

Positron-Impact Excitation of the Lowest Autoionizing State in Rubidium Atom Using Distorted Wave Method

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Abstract: Many calculations on atomic collisions and scattering processes have been performed on electron impact excitation of the lowest autoionizing state of rubidium, but not much attempt has been made with positron impact which is of equally fundamental importance and is receiving attention nowadays with the availability of improved positron beam experiments. So, in this study, total cross-sections, λ and the alignment parameter for positron impact excitation of the lowest autoionizing state of rubidium have been calculated using Distorted Wave method. The wave functions used are the Roothan Hatree Fock double zeta and multi zeta wave functions due to Clementi and Roetti. Variations in distortion potential have been made such that the static potential of the initial state of rubidium atom is used as the initial channel distortion potential and a linear combination of static potentials of the initial and final states as the final channel distortion potential to check its effect on cross-sections. Numerical calculations have been done using a modified DWBA1 FORTRAN computer program which was originally made for hydrogen atom. The results for positron impact excitation of the lowest autoionizing state of rubidium have been analyzed and compared with experimental and theoretical results for positron and electron impact excitation of the same state available in literature. From the comparison of the results, it is seen that in general the electron impact excitation cross section results are higher than the positron impact excitation cross section especially near excitation threshold energy. This can be attributed to the exchange process which takes place in the case of electron impact and not in the case of positron impact and also due to larger interaction between the projectile and the target in case of electron impact than in case of positron impact. It is also found from the alignment parameter results that the integral cross section results for $m=0$ level are larger compared to $m=1$ level for impact energies up to about 500 eV beyond which integral cross-sections for the magnetic sublevel $m=1$ become greater. The λ parameter indicates that more particles are scattered towards $m=0$ for electron impact compared to positron impact excitation near threshold energy.

Key Words: Positron Impact Excitation, Distorted Wave Method, Rubidium Atom, Integral Cross Section, Alignment Parameter.

INTRODUCTION

Collisions lead to excitation of atoms and ions to autoionizing states which are usually short-lived, approximately 10^{-13} to 10^{-14} seconds and thus can be described as resonances rather than normal bound states [1]. Borovik *et al.* [2] carried out an experimental study on the $4p^6$ autoionization cross section of rubidium atoms excited by low-energy electron impact at energy range of 15.3 eV up to 50 eV. In this work, rubidium $4p^6$ state excitation shows a resonance or quick rise of the autoionization cross section between 15.3 eV and 18.5 eV.

Collision problems are usually solved by making approximations which are classified into quantum mechanical approaches such as close coupling, R-matrix, variation method, perturbation series or semi classical approaches. Approximation methods are chosen depending on the impact energy. For example, at low impact energies, the close coupling approaches are preferred while at intermediate and higher energies, the perturbation series expansion approaches are preferable since they give results with good agreement to experimental work. At the same time the DWBA is less expensive computationally as compared to other reliable theories like R-matrix and close-coupling methods [3].

In this study positron impact excitation of the lowest lying autoionizing level in rubidium has been investigated by use of the Distorted Wave method. Integral cross sections are compared in the energy range of 15 eV to 1500 eV using multi zeta and double zeta wave functions as given in the Clementi and Roetti atomic data tables of 1974[4]. The results

for ICS have been compared to those of .Pangantiwar and Srivastava [5]) who studied electron and positron impact excitation of autoionizing levels in alkalis using Distorted Wave Method approach for incident particle energy varying up to 1000 eV using multi-zeta wave functions with the initial and final state static potentials as the distortion potentials for the initial and final distorted waves respectively. They presented results for positron and electron impact excitation of the lowest autoionizing state for rubidium though the near threshold autoionization integral cross section(ICS) for electron impact does not clearly predict the short lived resonance shown in the results for electron impact excitation of Borovik et al. [2]. Lamda parameter and alignment parameter for the excited state have also been calculated and compared to both theoretical and experimental results available in literature.

RESEARCH METHODOLOGY

The distorted wave method

We consider the scattering of a positron by a neutral atom. The total Hamiltonian for the system of collisions is expressed as

$$H = H_o + V \tag{1}$$

The operator H_o is a sum of the Hamiltonian for the isolated atom (target) and the isolated projectile, while V is the interaction potential between the projectile (positron) and the target which is given by

$$V = \frac{N}{r_o} - \sum_{i=1}^N \frac{N}{r_{oi}} \tag{2}$$

Here, r_o and r_{oi} represents magnitudes of the position vector of the projectile from the target nucleus and the displacement vector of the projectile relative to the i^{th} target electron respectively. The initial-state full scattering wave function ψ_i^+ is a solution of the Schrödinger’s equation

$$(H - E)\psi_i^+ = 0 \tag{3}$$

The plus (+) sign indicates the outgoing wave boundary conditions. In this case, the projectile positron experiences either elastic or inelastic collisions with N-electron atom, the exact transition matrix in the two-potential approach as derived in chapter three is given by

$$T_{if} = (N + 1)\langle \chi_f^-(0) \varphi_f(1, \dots, N) | V - U_f | A \psi_i^+(0, \dots, N) \rangle + \langle \chi_f^-(0) \varphi_f(1, \dots, N) | U_f | \varphi_i(1, \dots, N) \beta_i(0) \rangle. \tag{4}$$

φ_i and φ_f are properly antisymmetrized initial and final atomic wave functions for an isolated atom. Furthermore β_i is an initial-state plane wave [6]. A is the antisymmetrizing operator for $N + 1$ electron system. potential U_f is an arbitrary distorting potential for the projectile, which is used to calculate the distorted wave χ_f^- by solving the wave equation.

$$(T + U_f - E_f)\chi_f^- = 0 \tag{5}$$

solved using Numerov’s method. E_f is the final state energy of the projectile, T is the Hamiltonian of the isolated projectile and k_f is the final state wave vector for the projectile in atomic units. χ_i^+ is the distorted wave function representing the projectile in the initial state and is a solution to the wave equation

$$(T + U_i - E_i)\chi_i^+ = 0 \tag{6}$$

where U_i is the distortion potential in the initial state and \vec{K}_i is the incident wave vector. χ_i^+ satisfies the outgoing wave boundary condition.

Distortion potentials

In principle, U_i and U_f can be any distortion potential as long as χ_i^+ and χ_f^- fulfill the appropriate boundary conditions. In this study we choose the static potential of the target atom in its initial state as the distorting potential for the initial state of the projectile positron and a linear combination of the static potentials of the target atom in its initial and final states as the distortion potential for the final state of the positron. The reason behind this choice is that, in the initial state of the projectile, it only ‘sees’ the initial-state static potential of the target atom, but when the energy of the projectile is transferred to the atom, it takes some time before the atom goes to its final state. As a result, the projectile in its final state ‘sees’ an intermediate potential between the initial and final state static potentials of the target [7]. That is,

$$U_i = \langle \Phi_i | V | \Phi_i \rangle \tag{7}$$

$$U_f = \frac{1}{2} \langle \Phi_i | V | \Phi_i \rangle + \frac{1}{2} \langle \Phi_f | V | \Phi_f \rangle \tag{8}$$

V is the interaction potential between the projectile and the target and U is the distortion potential for the projectile, where subscript i (f) represent the initial (final) state of the target. The static potentials for the initial V_i and final V_f states take the form.

$$V_i = \langle \Phi(4p) | V | \Phi(4p) \rangle \quad (9)$$

$$V_f = \langle \Phi(5s) | V | \Phi(5s) \rangle \quad (10)$$

Atomic wave functions

Atomic wave functions used in this study are based on the RoothanHartree-Fock (RHF) expansion technique. The total wave function for an N -electron system is a Slater determinant given by

$$\psi^+ = A(\Phi_1^{(1)} \dots \Phi_n^{(n)}) \quad (11)$$

A is the antisymmetrizing operator and n is the total number of electrons and Φ_i^j are the spin orbital which are assumed orthogonal to each other. The orbital is expanded in terms of basis functions as

$$\Phi_{i\lambda\alpha} = \sum_p \chi_{p\lambda\alpha} C_{i\lambda p} \quad (12)$$

Subscript p refers to the p^{th} basis function of symmetry λ and C is the expansion coefficient.

The basis functions χ are Slater-type orbitals with integer quantum numbers, namely

$$\chi_{p\lambda\alpha}(r, \theta, \varphi) = R_{p\lambda}(r) Y_{\lambda\alpha}(\theta, \varphi) \quad (13)$$

The radial part is expressed as;

$$R_{p\lambda}(r) = N r^{n-1} e^{-\zeta r} \quad (14)$$

The normalization factor N takes the form

$$N = ((2n)!)^{-\frac{1}{2}} (2\zeta)^{n+0.5} \quad (15)$$

Here, n , and ζ represent the principal quantum number and orbital exponent zeta respectively while $Y_{\lambda\alpha}(\theta, \varphi)$ are normalized complex spherical harmonics. For Rubidium, the 4p state (initial state), the double zeta wave functions for the radial part as constructed by summing up all p^{th} basis functions given in the atomic data tables of Clementi and Roetti (1974)[4] such that

$$\Phi(4p) = \sum_p \chi_i C_i$$

$$\Phi(4p) = 0.00881\chi_1 + 0.12882\chi_2 + (-0.24895)\chi_3 + (-0.13864)\chi_4 + 0.61394\chi_5 + 0.51815\chi_6 \quad (16)$$

For the 5s state (final state),

$$\Phi(5s) = \sum_p \chi_f C_f$$

$$\Phi(5s) = 0.00018\chi_1 + 0.01441\chi_2 + 0.02387\chi_3 + (-0.07354)\chi_4 + 0.02451\chi_5 + 0.08837\chi_6 + (-0.16671)\chi_7 + (-0.07389)\chi_8 + 0.44807\chi_9 + 0.65575\chi_{10} \quad (17)$$

The procedure explained above is for the construction of double zeta functions, which is an approximate RHF function in which a given electron orbital is described by two Slater functions. The same procedure can be used to derive MZ functions, where an electron orbital is described by two or more Slater functions, by adjusting the C , ζ and N parameters as given in the Clementi and Roetti tables[4].

Evaluation of transition matrix elements and cross sections

Generally, the matrices involved are; direct matrix elements and exchange matrix elements, but for positron (e^+) projectile, exchange between projectile and target electron does not occur since the particles are not identical. The excitation process for any alkali metal atom A is expressed as follows[5].

$$e^+ + A[np^6(n+1)s] {}^2S_{\frac{1}{2}} \rightarrow e^+ + A[np^5(n+1)s^2] {}^2P_{\frac{1,3}{2}} \quad (18)$$

For rubidium atom and we consider the transition $4p \rightarrow 5s$ and the excitation process for the positron impact excitation of rubidium takes the form

$$e^+ + A[4p^65s] {}^2S_{\frac{1}{2}} \rightarrow e^+ + A[4p^55s^2] {}^2P_{\frac{1,3}{2}} \quad (19)$$

With the general expression for the transition matrix in the absence of exchange given as

$$T = \langle \chi_f^-(\mathbf{r}_o) \varphi_f(\mathbf{r}_1) | V(\mathbf{r}_o, \mathbf{r}_1) | \varphi_i(\mathbf{r}_1) \chi_i^+(\mathbf{r}_o) \rangle \quad (20)$$

\mathbf{r}_0 and \mathbf{r}_1 are the position vectors of the incident positron and atomic electron undergoing a transition relative to the target nucleus taken as the origin of the center of mass respectively, while \mathbf{r}_{01} is the column vector between the positron and the

target electron. The wave functions φ_i and φ_f represents atomic orbitals for the initial and final states. The distorted waves χ_f^- and χ_i^+ are first expanded in terms of partial waves as follows:

$$|\chi_i^+\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_i r} \sum_{l_i m_i} i^{l_i} \chi_{l_i}(k_i, r) Y_{l_i m_i}(\hat{r}) Y_{l_i m_i}^*(\hat{k}_i) \quad (21)$$

$$|\chi_f^-\rangle = \sqrt{\frac{2}{\pi}} \frac{1}{k_f r} \sum_{l_f m_f} i^{l_f} \chi_{l_f}^*(k_f, r) Y_{l_f m_f}(\hat{r}) Y_{l_f m_f}^*(\hat{k}_f) \quad (22)$$

Here, Y_{lm} is a spherical harmonic. In the expansion of χ_f^- , the radial distorted wave is taken as complex conjugate so that it satisfies the incoming wave boundary conditions. Substituting (21) and (22) in equation (6) and (5) respectively, it can be shown that the radial distorted waves are solutions of the differential equation

$$\left(\frac{d^2}{dr^2} - \frac{l_s(l_s + 1)}{r^2} - U_s(r) + k_s^2 \right) \chi_{l_s}(r) = 0 \quad (23)$$

The radial distorted wave equations are solved by using Numerov's method [6]. Here $s=i$ for the initial state and $s=f$ for the final state distorted waves. In the asymptotic region, they satisfy the boundary condition

$$\lim_{r \rightarrow \infty} \chi_{l_s}(k_s, r) = j_{l_s} + \alpha_l(-\eta_{l_s} + i j_{l_s}) \quad (24)$$

Here, j_l and η_l are regular and irregular Ricatti-Bessel functions [8], while $\alpha_l = \exp(i\delta_l) \sin \delta_l$ where δ_l is the elastic scattering phase shift. The differential cross-sections summed over the magnetic sub levels are obtained using the relation

$$\left(\frac{d\sigma}{d\Omega} \right)_{4p \rightarrow 5s} = \frac{1}{4\pi^2} \frac{k_f}{k_i} \sum_{m=-1}^1 |T_{4p \rightarrow 5s}|^2 \quad (25)$$

and the differential cross section (DCS) for excitation of specific magnetic sublevel m can be obtained as

$$\sigma_m = \left(\frac{d\sigma}{d\Omega} \right)_{m^{4p \rightarrow 5s}} = \frac{1}{4\pi^2} \frac{k_f}{k_i} |T_{m^{4p \rightarrow 5s}}|^2 = \frac{k_f}{k_i} |f_m(\theta, \phi)|^2 \quad (26)$$

The scattering amplitude is given by;

$$f_m(\theta, \phi) = -\frac{1}{2\pi} T_m \quad (27)$$

Here, T_m is the transition matrix for the excitation of magnetic sublevel m . By summing up the differential cross sections, we obtain the total or integral cross section given by;

$$\sigma = \int_0^{2\pi} \int_0^\pi \frac{d\theta}{d\Omega} \sin\theta d\theta d\phi \quad (28)$$

Angular correlation parameters

Angular correlation parameters between the scattered positron when the atom is excited from $np \rightarrow (n+1)s$ state and the emitted photon from transition $(n+1)s \rightarrow np$ after excitation, are measured in order to obtain details regarding population of magnetic sub-states. The positron-photon coincidence parameter λ is expressed as

$$\lambda = \frac{\sigma_0(\theta, \phi)}{\sigma_0(\theta, \phi) + 2\sigma_1(\theta, \phi)} \quad (29)$$

Here, $\sigma_0(\theta, \phi) + 2\sigma_1(\theta, \phi)$ is the total differential cross section summed over all magnetic sublevels $m=0$ and $m=1$.

The alignment parameter (A_{20}) of the autoionizing excited state $[np^5(n+1)s^2]^2P_{3/2}$ is such that

$$A_{20} = \frac{\sigma(np_1) - \sigma(np_0)}{\sigma(np_0) + 2\sigma(np_1)} \quad (30)$$

Here, $\sigma(np_m)$ is the total cross section of anp_m electron excited to a $(n+1)s$ state [9]. The transition matrix elements, target wave functions, cross sections and angular correlation parameters have been evaluated using a DWBA1 FORTRAN computer code developed by Madison and Bartschat[5] for electron-hydrogen scattering. The modifications made on subroutines enable generate results for p -transition, changing hydrogen wave functions to rubidium, static potentials, generation of cross sections for energies above 200 eV and calculation of λ and A_{20} (alignment) parameters. The version 8 Origin Lab computer software was used for analysis of data which includes generation of graphs of cross sections and angular correlation parameters.

RESULTS AND DISCUSSION

Both DZ and MZ wave functions have been used in this work. The distortion potential is such that the initial state static potential is the initial channel distortion potential while a linear combination of initial and final state static potentials is taken as the final channel distortion potential. We have compared our results with those of Pangantiwar and Srivastava [5] and Borovik *et al.* [2] for electron and positron impact excitation of the lowest autoionizing state of rubidium. The result for Borovik *et al.* [2] was obtained through experiment, while the results for Pangantiwar and

Srivastava [5] is a calculation using the distorted wave method where the initial state static potential is the initial channel distortion potential while the final state static potential is the final channel distortion potential.

Integral cross sections

Integral cross sections for positron and electron impact excitation of the $4p^55s^2$ state of Rb are compared to those in the work of Srivastava and Pangantiwar [5] and Borovik *et al.* [2] results with both double zeta (DZ) and multi zeta (MZ) wave functions above threshold energy of 15.73 eV up to 1500 eV. Distorted wave calculations with exchange (DWE) and distorted wave calculations without exchange (DWD) graphs are presented.

The present integral cross section results (Fig-1) results indicate that multi zeta wave functions generate larger cross sections compared to those of double zeta wave functions at all energies. This study also reveals larger cross sections compared multi zeta results in the work of Srivastava and Pangantiwar [5] mainly at intermediate energies. This can be attributed to the choice of distortion potential used in this study.

At low impact energies up to around 40 eV, all the three integral cross section results for positron impact excitation are in good qualitative agreement, but not at intermediate energies. At higher energies approaching 1000 eV, the cross sections tend towards each other. The disagreement is therefore at intermediate energies.

It is clear (Fig-2) that the near threshold resonance (sharp increase in cross sections near the threshold excitation energy due to the existence of an extra electron in the vicinity of the target atom electron cloud which makes the target behave like a negative ion) for electron impact does not appear for positron impact. This is due to exchange effects between projectile electron and atomic electron during impact. This is not the case for positron impact which do not exchange with electrons during collision. Another reason for the resonance behavior is due to attraction of the electron projectile by the positive nucleus which results in more interaction with target electrons. Unlike electrons, positrons experience a repulsive force from the nucleus once they penetrate the electron cloud, hence less interaction in the atom. Because of this, the near threshold resonance is not observed.

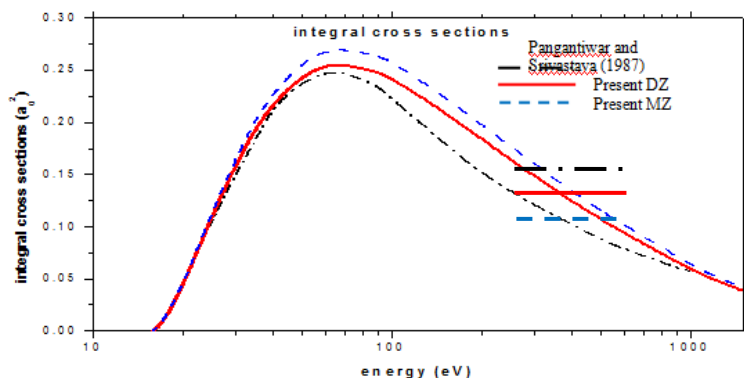


Fig-1: Integral cross sections results for positron impact excitation of the lowest autoionizing state in rubidium; - . - .,Pangantiwar and Srivastava [5] results; —,present DZ results; - - -, present MZ results

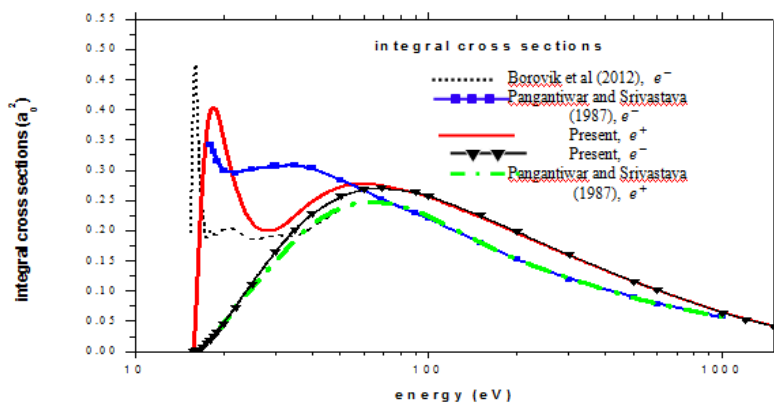


Fig-2. Integral cross sections results for electron and positron impact excitation of the lowest autoionizing state in rubidium;.....,Borovik et al. [2] electron impact results; —,present electron impact DWE-MZ results; —■—,Pangantiwar and Srivastava [5] electron impact results; —■—,Pangantiwar and Srivastava [5] positron impact results; —▼—,present positron impact MZ results.

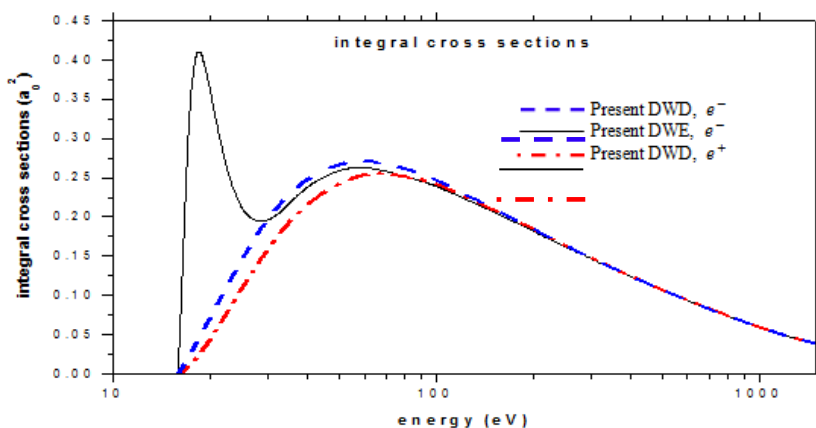


Fig-3. Present Integral cross sections DZ results for electron and positron impact excitation of the lowest autoionizing state in rubidium; —, DWE electron impact results; . . . ,DWD positron impact results; - - -,DWD electron impact results.

Alignment parameter A_{20}

The present alignment parameter result is compared with the work of Pangantiwar and Srivastava[5] for positron impact excitation at an energy range of 0 eV to 1000 eV. The present alignment parameter results for positron impact (Fig-4) are in good qualitative agreement with the results of Pangantiwar and Srivastava [5] at almost throughout the energy range of 20-1000 eV. The small difference between the two results can be attributed to the choice of distortion potential. The present results for positron and electron impact (Fig-5) disagree at energies near excitation threshold due to high electron interaction and exchange effects. The two results tend to converge at higher energies similar to the results for integral cross sections for electron and positron impact. From the formula for the alignment parameter, if A_{20} is negative, then $\sigma_0 \gg \sigma_1$ implying that the excited states are aligned more to the magnetic sub-state $m=0$ or this sub-state is largely populated compared to the magnetic sub-state $m=1$. Otherwise $m=1$ is largely populated (see equation 4.45).

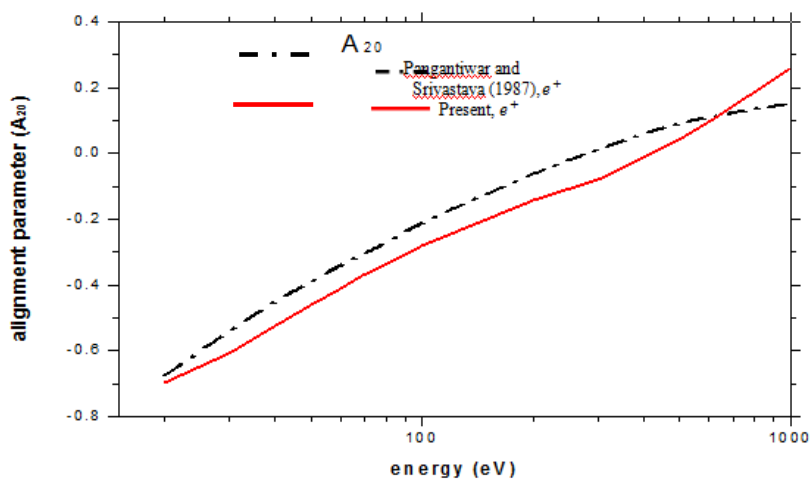


Fig-4: Alignment parameter results for positron impact excitation of the lowest autoionizing state in rubidium; —,present MZ results; - - -,Pangantiwar and Srivastava [5] results.

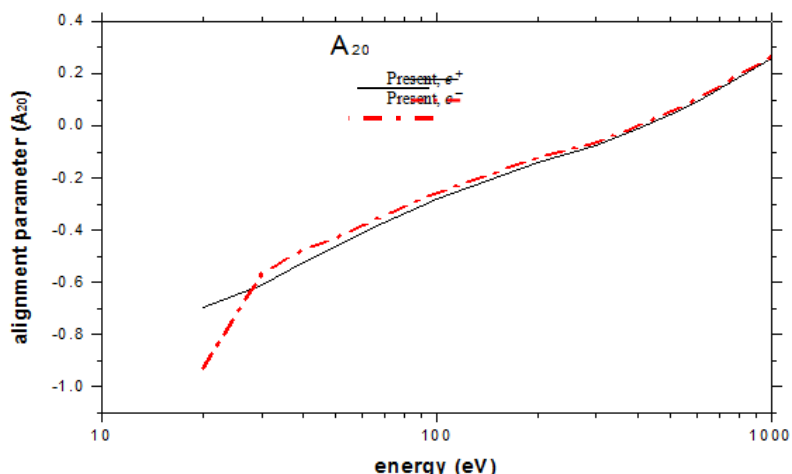


Fig-5: Present alignment parameter results for positron and electron impact excitation of the lowest autoionizing state in rubidium; , electron impact DZ results; ———, positron impact DZ results.

Lambda parameter λ

Results for lambda parameter are presented at 20eV and 100 eV projectile energies. Tables 5.8 and 5.9 give present lambda parameter results for electron impact excitation of the lowest autoionizing state in rubidium atom at various incident energies.

Fig-6 show that, apart from the result at 20 eV which is closer to the excitation energy, all other results give a similar trend for positron and electron impact results. The disparity at 20 eV is due to the behavior of electrons to interact more with the target electrons at energies near excitation threshold. At the small and large angles, that is close to 0^0 and 180^0 , particles are scattered more to the magnetic sub-state $m=0$ since from the formula (4.41) it is clear that for $\lambda=1$, $\sigma_0 \gg \sigma_1$. At intermediate angles σ_0 decreases and σ_1 increases, but still in most cases $\sigma_0 > \sigma_1$ except for 100 eV where $\sigma_0 < \sigma_1$ for 80^0 - 160^0 for positron impact (fig-7). If $\sigma_0 = \sigma_1$, the value of lambda is approximately 0.3. This happens when the magnetic sub-states are equally populated after excitation. For $\sigma_0 < \sigma_1$, $\lambda < 0.3$. From the electron impact results at 20 eV, it is clear that scattering is mainly towards the magnetic sub-state $m=0$, but at higher energies, this is not the case.

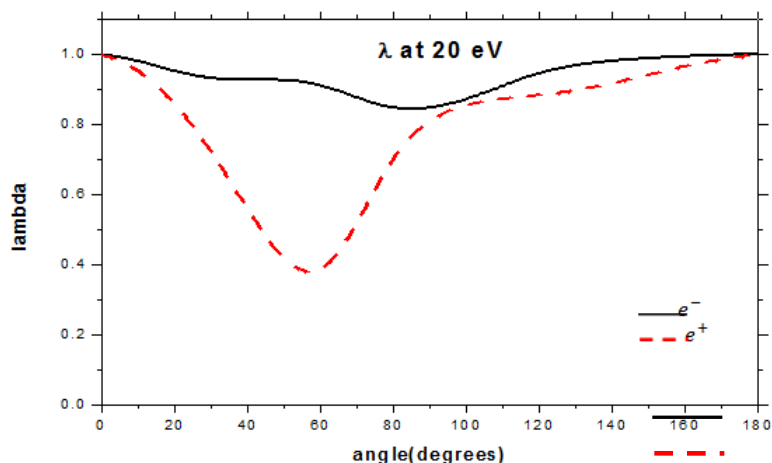


Fig-6: Present lambda parameter results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 20 eV; ———, electron impact results; - - - , positron impact results.

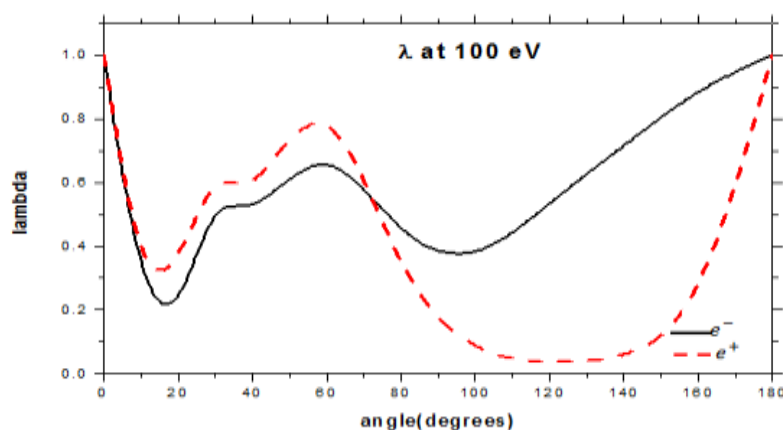


Fig-7: Present lambda parameter results for electron and positron impact excitation of the lowest autoionizing state in rubidium at 100 eV; ———,electron impact results; - - -,positron impact results.

CONCLUSIONS

From this study, the DWM integral cross section results for positron impact excitation of the lowest autoionizing state of rubidium obtained in the present study and those of Pangantiwar Srivastava[5] are in good agreement at near threshold and higher energies, but there is disagreement at intermediate energies; this is not the case for the results of electron impact excitation where at low impact energies these two results are in disagreement.

The near threshold strong negative ion resonances that appear for electron impact excitation results do not appear in positron impact excitation results due to lack of exchange between target electrons and the projectile positron. Low interaction between a positron and the target electrons (due to repulsion by the positive nucleus) is also a reason for the low cross sections in case of positron impact. Theoretical cross sections due to MZ wave functions in this study are generally larger at all energies compared to those of DZ wave functions. The lambda parameter indicates that more particles are scattered towards the magnetic sublevel $m=0$ for electron impact excitation compared to positron impact excitation at energies close to excitation threshold, for example at 20 eV. The alignment parameter results indicates that integral cross sections for $m=0$ are larger compared to $m=1$ up to about 500 eV.

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