Stokes Parameters of Excited Mg Atom

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ABSTRACT

In this paper we have reported the Stokes Parameters of excited Magnesium atom using non-relativistic (DW) and relativistic distorted wave approximation theories (RDW) at incident electron energies 15 and 45 eV. Good agreement has been found on comparison of both DW and RDW methods with each other and the importance of relativistic effect is also explored.

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Introductions

Electron impact excitation of atoms has been most extensively studied subject in the field of atomic collision. In recent years, there has been considerable interest and progress in the study of electron impact excitation process both the theoretically and experimentally. Most of earlier studies on electron impact excitation of atoms have been confined on the S-S and S-P transitions [1-3]. In this paper we have focused on study the D state of Mg. The study of D state excitation is confined to simpler like Helium [4-8]. We have used both the non relativistic and relativistic distorted wave methods and present the results for Stokes parameter at incident electron impact energies 15 and 45 eV. Comparison of results obtained from both the non-relativistic and relativistic methods are made with each other and the importance of relativistic effects is also explored.

Theoretical Considerations:

T-Matrix in DW Approximation:-

The transition matrix for the electron impact excitation of alkaline earth atoms (Mg) from its initial state i to a final magnetic sub-state f_M in the distorted wave approximation (DW) can be written as

$$T_{if_M} = \left\langle \chi_{f_M}^- \left| V - U_f \right| A\chi_i^+ \right\rangle \tag{1}$$

Where A is the antisymmetrization operator which takes into account the electron exchange effect between projectile and target electrons, V is the total interaction potential between the target alkaline earth atom and the projectile electron given by (atomic units are used throughout)

$$V = -\frac{2}{r_3} + \frac{1}{|r_2 - r_3|} + \frac{1}{|r_1 - r_3|} + V^{core}(r_3) \tag{2}$$

Here r_1, r_2 and r_3 are respectively the position co-ordinates of the target valence electrons and the projectile electron with respect to the target nucleus. Further, the core potential V^{core}, of the alkaline earth atom is given by

$$V^{core} = \sum_{n=1}^{j} N_{nl} \int \frac{|R_{nl}(r)|^2 r^2 dr}{r_>} \tag{3}$$

Where N_{nl} represents the occupation number of the electrons in different orbitals referred to by n and l quantum numbers and R_{nl} is the corresponding radial wave functions.

$\chi_i^+ (\chi_{f_M}^-)$ is the combined wave function of the distorted wave projectile electron and target state of alkaline atoms in the initial (final) channel. It is defined as

$$\chi_{i(f_M)}^{+(-)} = F^{+(-)}(k_{i(f)}, r_3)\, \Psi_{i(f_M)}(r_1, r_2)\, S_{i(f)}(1,2,3) \tag{4}$$

Where is the initial (final) state wave function of the target alkaline atom and $S_{i(f)}(1,2;3)$ is the initial (final) state spin function for the composite system consisting of the incident projectile and the target. $F_{i(f)}^{+(-)}$ represents the initial (final) channel projectile

distorted wave with the wave vector $k_i(k_f)$ and the associated superscript +(-) indicates the usual outgoing (incoming) wave boundary condition. The distorted waves are the solution of

$$[\nabla_3^2 + k_{i(f)}^2 - 2U_{i(f)}(r_3)]F^{+(-)}(k_{i(f)}, r_3) = 0 \tag{5}$$

Here $U_{i(f)}$ is the distorted potential in the initial (final) channel.

Further, on substituting the expressions for χ_i^+ and $\chi_{f_M}^-$ from equation (4) into the expression of the T-matrix equation (1) we get

$$T_{if_M} = \left\langle F^-(k_f, r_3)\Psi_{f_M}(r_1, r_2)S_f(1,2;3) \,|V - U_f|\, F^+(k_i, r_3)\Psi_i(r_1, r_2)S_i(1,2;3) \right\rangle$$
$$- \left\langle F^-(k_f, r_3)\Psi_{f_M}(r_1, r_2)S_f(1,2;3) \,|V - U_f|\, F^+(k_i, r_1)\Psi_i(r_3, r_2)S_i\,3,2;1 \right\rangle \tag{6}$$

Further, the scattering amplitude a_M in the 'collision frame of reference' for the electron impact excitation of the atom from an initial state i to a final magnetic sub state f_M is related to the DW transition matrix element T_{if_M} by

$$a_M = -\left(\frac{1}{2\pi}\right)T_{if_M} \tag{7}$$

The expression for the T-matrix equation (6) can be simplified further for a specific transition by carrying out the integration over the spin co-ordinates.

In the present paper work we consider only singlet to singlet transitions (n^{1}S to n^{1}D), (n=3) for Mg atom we give here brief outline to evaluate the T-matrix for SS excitation process.

In the singlet-singlet excitation the scattering takes place in the doublet mode i.e. the total spin of the system S = 1/2. The doublet mode spin function $S_i(S_{sf})$ in terms of the usual Dirac matrices α and β for the composite system is given by (Schiff [9]).

$$S_{i(f)}(1,2,3) = \frac{1}{\sqrt{2}}\alpha_3[\alpha_1\,\beta_2 - \alpha_2\beta_1] \tag{8}$$

Substituting $S_{i(f)}$ in equation [6] and carrying out the spin integrations using the usual orthogonal properties of individual spin function which is given below :

$$< \alpha_i \,|\, \alpha_j > = \delta_{ij}$$
$$< \beta_i \,|\, \beta_j > = \delta_{ij}$$
$$< \alpha_i \,|\, \beta_j > = 0$$

we get

$$T_{if_M} = T_{if_M}^d - T_{if_M}^{ex} \tag{9}$$

In equation (9), $T_{if_M}^d$ and $T_{if_M}^{ex}$ are the spin averaged direct and exchange T-matrices expressed as

$$T_{if_M}^d = \int F^{-*}(k_f, r_3)\Psi_{f_M}^*(r_1, r_2)(V - U_f(r_3))F^+(k_i, r_3)\Psi_i(r_1, r_2)\,dr_1 dr_2 dr_3 \tag{10}$$

$$T_{if_M}^d = \int F^{-*}(k_f, r_3)\Psi_{f_M}^*(r_1, r_2)(V - U_f(r_3))F^+(k_i, r_1)\Psi_i(r_3, r_2)\,dr_1 dr_2 dr_3 \tag{11}$$

In order to evaluate integrals equations [10, 11], we require the wave functions for Mg atom in their initial to final states. For this purpose the Hartree-Fock wave functions have been used which are obtained from the Fischer's computer code [10].

The RDW Calculation :-

Similarly, in order to evaluate the relativistic T-matrix, we require the wave function for target atom in its initial and final states. The Dirac Wave Function has been used to represent bound states of the atoms. These wave functions are obtained using Graps 92 programme of Prapia et al. [11]. There after the distortion potential and distorted waves are obtained to calculate the T-matrix finally. The configuration of SS states are taken to be same type of multi configuration ground state (MCGS) calculation as in Muktavat et al. [12] and Srivastava et al. [13].

Stokes Parameters P_i (i = 1 - 4) :-

The differential Stokes parameters P_i (i = 1 - 3) for the photon emitted after the excitation of atoms by electrons, measured perpendicular to the scattering plane are

$$P_1 = \frac{I(0°) - I(90°)}{I(0°) + I(90°)} \tag{12}$$

$$P_2 = \frac{I(45^\circ) - I(135^\circ)}{I(45^\circ) + I(135^\circ)} \tag{13}$$

$$P_3 = \frac{I(RHC) - I(LHC)}{I(RHC) + I(LHC)} \tag{14}$$

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

$$P_4 = \frac{I(0^\circ) - I(90^\circ)}{I(0^\circ) + I(90^\circ)} \tag{15}$$

where $I(\phi)$ 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.

In order to calculate theoretically the Stokes parameters of the light emitted from an excited state on its decay by photon emission we relate these to the state multipoles containing information of the excited atom. A general expression for the polarization density matrix of the emitted photons in terms of state multipoles has been given for example by Blum [14] from which Stokes parameters can rapidly be delivered. In this Section we briefly take this derivation and then finally give expression for Stokes parameters in terms of state multipoles of the excited atom.

The Stokes parameters of the emitted photons can be related to the elements of the its density matrix, ρ. Denoting the elements of ρ by $\rho_{\lambda'\lambda} \equiv <\lambda'|\rho|\lambda>$ we write.

$$\rho = \begin{pmatrix} \rho_{+1,+1} & \rho_{+1,-1} \\ \rho_{-1,+1} & \rho_{-1,-1} \end{pmatrix} \tag{16}$$

where, $\rho_{+1,-1} = \rho_{-1,+1}$ because of Hermit city. The components of the photon spin along the direction of propagation $\hat{n}$, which we denote by symbol λ, can have values $\lambda = +1$ ("spin up") and $\lambda = -1$ ("spin down"). It is important to note that the two photon states with spin up and spin down with respect to $\hat{n}$ as quantization axis has direct physical meaning. Since the component of the orbital ongular momentum vanishes in the direction of propagation $\hat{n}$ we have $J.\hat{n} = (L+S)\hat{n} = S.\hat{n} = \lambda$.

This implies λ is the component of the total angular momentum of the photon in the direction of propagation $\hat{n}$. These photon states are helicity states.

The trace of the density matrix gives the total intensity

$$I = \rho_{+1,+1} + \rho_{-1,-1} \tag{17}$$

In order to obtain η_3 we have to calculate the intensities I(0°) and I(90°) which are

$$I(0^\circ) = <e_x|\rho|e_x> \tag{18}$$

$$I(90^\circ) = <e_y|\rho|e_y> \tag{19}$$

where, the light beams which are completely linearly polarized along the x and y axes respectively are

$$|e_x> = \frac{-1}{\sqrt{2}}(|+1> - |-1>) \tag{20}$$

$$|e_y> = \frac{1}{\sqrt{2}}(|+1> + |-1>) \tag{21}$$

where the basis states are

$$|+1> = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-1> = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{22}$$

hence,

$$I(0^\circ) = \frac{1}{2}(-1, +1)\begin{pmatrix} \rho_{11} & \rho_{1,-1} \\ \rho_{-1,1} & \rho_{-1,-1} \end{pmatrix}\begin{pmatrix} -1 \\ +1 \end{pmatrix} \tag{23}$$

$$= \frac{1}{2}(\rho_{11} - \rho_{1,-1} - \rho_{-1,1} + \rho_{-1,-1}) \tag{24}$$

Similarly, we obtain

$$I(90°) = \frac{1}{2}(-i, -i)\begin{pmatrix} \rho_{11} & \rho_{1,-1} \\ \rho_{-1,1} & \rho_{-1,-1} \end{pmatrix}\begin{pmatrix} i \\ i \end{pmatrix}$$

(25)

$$= \frac{1}{2}(\rho_{11} + \rho_{1,-1} + \rho_{-1,1} + \rho_{-1,-1})$$

(26)

Therefore, it follows that

$$I\eta_3 = -(\rho_{1,-1} + \rho_{-1,1})$$

(27)

In a similar way we calculate the parameter $I\eta_1$ for which I(45°) and I(135°) need to be evaluated. In this case the axes of transmission of the Nicols are set at angles 45° and 135° to the x axes, respectively.

$$I(45°) = <e_1|\rho|e_1>$$

(28)

$$I(135°) = <e_2|\rho|e_2>$$

(29)

where, $|e_1>$ denotes a photon state which is fully transmitted by the first prism set at 45°.

$$|e_1> = \frac{1}{\sqrt{2}}(|e_x> + |e_y>)$$

(30)

Similarly, $|e_2>$ is a photon state which is fully transmitted by the second prism set at 135°.

$$|e_2> = \frac{1}{\sqrt{2}}(-|e_x> + |+|e_y>)$$

(31)

Transforming $|e_x>$ and $|e_y>$ to the helicity basis gives

$$I\eta_1 = -i(\rho_{1,-1} - \rho_{-1,1})$$

(32)

and

$$I\eta_2 = \rho_{11} - \rho_{-1,-1}$$

(33)

Hence the photon density matrix is expressed in terms of the Stokes parameters as

$$\rho = \frac{1}{2}\begin{pmatrix} 1+\eta_2 & -\eta_3 + i\eta_1 \\ -\eta_3 - i\eta_1 & 1-\eta_2 \end{pmatrix}$$

(34)

From Blum (14) the density matrix elements of photons emitted from an atom on its decay from the state $J \to J_f$ can be expressed as

$$\rho(n)_{\lambda,\lambda} = \frac{G(\omega)}{\gamma}\sum_{KQ_q}|<J_f \| r \| J>|^2 (-1)^{J+J_f+\lambda}(2K+1)^{\frac{1}{2}}\begin{pmatrix} 1 & 1 & K \\ -\lambda' & \lambda & q \end{pmatrix}$$

$$x\begin{Bmatrix} 1 & 1 & K \\ J & J & J_f \end{Bmatrix} D(0\theta\Phi)_{qQ}^k <T(J)_{KQ}^+ >$$

(35)

where, the above equation gives the polarization density matrix elements of photons observed in the direction **n**. Corresponding to the helicity $(\lambda = \pm 1)$ the rotation matrices $D(0\theta\Phi)_{qQ}^K$ are determined. J and J_f are the total angular momentum of the initial and final atomic state, γ is the decay constant and

$$G(\omega) = \frac{e^2\omega^4 d\Omega}{2\pi c^3 h}$$

(36)

where $d\Omega$ is the element of solid angle into which the photons are emitted, ω is the frequency of the emitted photon and c is the velocity of light and $|<J_f \| r \| J>|^2$ is related to the oscillator strength of the radiative transition.

Using the properties of rotation matrices and determining $\rho_{11}, \rho_{+1,-1} \rho_{-1,+1}$ and $\rho_{-1,-1}$ we obtain the Stokes parameters from equations (17), (27), (32) and (33) in terms of state multipoles as.

$$I\eta_3(\Theta, \Phi) = \frac{G(\omega)}{\gamma} |\langle J_f \| r \| J \rangle|^2 (-1)^{J+J_f} \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix}$$

$$\times [\{ \mathrm{Re}\langle T(J)_{22}^+ \rangle (1 + \cos^2 \Theta) \cos 2\Phi + \mathrm{Re}\langle T(J)_{21}^+ \rangle \sin 2\Theta \cos \Phi$$

$$+ \frac{\sqrt{3}}{2} \langle T(J)_{20}^+ \rangle \sin^2 \Theta \}$$

$$- \{ \mathrm{Im}\langle T(J)_{22}^+ \rangle (1 + \cos^2 \Theta) \sin 2\Phi + \mathrm{Im}\langle T(J)_{21}^+ \rangle \sin 2\Theta \sin \Phi \}]$$

$$(37)$$

$$I\eta_1(\Theta, \Phi) = -\frac{G(\omega)}{\gamma} |\langle J_f \| r \| J \rangle|^2 (-1)^{J+J_f} \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix}$$

$$\times [\{ \mathrm{Re}\langle T(J)_{22}^+ \rangle 2\cos \Theta \sin 2\Phi + \mathrm{Re}\langle T(J)_{21}^+ \rangle 2\sin \Theta \sin \Phi \}$$

$$+ \{ IM \langle T(J)_{22}^+ \rangle 2\cos \Theta \cos 2\Phi + \mathrm{Im}\langle T(J)_{21}^+ \rangle 2\sin \Theta \cos \Phi \}]$$

$$(38)$$

$$I\eta_2(\Theta, \Phi) = \frac{G(\omega)}{\gamma} |\langle J_f \| r \| J \rangle|^2 (-1)^{J+J_f} \begin{Bmatrix} 1 & 1 & 1 \\ J & J & J_f \end{Bmatrix}$$

$$\times [\{ \mathrm{Im}\langle T(J)_{11}^+ \rangle 2\sin \Theta \sin \Phi - \mathrm{Re}\langle T(J)_{11}^+ \rangle 2\sin \Theta \cos \Phi \}$$

$$+ \sqrt{2} \langle T(J)_{10}^+ \rangle \cos \Theta]$$

$$(39)$$

$$I(\Theta, \Phi) = \frac{G(\omega)}{\gamma} |\langle J_f \| r \| J \rangle|^2 (-1)^{J+J_f} \left(\frac{2(-1)^{J+J_f}}{3(2J+1)^{1/2}} \langle T(J)_{00}^+ \rangle \right.$$

$$- \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix} [\{ \mathrm{Re}\langle T(J)_{22}^+ \rangle \sin^2 \Theta \cos 2\Phi - \mathrm{Re}\langle T(J)_{21}^+ \rangle \sin 2\Theta \cos 2\Phi$$

$$+ \sqrt{\frac{1}{6}} \langle T(J)_{20}^+ \rangle 3\cos^2 \Theta - 1) \}$$

$$+ \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix} \{ \mathrm{Im}\langle T(J)_{22}^+ \rangle \sin^2 \Theta \sin 2\Phi - \mathrm{Im}\langle T(J)_{21}^+ \rangle \sin 2\Theta \sin \Phi$$

$$(40)$$

The state multipoles $\langle T(J)_{KQ}^+ \rangle$ do not take into account the depolarization due to the hyperfine splitting of the atomic nucleus, this is taken into account by multiplying $G_K(J)$ coefficients to every state multipoles, which are defined as

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

t   (41)

where, I = nuclear spin and F = J+I is the total angular momentum of the atom. The coefficients $G_K(J)$ are normalized such that $G_0(J)=1$.

Usually the experimentalists measure the differential Stokes parameters $P_i, (i = 1-3)$ for the photon detection perpendicular to the scattering plane $(\Theta = \Phi = 90°)$. And the stock parameter P_4 is also generally defined which is measured parallel to the scattering plane $(\Theta = 90, \Phi = 0°)$. Than these equation [37-40] can be written as

$$P_1 = \eta_3^y = \frac{1}{I^y} \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_r \end{Bmatrix} \times \left[\frac{\sqrt{3}}{2} G_2(J)\langle T(J)_{20}^+ \rangle - G_2(J) \mathrm{Re}\langle T(J)_{22}^+ \rangle \right]$$

$$(42)$$

$$P_2 = \eta_1^y = -\frac{2}{I^y} \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix} G_2(J) \mathrm{Re}\langle T(J)_{21}^+ \rangle$$

$$(43)$$

$$P_3 = \eta_2^y = -\frac{2}{I^y} \begin{Bmatrix} 1 & 1 & 1 \\ J & J & J_f \end{Bmatrix} G_1(J) \, \mathrm{Im}\left\langle T(J)_{11}^+ \right\rangle \tag{44}$$

$$P_4 = \eta_3^x = \frac{1}{I^x} \begin{Bmatrix} 1 & 1 & 1 \\ J & J & J_f \end{Bmatrix} \times \left[\frac{\sqrt{3}}{2} G_2(J)\left\langle T(J)_{20}^+ \right\rangle + G_2(J) \, \mathrm{Re}\left\langle T(J)_{22}^+ \right\rangle \right] \tag{45}$$

where I^y and I^x are given by

$$I^y = \left[\frac{2(-1)^{J+J_f}}{3\sqrt{2J+1}} G_0(J)\left\langle T(J)_{00}^+ \right\rangle \right.$$

$$\left. + \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix} \left(\frac{1}{\sqrt{6}} G_2(J) \, \mathrm{Re}\left\langle T(J)_{20}^+ \right\rangle + G_2(J) \, \mathrm{Re}\left\langle T(J)_{22}^+ \right\rangle \right) \right] \tag{46}$$

and

$$I^x = \left[\frac{2(-1)^{J+J_f}}{3\sqrt{2J+1}} G_0(J)\left\langle T(J)_{00}^+ \right\rangle \right.$$

$$\left. + \begin{Bmatrix} 1 & 1 & 2 \\ J & J & J_f \end{Bmatrix} \left(\frac{1}{\sqrt{6}} G_2(J) \, \mathrm{Re}\left\langle T(J)_{20}^+ \right\rangle + G_2(J) \, \mathrm{Re}\left\langle T(J)_{22}^+ \right\rangle \right) \right] \tag{47}$$
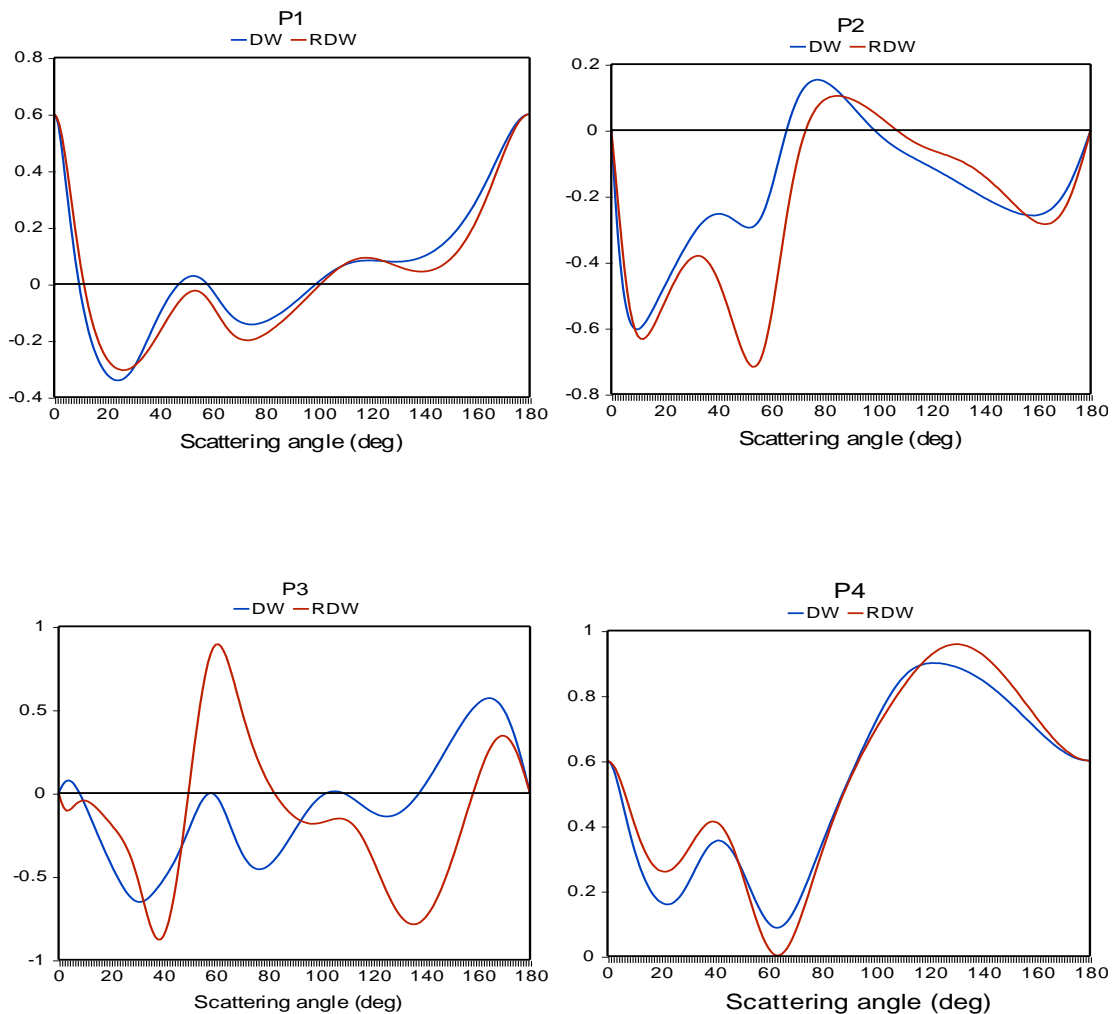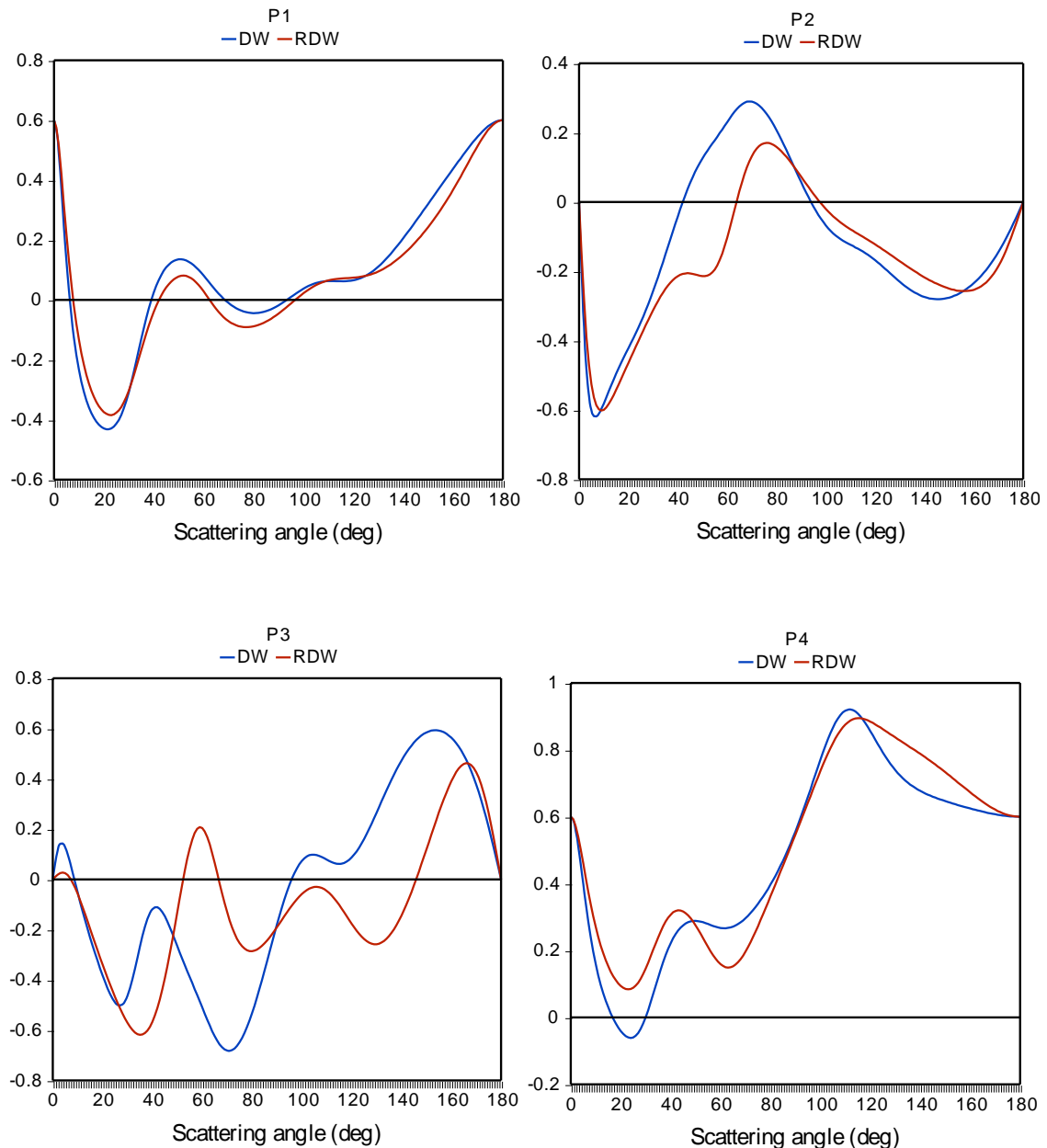
Figures:-

Figure 1 - Stokes Parameters (P_1, P_2, P_3, P_4) for the excitation of the ^1D state of Mg atom at 15 eV.

Figure 2 - Stokes Parameters (P_1, P_2, P_3, P_4) for the excitation of the 3^1D state of Mg atom at 45 eV.

Results and Discussion:-

In this paper we consider the results of the Stokes Parameters of the emitted photons while the excited $n\,^1D$ state of Mg (n=3) decay to their corresponding lower $n\,^1P$ states. This P state may further subsequently decay by another cascading photon emission to a still lower S state.

In figures 1 to 2 we have presented our DW and RDW results of the Stokes parameters (P_1, P_2, P_3, P_4) for the excitation of 3^1D state of Magnesium atom at incident electron energies 15 and 45 eV. We find that both the DW and RDW calculations agree qualitatively and quantitatively in reasonable manner at these energy levels. It is interesting to note that the shape of the Stokes parameters P_3 for both the energies at 15 and 45 eV slightly differ in forward scattering. Consequently, the RDW calculation suggest the violation of the propensity rule while DW calculation obey it and behave in normal manner. This is due to the effect of relativistic contribution which need to be verified by future experiment.

Conclusions:-

We have reported Stokes Parameters for the excitation of the lower lying D states of the Mg at 15 and 45 eV. A reasonable agreement is found between the results predicted by the DW and RDW theories. The contribution of relativistic effects is also discussed in the results. We believe that our present results would be helpful in guiding the future experimental measurements and more theoretical calculations.

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