\frac{3}{2}} G_2(L_f) \left\langle T(L_f)_{20}^+ \right\rangle - G_2(L_f) \left\langle T(L_f)_{22}^+ \right\rangle \right] \tag{22}$$

$$P_2 = \frac{1}{I^Y} \begin{Bmatrix} 1 & 1 & 2 \\ L_f & L_f & L_d \end{Bmatrix} \left[2G_2(L_f) \left\langle T(L_f)_{21}^+ \right\rangle \right] \tag{23}$$

$$P_3 = \frac{1}{I^Y} \begin{Bmatrix} 1 & 1 & 1 \\ L_f & L_f & L_d \end{Bmatrix} \left[2iG_1(L_f) \left\langle T(L_f)_{11}^+ \right\rangle \right] \tag{24}$$

$$P_4 = \frac{1}{I^x} \begin{Bmatrix} 1 & 1 & 2 \\ L_f & L_f & L_d \end{Bmatrix} \left[\sqrt{\frac{3}{2}} G_2(L_f) \left\langle T(L_f)_{20}^+ \right\rangle + G_2(L_f) \left\langle T(L_f)_{22}^+ \right\rangle \right] \tag{25}$$

where

$$I^Y = \frac{2(-1)^{L_f+L_d}}{3(2L_f+1)^{1/2}} G_0(L_f) \left\langle T(L_f)_{00}^+ \right\rangle + \begin{Bmatrix} 1 & 1 & 2 \\ L_f & L_f & L_d \end{Bmatrix} \left[\frac{G_2(L_f)}{\sqrt{6}} \left\langle T(L_f)_{20}^+ \right\rangle + G_2(L_f) \left\langle T(L_f)_{22}^+ \right\rangle \right] \tag{26}$$

and

$$I^x = \frac{2(-1)^{L_f+L_d}}{3(2L_f+1)^{1/2}} G_0(L_f) \left\langle T(L_f)_{00}^+ \right\rangle + \begin{Bmatrix} 1 & 1 & 2 \\ L_f & L_f & L_d \end{Bmatrix} \left[\frac{G_2(L_f)}{\sqrt{6}} \left\langle T(L_f)_{20}^+ \right\rangle - G_2(L_f) \left\langle T(L_f)_{22}^+ \right\rangle \right]. \tag{27}$$

The fine-structure depolarization coefficient $G_K(L_f)$ can be written as

$$G_K(L_f) = \frac{1}{(2S_f+1)} \sum_{J_f} (2J_f+1)^2 \begin{Bmatrix} L_f & J_f & S_f \\ J_f & L_f & K \end{Bmatrix}^2 \quad (28)$$

where S_f is the electronic spin and $\mathbf{J}_f = \mathbf{L}_f + \mathbf{S}_f$ is the total angular momentum of the atom. The $G_K(L_f)$ are normalized such that $G_0(L_f) = 1$ for all L_f.

Further, the state multipole $\langle T(L_f)^+_{KQ} \rangle$ with $-K \leq Q \leq K$ and $0 \leq K \leq 2L_f$ of the excited state with orbital angular momentum L_f are related to the complex scattering amplitudes a_M of the magnetic sub state M by

$$\left\langle T(L_f)^+_{KQ} \right\rangle = \sum_{M',M} (-1)^{L_f - M'} (2K+1)^{1/2} \begin{pmatrix} L_f & L_f & K \\ M' & -M & -Q \end{pmatrix} \langle a_{M'} a^*_M \rangle \quad (29)$$

where spin average $\langle a_{M'} a^*_M \rangle$ is defined as

$$\langle a_{M'} a^*_M \rangle = \frac{1}{2(2S_i+1)} \sum_s (2S+1) a^s_{M'} a^{s*}_M \quad (30)$$

here S_i is the atomic spin in the initial state and S is the total spin of the system which in the present calculation can be zero and unity respectively in singlet and triplet modes.

Further, in order to give a better physical meaning to the Stokes parameters P_i $(i = 1{-}4)$ as well as to characterize the excited state charge cloud of the atom immediately after the excitation, Andersen et al. [1] defined a set of four alignment and orientation parameters. They are the alignment angle γ, the linear polarization P_ℓ, the angular momentum transferred perpendicular to the scattering plane $L_\perp$ and relative height of charge cloud ρ_{00}. These parameters can be expressed [1] in terms of the reduced Stokes parameters $\bar{P}_1 - \bar{P}_4$ which can be obtained by using the same relations as for measured Stokes parameters given by equations (22–25), but with values of all the $G_K(L_f)$ taken as unity, as the alignment and orientation parameters are defined for the nascent charge cloud.

2.2.3 Stokes parameters for the fine structure resolved states

For the radiative decays $5\ ^2\mathrm{P}_{1/2,3/2} \rightarrow 5\ ^2\mathrm{S}_{1/2}$ in Rb, the Stokes parameters $P_i(J_f)$, $(i = 1, 4)$ at a fixed scattering angle θ can be obtained using the following relations. J_f refers angular momentum of the excited state [20]

$$P_1\left(\frac{3}{2}\right) = \frac{3G_2\left(\frac{3}{2}\right)(\sigma_0 - 2\sigma_1)}{\left(4 + G_2\left(\frac{3}{2}\right)\right)(\sigma_0 + 2\sigma_1)} \quad (31)$$

$$P_2\left(\frac{3}{2}\right) = \frac{18G_2\left(\frac{3}{2}\right) \mathrm{Re}\left[(f_0 g_1^* + g_0 f_1^*) - 2(f_0 f_1^* + g_0 g_1^*)\right]}{\sqrt{30}\left(4 + G_2\left(\frac{3}{2}\right)\right)(\sigma_0 + 2\sigma_1)} \quad (32)$$

$$P_3\left(\frac{3}{2}\right) = \frac{5\sqrt{2}G_1\left(\frac{3}{2}\right) \mathrm{Im}\left[2(f_0 f_1^* + g_0 g_1^*) - (f_0 g_1^* + g_0 f_1^*)\right]}{(4 + G_2\left(\frac{3}{2}\right))(\sigma_0 + 2\sigma_1)} \quad (33)$$

$$P_4\left(\frac{3}{2}\right) = \frac{3G_2\left(\frac{3}{2}\right)\sigma_0}{\left(4 + G_2\left(\frac{3}{2}\right)\right)\sigma_0 + (8 - 4G_2\left(\frac{3}{2}\right))\sigma_1} \quad (34)$$

$$P_1\left(\frac{1}{2}\right) = P_2\left(\frac{1}{2}\right) = P_4\left(\frac{1}{2}\right) = 0 \quad (35)$$

and

$$P_3\left(\frac{1}{2}\right) = \frac{\sqrt{2}G_1\left(\frac{1}{2}\right) \mathrm{Im}\left[2(f_0 f_1^* + g_0 g_1^*) - (f_0 g_1^* + g_0 f_1^*)\right]}{(\sigma_0 + 2\sigma_1)} \quad (36)$$

where Re and Im refer respectively the real and imaginary parts of the bracketed quantity, σ_M are the different cross-section at scattering angle θ with $M = 0, \pm 1$ for the unresolved excited $5\ ^2\mathrm{P}$ state and f_M and g_M are respectively the direct and exchange amplitudes given by

$$f_M = -\frac{1}{2\pi} T^d_{if}(M) \quad (37)$$

and

$$g_M = -\frac{1}{2\pi} T^{ex}_{if}(M). \quad (38)$$

In equations (31–36), $G_K(J_f)$ are the hyperfine depolarization coefficients given by

$$G_K(J_f) = \frac{1}{(2I+1)} \sum_F (2F+1)^2 \begin{Bmatrix} J_f & F & I \\ F & J_f & K \end{Bmatrix}^2 \quad (39)$$

where I is the nuclear spin of the Rb atom and its value is 5/2. Further $\mathbf{F} = \mathbf{I} + \mathbf{J}_f$ is the full quantum number of the atom.

Similarly for the radiative decays $4\ ^2\mathrm{D}_{5/2} \rightarrow 5\ ^2\mathrm{P}_{3/2}$ and $4\ ^2\mathrm{D}_{3/2} \rightarrow 5\ ^2\mathrm{P}_{1/2}$ in Rb, the Stokes parameters $P_i(J_f)$, $(i = 1, 4)$ at scattering angle θ can be derived in terms of the differential cross-sections σ_M and the amplitudes f_M and g_M, at scattering angle θ with $M = 0$, ± 1, ± 2 for the unresolved excited $4\ ^2\mathrm{D}$ state.

2.2.4 The complete experiment parameters

The scattering amplitudes as given in earlier sections have been written in the "collision frame of reference" in which the incident electron direction has been chosen as quantization axis and is along the z-axis while x–z-plane is the scattering plane. However, often experimental observables can be interpreted more easily in the "natural frame of reference" where the projectile electron is incident along x-axis and the x–y-plane is the scattering plane. The natural co-ordinate system can be obtained by rotating the collision frame of reference through Euler angles $\alpha = -\pi/2$, $\beta = -\pi/2$, $\gamma = 0$. A set of complete parameters for the 5 ^{2}S $\rightarrow$ 5 ^{2}P excitation in Rb, can be defined in terms of the scattering amplitudes in "natural frame of reference". Since the scattering can take place in $S = 0$ singlet (s) and $S = 1$ triplet (t) modes, the corresponding scattering amplitudes in the "natural frame" can be expressed as a'^t_M and a'^s_M with $M = \pm 1$. Note that in the "natural frame" amplitude with $M = 0$ does not survive due to reflection symmetry along the scattering plane. The amplitudes in the "natural frame" are related to the corresponding scattering amplitudes that we calculated in the "collision frame" by

$$a'_{\pm 1} = \mp\sqrt{\frac{1}{2}}a_0 - ia_1. \tag{40}$$

Let us further express these amplitudes by the following complex quantities

$$a'^t_{+1} = \alpha_+ e^{i\phi_+} \tag{41}$$

$$a'^t_{-1} = \alpha_- e^{i\phi_-} \tag{42}$$

$$a'^s_{+1} = \beta_+ e^{i\psi_+} \tag{43}$$

$$a'^s_{-1} = \beta_- e^{i\psi_-} \tag{44}$$

where $\alpha_\pm$, $\beta_\pm$, $\phi_\pm$ and $\psi_\pm$ are real numbers. Neglecting an overall phase, we thus need seven independent parameters at each scattering angle θ to characterize the scattering amplitudes given by equations (41–44) completely. In addition to differential cross-sections σ_u corresponding to unpolarized incident electron beam, we require six dimensionless parameters i.e. three relative amplitudes and three relative phase angles. Consequently, a following set of complete experiment parameters have been defined [2]:

$$(\sigma_u, \omega^t, L^t_\perp, L^s_\perp, \gamma^t, \gamma^s, \Delta^+) \tag{45}$$

which allow for a complete description of the 5 ^{2}S $\rightarrow$ 5 ^{2}P scattering process. These quantities can be expressed in terms of the real numbers $\alpha_\pm$, $\beta_\pm$, $\phi_\pm$ and $\psi_\pm$ of the equations (41–44) as given in Andersen et al. [2].

2.2.5 Generalized STU parameters

The complete set of parameters discussed in the earlier section can not be realized experimentally with the measurements of the Stokes parameters only. The experimental measurements of the generalized STU parameters are also required [1]. The generalized STU parameters are: σ_u, the differential cross-section for the scattering of unpolarized projectiles from unpolarized targets, the polarization function S_P (which gives the polarization of an initially unpolarized projectile beam after the collision), the asymmetry function S_A (determines a left-right asymmetry in the differential cross-section for scattering of a spin-polarized beam), the contraction parameters T_x, T_y, T_z (describe the change of an initial polarization component along the three Cartesian axes) and the parameters U_{xz} and U_{zx} (determine the rotation of a polarization component in the scattering plane).

The seven, polarization, asymmetry, contraction and rotation parameters for each of the fine structure transitions 5 ^{2}S$_{1/2}$ $\rightarrow$ 5 ^{2}P$_{1/2,3/2}$ in Rb can be written in terms only four independent parameters as defined below. The superscripts 1/2 and 3/2 denote the values corresponding to the excitations ^{2}P$_{1/2}$ and ^{2}P$_{3/2}$ respectively

$$S_P \equiv S_P^{1/2} = -2S_P^{3/2} \tag{46}$$

$$S_A \equiv S_A^{1/2} = -2S_A^{3/2} \tag{47}$$

$$T \equiv T_x^{1/2} = T_y^{1/2} = T_z^{1/2} = T_x^{3/2} = T_y^{3/2} = T_z^{3/2} \tag{48}$$

and

$$U \equiv U_{zx}^{1/2} = U_{xz}^{1/2} = -2U_{zx}^{3/2} = -2U_{xz}^{3/2}. \tag{49}$$

These above set of four parameters S_P, S_A, T and U can be expressed in terms of the real numbers $\alpha_\pm$, $\beta_\pm$, $\phi_\pm$ and $\psi_\pm$ of the equations (41–44) as given in Andersen et al. [2].

3 Results and discussion

Using the DWA method described in the earlier section we calculated various collisional parameters mentioned in Section 2.2. These are the DCS and TCS for 5 ^{2}P, 6 ^{2}S and 4 ^{2}D excitations, the Stokes parameters and alignment and orientation parameters for 5 ^{2}P and 4 ^{2}D excitations as well as set of complete experiment parameters and STU parameters for 5 ^{2}P excitation. Atomic target wave functions for the ground 5 ^{2}S and the excited 5 ^{2}P, 6 ^{2}S and 4 ^{2}D states are obtained from the Hartree-Fock atomic structure code of Fischer [21]. These are also used to obtain the distortion potential for obtaining the distorted waves in equation (6). The calculations are performed in the incident electron energy range from 10 to 200 eV. However, here only selected few results mainly at 20 and 40 eV of incident electron energies have been presented and rest of the results can be obtained from us.

In Figure 1, we present results of differential cross-sections for the individual 5 ^{2}P, 6 ^{2}S and 4 ^{2}D excitations and for the combined (6 ^{2}S + 4^{2}D) excitations of Rb atom at 10, 20 and 40 eV incident electron energies. Our results are compared with the only available experimental data from Vuskovic et al. [4] for 5 ^{2}P excitation and for the combined (6 ^{2}S + 4 ^{2}D) excitations at 10 and 20 eV. We also compare our results for 5 ^{2}P excitation with the available RDW calculations of Zeman et al. [8] at 20 and 40 eV.

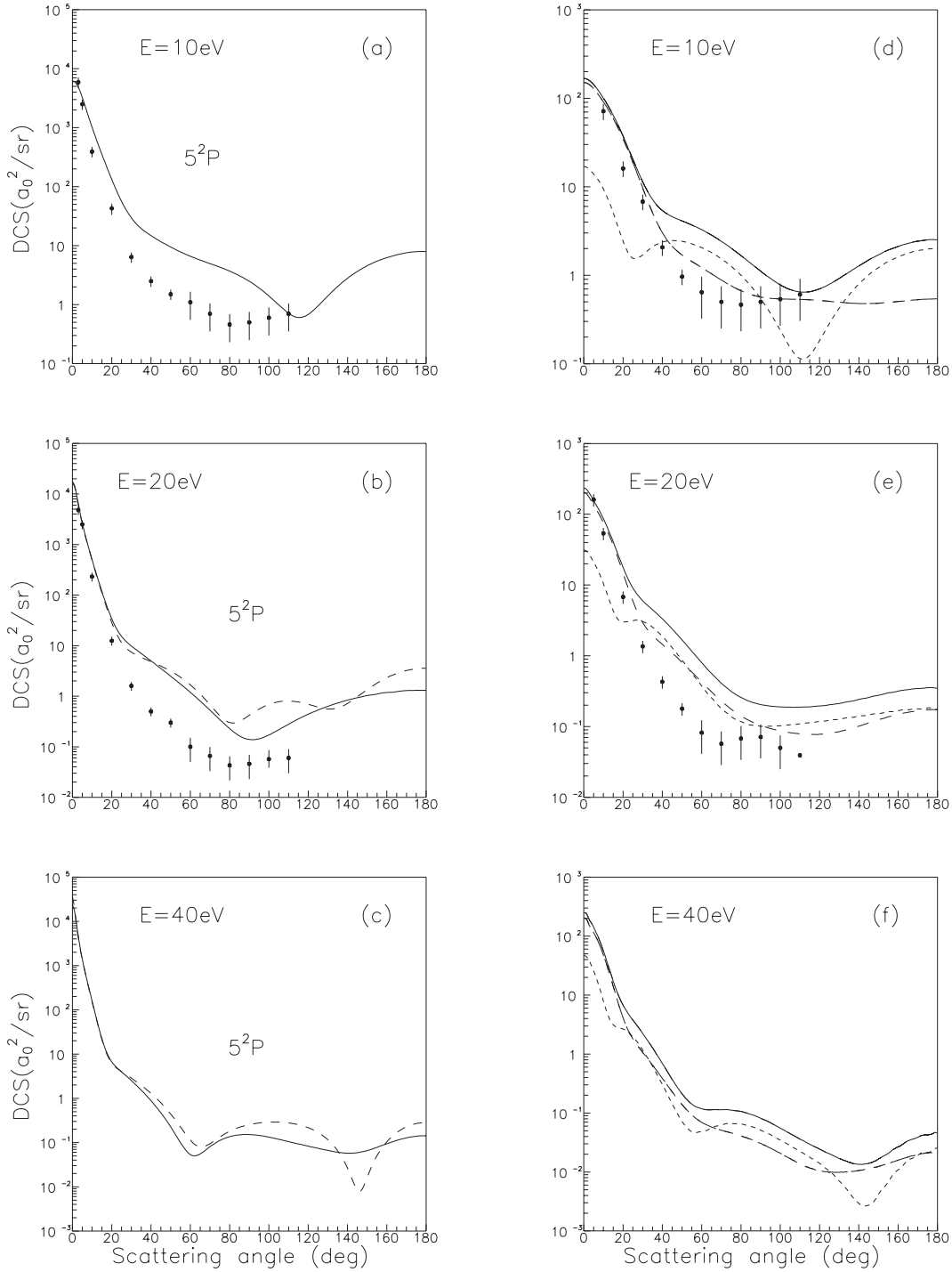

Fig. 1. Differential cross-sections in atomic units for the excitation of the 5 ^{2}P, 4 ^{2}D and 6 ^{2}S states of Rb by electron impact at 10, 20 and 40 eV. For (a), (b), (c): (——) present DWA; (- - - - -) RDW [8]; (•) experiment [4]. For (d), (e), (f): (——) (6 ^{2}S+4^{2}D); (- - - - -) 6 ^{2}S; (– — –) 4 ^{2}D; (•) (6 ^{2}S + 4^{2}D) experiment [4].

Our results for 5 ^{2}P excitation as shown in Figures 1a, 1b and 1c show very good agreement with the RDW calculations up to scattering angles of 80° and there after the small structures seen in RDW results are not reproduced by our DWA calculations. However, the agreement of both the calculations with the experimental data is only in the near forward scattering angles while at larger scattering angles the theoretical results lie relatively higher. It should be noted that with the experimental errors are listed [4] as 20% at scattering angles less than 50 degrees and between 30 and 50% for scattering angles greater than 50 degrees. Thus one can say that at small scattering angles our calculations are in good agreement with experiment. Figures 1d, 1e and 1f show the comparison of our results for

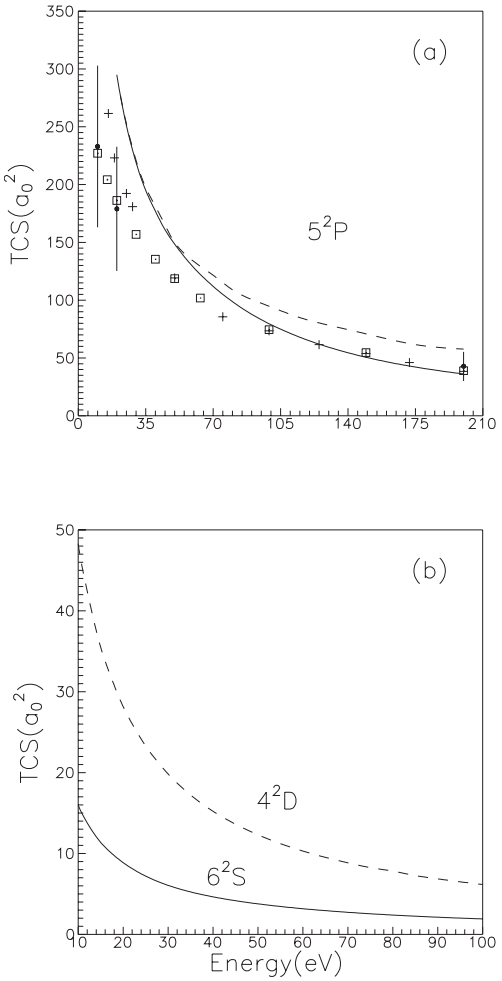

Fig. 2. Total cross-sections in atomic units for the excitation of the 5 ^{2}P, 4 ^{2}D and 6 ^{2}S states of Rb atom by electron impact. For (a): (——) present DWA; (-----) RDW [8]; (•) experiment [4]; (+) experiment [6]; (□) experiment [5]. For (b): (——) 6 ^{2}S; (– – – –) 4 ^{2}D.

the 6 ^{2}S and 4 ^{2}D excitations. We find from these figures that the over all agreement of the experimental results for the combined (6 ^{2}S + 4 ^{2}D) excitations with our DWA calculations is similar to that of the 5 ^{2}P excitation. We also notice that the combined (6 ^{2}S + 4 ^{2}D) results are in fact dominated by the contribution of the 4 ^{2}D state as compared to that of the 6 ^{2}S excitation.

In Figure 2, the total excitation cross-section results are presented for the 5 ^{2}P, 6 ^{2}S and 4 ^{2}D excitations of the Rb atom. We compare our DWA results of TCS for 5 ^{2}P state with the experimental data of Chen and Gallagher [5], Zapesochnyi et al. [6] and Vuskovic et al. [4]. Our results show good agreement with experimental data at higher energies and better than the RDW calculations. We also present our TCS results for 4 ^{2}D and 6 ^{2}S excitations for which though there are no other calculations or experimental results available for comparison.

In Figure 3, we present Stokes parameters (viz. P_1, P_2 and P_3) of the photons emitted from the decay of the excited fine structure unresolved 5 ^{2}P state to 5 ^{2}S at 20 and 40 eV. Here P_4 Stokes parameters are not shown being close to unity. Our results are compared with the RDW calculations and the only available experimental data of Hall et al. [9] for P_3 at 20 eV. In general our results for all the Stokes parameters are in over all close agreement with the RDW calculations. However, the additional structure seen at the backward scattering angles in each of the Stokes parameter results of the RDW calculation is absent in our DWA results. The comparison of our P_3 results with the experiment is quite satisfactory and better than the RDW results.

In Figure 4, we show results at 20 and 40 eV for the Stokes parameters $P_1(3/2)$, $P_2(3/2)$ and $P_3(3/2)$ of the emission from the fine structure resolved 5 ^{2}P$_{3/2}$ state decaying to the 5 ^{2}S$_{1/2}$ state. There are no experimental results for comparison but we compare our results with the RDW calculations. Here again in general for all the Stokes parameters, the agreement between our DWA and the RDW calculations is quite good except that of the additional sharp structure present at backward scattering angle in the RDW calculations, which is more pronounced at 40 eV. Note that for the decay of the excited 5 ^{2}P$_{1/2}$ state to the ground 5 ^{2}S$_{1/2}$ state of Rb the linear polarization $P_1(1/2)$ and $P_2(1/2)$ are zero and the circular polarization $P_3(1/2)$ is only nonzero. However, from equations (33, 36) we can see that $P_3(3/2)$ and $P_3(1/2)$ are related by multiplication of a constant factor only and therefore can be easily obtained from one another.

For the Stokes parameters (P_1, P_2, P_3) of the decay of photons from the excited 4 ^{2}D state to 5 ^{2}P state there are no other theoretical or experimental data available. We have therefore presented our DWA calculations at 20 and 40 eV for the Stokes parameters of fine structure unresolved 4 ^{2}D–5 ^{2}P transition and for the fine structure resolved 4 ^{2}D$_{3/2}$–5 ^{2}P$_{1/2}$ transition in Figure 5. We hope that the future other calculations and experimental measurements will provide meaningful comparison. We would like to mention here that we calculated the Stokes parameters for fine structure resolved 4 ^{2}D$_{5/2}$–5 ^{2}P$_{3/2}$ transition which are though not presented here but we found that these are having the similar shape to those we obtained for the fine structure resolved 4 ^{2}D$_{3/2}$–5 ^{2}P$_{1/2}$ transition and also $P_i(3/2) \approx P_i(5/2)$ ($i = 1$ and 4).

In Figure 6, we present the STU parameters (S_A, T, U) for the excitation of fine structure states of the 5 ^{2}P of Rb at 20 and 40 eV and compare them with the RDW calculations. We have not shown the results for the S_P parameter as both the DWA and RDW calculations show that $S_A \approx S_P$ at these two energies. Our S_A, T and U results show overall reasonable agreement with the RDW calculations. The agreement at 20 eV is much better than at 40 eV. We notice that the value of the T parameter is nearly unity. The magnitudes of S and U parameters appear to be appreciable and hence would be measure experimentally.

We aim to present the results of the complete set of parameters ($\sigma_u, \omega^t, L_\perp^t, L_\perp^s, \gamma^t, \gamma^s, \Delta^+$) for the 5 ^{2}S–5 ^{2}P excitation of Rb at 20 and 40 eV. The DCS results σ_u at both these energies have already been presented in Figure 1 and

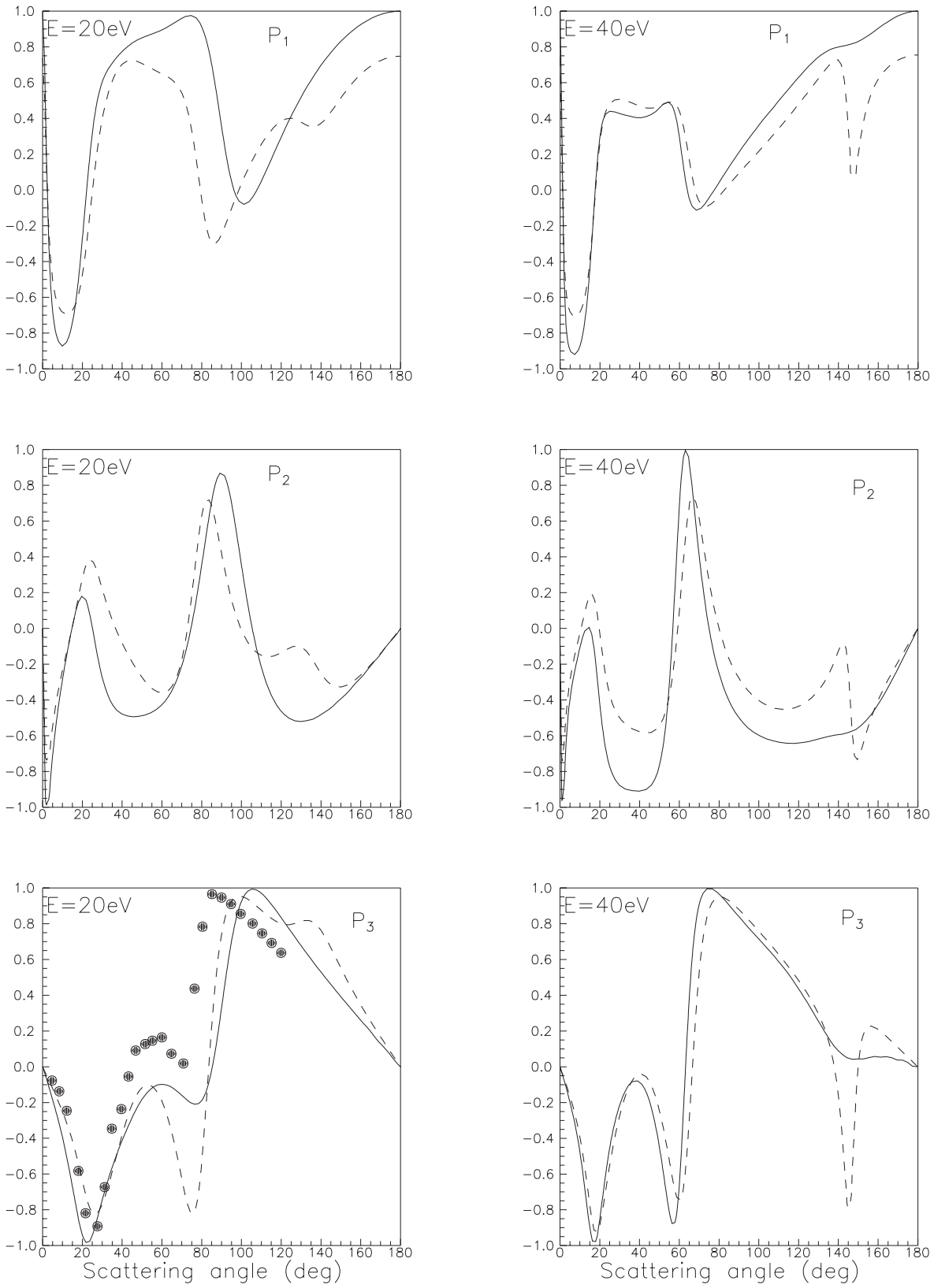

Fig. 3. Fine structure unresolved Stokes parameters P_1, P_2, P_3 for the emitted photons from the excited 5 ^{2}P state decaying to 5 ^{2}S state of Rb atom at 20 and 40 eV of incident electron energies. (——) Present DWA; (- - - - -) RDW [8]; (•) experiment [9].

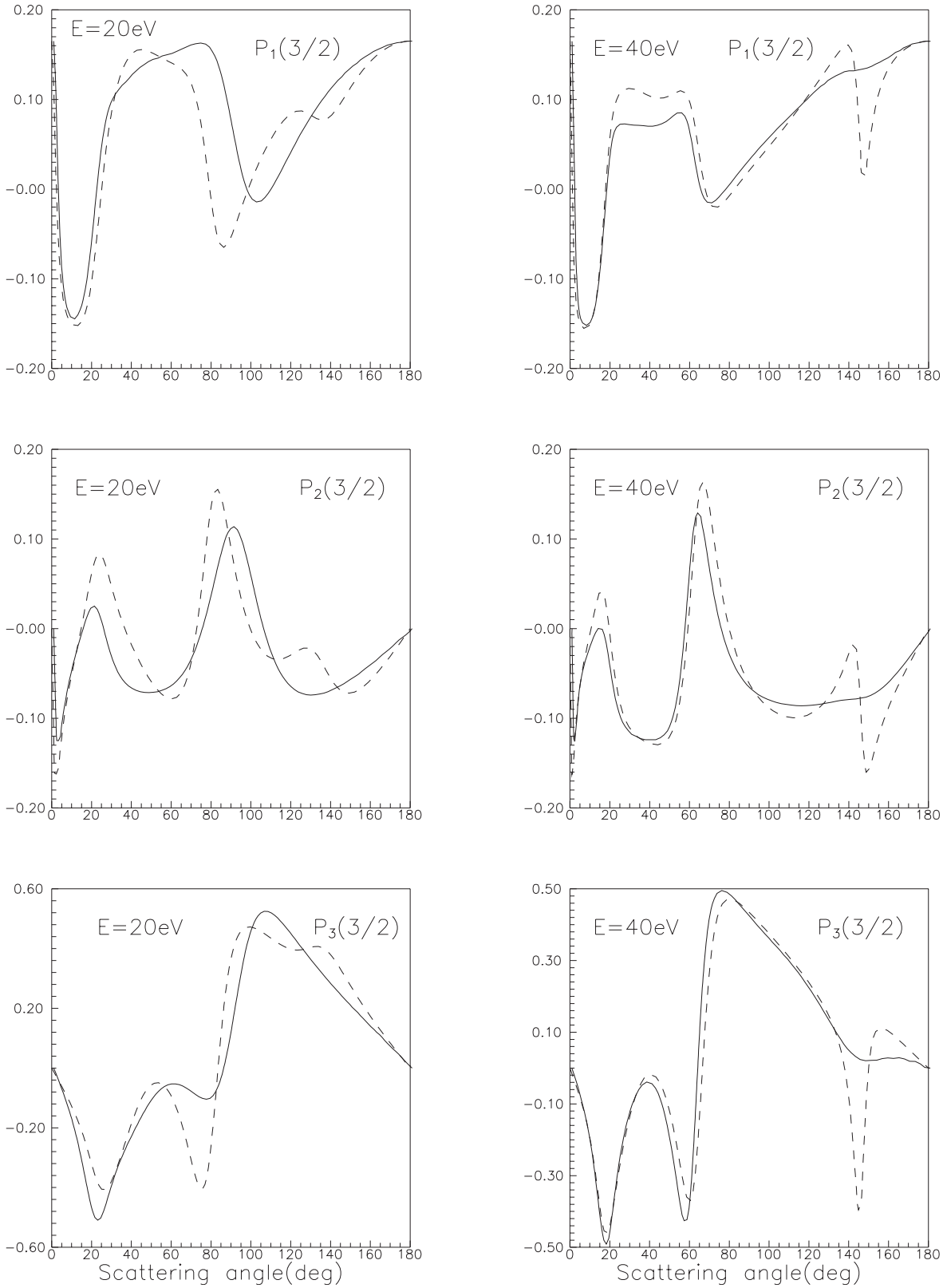

Fig. 4. Fine structure resolved Stokes parameters $P_i(3/2)$ $(i = 1, 3)$ of the emission of photon from the excited 5 $^2P_{3/2}$ state decaying to 5 $^2S_{1/2}$ ground state of Rb atom at 20 and 40 eV of incident electron energies. Figure captions are the same as in Figure 3.

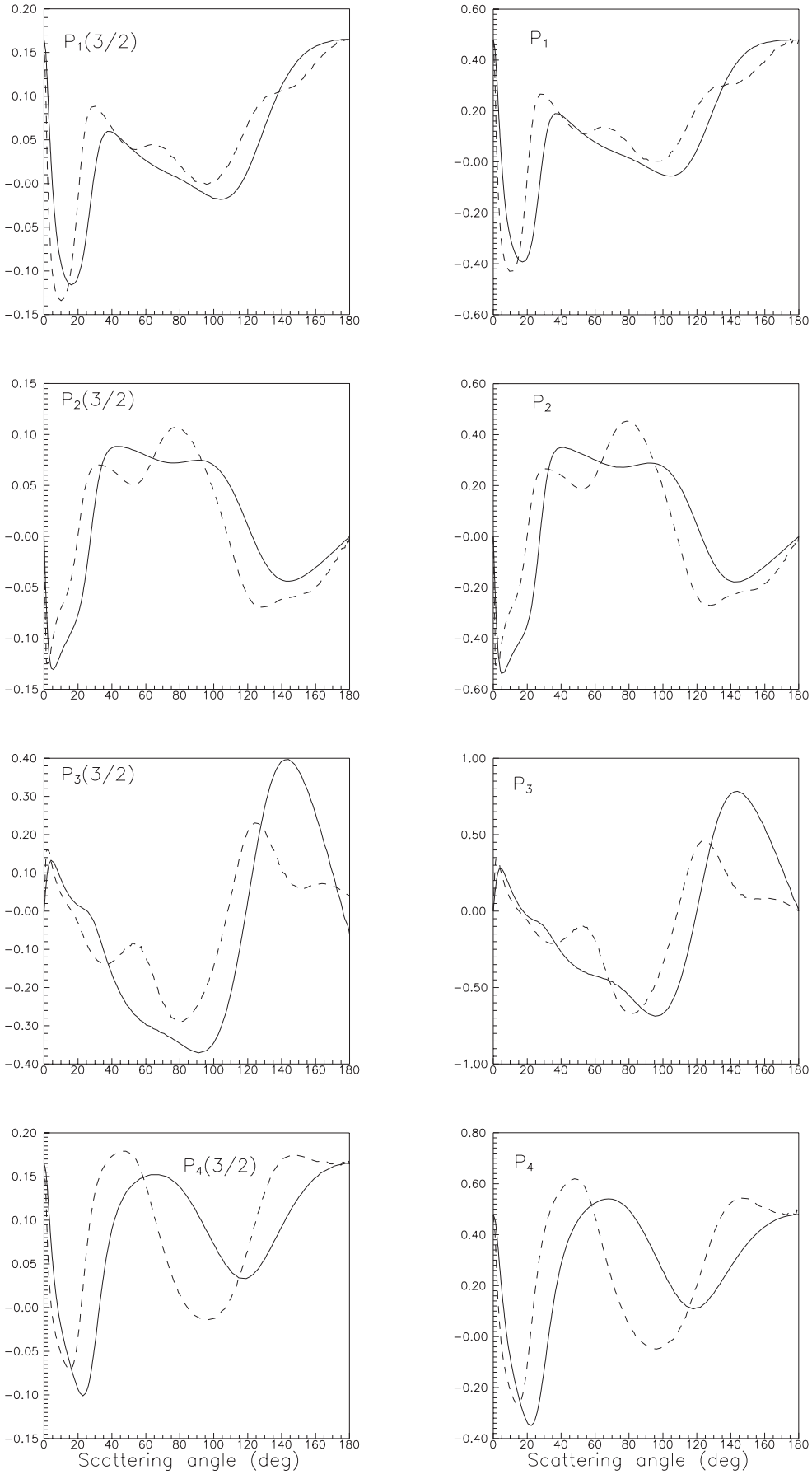

Fig. 5. Left side figures: resolved fine structure Stokes parameters $P_i(3/2)$ $(i = 1, 4)$ of the emission from the excited 4 $^2D_{3/2}$ state decaying to 5 $^2P_{1/2}$ state of Rb atom. Right side figures: unresolved fine structure Stokes parameters P_i $(i = 1, 4)$ of the emission from the excited 4 ^2D state decaying to 5 ^2P state of Rb atom. Results are at the incident electron energies. (——) 20 eV; (– – –) 40 eV.

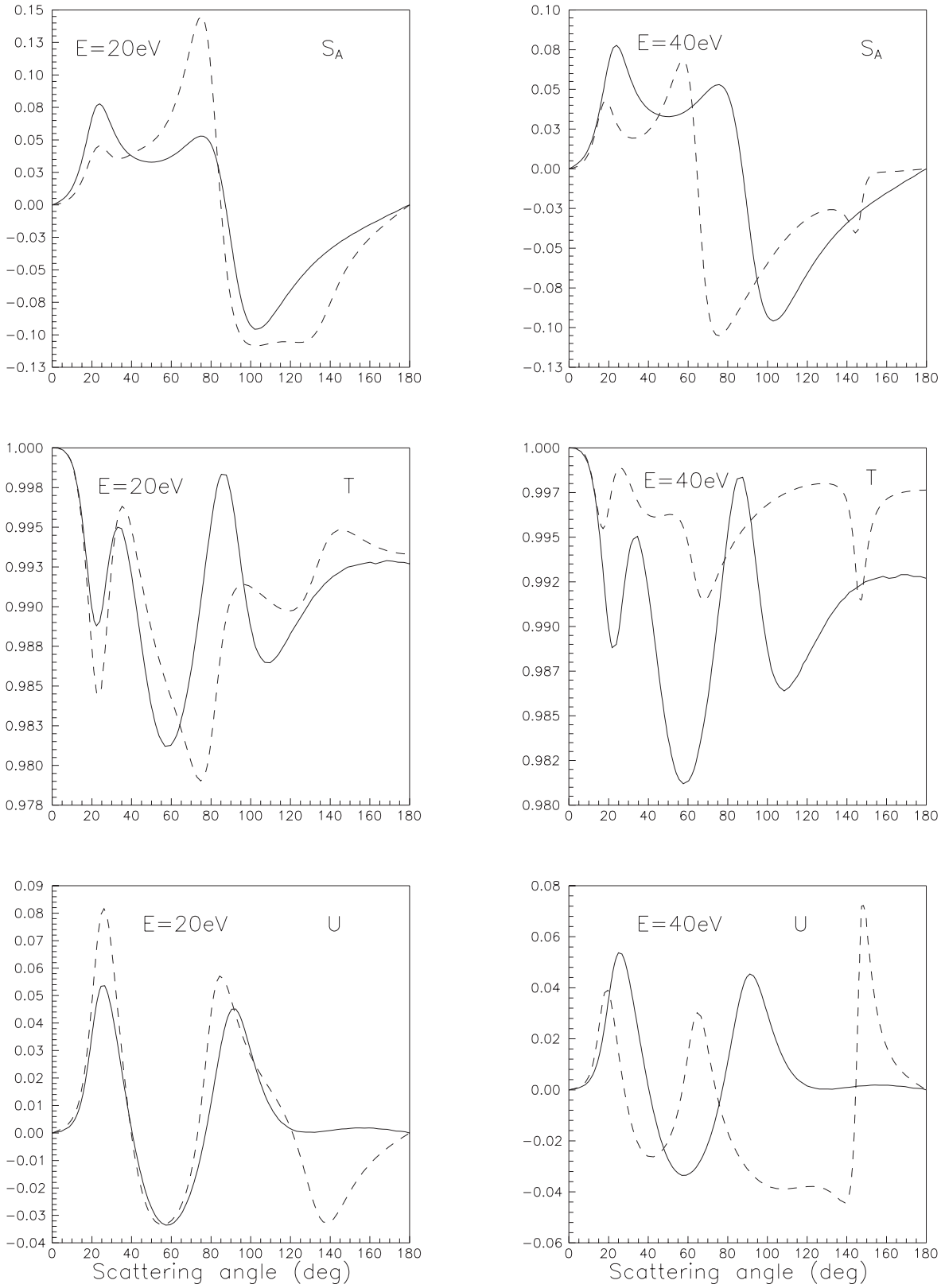

Fig. 6. STU parameters (S_A, T, U) for the excitation of the resolved fine structure states of the 5 ^{2}P in Rb atom by electron impact at 20 and 40 eV. Figure captions are same as in Figure 3.

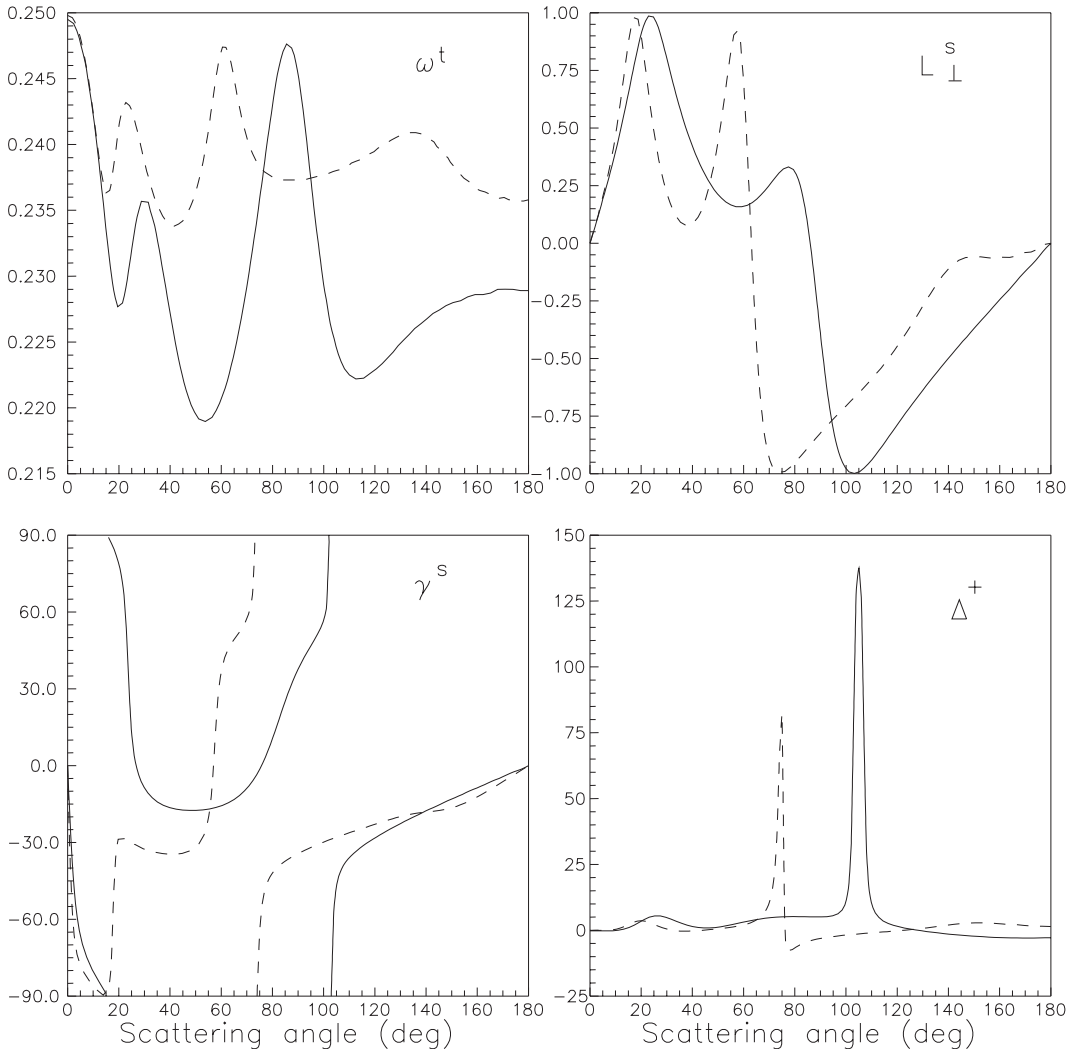

Fig. 7. Complete set of parameters $(\omega^t, L^s_\perp, \gamma^s, \Delta^+)$ for the excitation 5 ^{2}S–5 ^{2}P in Rb atom by electron impact at 20 and 40 eV. Figure captions are same as in Figure 5.

we found that $L^s_\perp \approx L^t_\perp$ and $\gamma^s \approx \gamma^t$. We show therefore through Figure 7 only the parameters $(\omega^t, L^s_\perp, \gamma^s, \Delta^+)$. Unfortunately there are no other calculations reported so far for these parameters.

Although we have not analyzed the complete set of parameters in case of the 5 ^{2}S–4 ^{2}D excitation, we present through Figure 8 the alignment and orientation parameters P_ℓ, γ, ρ_{00} and $L_\perp$ for this transition at 20 and 40 eV for sake of the completeness. It is interesting to note that in the near forward scattering angles the results for $L_\perp$ are having negative values (rather than positive) which thus show violation of the propensity rule in case of the excitation of the 4 ^{2}D state of the Rb. It would be interesting therefore to verify this experimentally.

4 Conclusions

In this paper we have presented our DWA calculations of the various collisional parameters in detailed manner for the 5 ^{2}S–5 ^{2}P resonance excitation of Rb atom and compared them with the RDW calculations and scarcely available experimental data. The agreement of our calculations with these results has been quite reasonable. The close agreement of the DWA and RDW calculations for the DCS and various sensitive parameters suggest that the relativistic effects may not be very important here. Similar to 5 ^{2}P excitation our calculations of the DCS for 6 ^{2}S and 4 ^{2}D excitations show satisfactory agreement with the experimental data. We feel that our results for various parameters of the different excitations reported here would be quite reliable and useful for the future comparison purposes.

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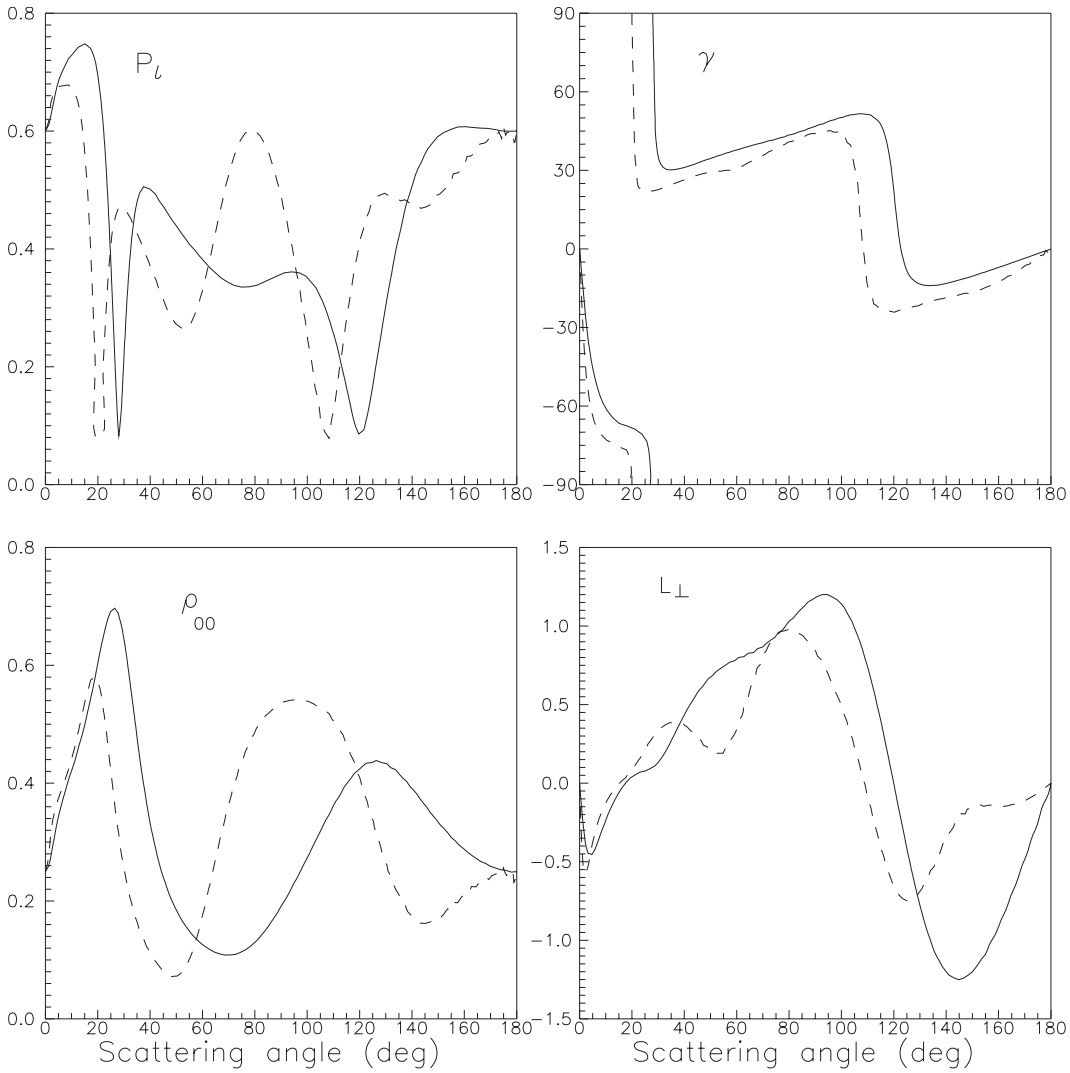

Fig. 8. For P_ℓ, γ, ρ_{00} and $L_\perp$ parameters for the excitation of 4 ^{2}D state of Rb atom by electron impact at 20 and 40 eV. Figure captions are same as in Figure 5.

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