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Positron-Helium Atom Excitation Using the Distorted Wave Method at Intermediate Impact Energy Range

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ABSTRACT

Positron-atom scattering provides an opportunity for positive-negative projectile comparison. This is because positrons are opposite sign to electron projectiles commonly used in scattering experiments. Calculations are done for cross-section for positron-helium scattering for the excitation of 1^1S to 2^1S state at impact energy range of 24eV-500eV using a distorted wave method. There is a systematic change on the angle-position of a dip with varying incident energy. The comparison made with the available theoretical results show interesting features of agreement at higher energies as well as disagreements as the impact energy is lowered. The observed agreement between calculated and experimental tread for the integral cross section results is encouraging.

Keywords: *Excitation of Helium on Positron Impact Using a Distorted Wave Method.*

1. INTRODUCTION

The availability of positron beam in the past few decades has enabled experimental procedures for positron-atom scattering processes. Positron as a projectile eliminates the complexity of exchange process (with the target electron) experienced when the projectile is an electron. Nevertheless, positron presents most of the possible outcomes of scattering processes such as target excitation, positronium formation, ionization and annihilation.

A number of theoretical approaches have been presented to study positron-helium scattering. Some of these includes; first-order distorted wave approximation close coupling approximation (DWBA) [9], convergent close coupling method (CCC) of Utamuratov[17], (CCA) of Wu [19] Puspitapallab [11]), and Hewitt [4] including the distorted wave method (DWA) of Mukesh [8] and Parcel [10].

In the present calculations, we have applied the distortion potentials suggested by Singh, 2004 [13] such that; the distortion potential in the initial channel is taken as the static potential of the target atom in its initial state, and the final channel distorted wave was generated by a potential taken as one-half of the initial state static potential and one-half of the final state static potential of the helium atom. This was arrived at from the fact that when the positron is in the initial state, for all the time it is in this field of the initial state of the target. Hence the distortion potential for the projectile positron in the initial state is taken as the static potential of the target atom in its initial state. After the energy transfer to the target atom, there is a time lag before the atom reaches its final state. Thus, the positron in its final state sees a potential which is intermediate between the initial- and final-state static potentials.

The form of the distorted wave method applied by Parcel *[9]*, used distortions by static potential incorporating various polarization potentials in the final channel, (Mukesh [8]). Saxena [12] employed distortion in both channels by the coulomb potential, and that used by Willis [18] involved taking the distortions in both channels in the field of static and polarization potentials of the target ground state.

2. THEORY

2.1. Two-Potential Scattering Model

The interaction of particles in two-potential scattering model can be split into two parts with one part being solved exactly and the other part by approximation. The total Hamiltonian of the system shall be given by (Gell-Mann and Goldberger, 1953)

$$H = H_0 + V \tag{1}$$

where H_0 is the unperturbed Hamiltonian of the collision system. V is the interaction potential between the projectile and the target and can also be split such that;

$$W = V - U \tag{2}$$

where U is the distortion potential.

The transition probabilities that an incident projectile will be scattered per unit time, per unit target scatterer and per unit incident flux is called the differential cross section given by

$$\frac{d\sigma}{d\Omega}=(2\pi)^4\frac{k_f}{k_i}\left|T_{fi}\right|^2 \qquad (3)$$

where k_i and k_f are the initial and final momentum of the scattering electrons (in atomic units). T_{fi} is the transition-matrix which gives the probability of finding a system in final channel state $\left|\phi_f\right\rangle$ after collision which was initially in collision state $\left|\Psi_i^{(+)}\right\rangle$ and is given by

$$T_{fi}=\left\langle\phi_f\right|V\left|\Psi_i^{(+)}\right\rangle \qquad (4)$$

3.2 The Distorted Wave Born Approximation Method

Inclusion of distortion potential in the unperturbed part of the Hamiltonian, transforms the Schrodinger equations governing the interaction to, (Gell-Mann and Goldberger, 1953)

$$(E-K-H_t-U)\left|\Psi_i^{(\pm)}\right\rangle=(V-U)\left|\Psi_i^{(\pm)}\right\rangle \qquad (5)$$

and

$$(E-K-H_t-U)\left|\mathrm{X}_i^{(\pm)}\right\rangle=0 \qquad (6)$$

respectively.

The Schrodinger equations (5) and (6) will give Lippmann-Schwinger equations of the form

$$\left|\Psi_i^{(\pm)}\right\rangle=\left|\mathrm{X}_i^{(\pm)}\right\rangle+\frac{1}{E-K-H_t-U\pm i\varepsilon}(V-U)\left|\Psi_i^{(\pm)}\right\rangle \qquad (7)$$

and

$$\left|\mathrm{X}_i^{(\pm)}\right\rangle=\left|\phi_i\right\rangle+\frac{1}{E-K-H_t\pm i\varepsilon}U\left|\mathrm{X}_i^{(\pm)}\right\rangle \qquad (8)$$

Thus, the T-matrix in equation (4) can be written in terms of $\left|\mathrm{X}_i^{(\pm)}\right\rangle$ above to get

$$T_{fi}=\left\langle\mathrm{X}_f^{(-)}\right|V\left|\Psi_i^{(+)}\right\rangle-\left\langle\mathrm{X}_f^{(-)}\right|U\ \frac{1}{E-K-H_t+U\pm i\varepsilon}V\left|\Psi_i^{(+)}\right\rangle \qquad (9)$$

Which after some mathematical manipulations becomes the distorted wave formula for two potential scattering model written as;

$$T_{fi}=\left\langle\mathrm{X}_f^{(-)}\right|U\left|\phi_i\right\rangle+\left\langle\mathrm{X}_f^{(-)}\right|V-U\left|\Psi_i^{(+)}\right\rangle \qquad (10)$$

Taking $\left|\mathrm{X}_i^{(\pm)}\right\rangle=\left|\varphi_i\chi_i^{(\pm)}\right\rangle$ explicitly, then equation (10) is written in terms of the final target state as

$$T_{fi}=\left\langle\chi_f^{(-)}\varphi_{f\varphi}\right|U\left|\varphi_i\right\rangle+\left\langle\chi_f^{(-)}\varphi_f\right|V-U\left|\Psi_i^{(\pm)}\right\rangle \qquad (11)$$

The first order distorted wave born approximation (DWBA) is obtained by considering the first term (only) of equation (7) such that

$$\left|\Psi_i^{(\pm)}\right\rangle\approx\left|\mathrm{X}_i^{(\pm)}\right\rangle=\left|\chi_i^{(\pm)}\varphi_i\right\rangle \qquad (12)$$

And thus, the T-matrix in equation (11) becomes

$$T_{fi}=\left\langle\chi_f^{(-)}\varphi_{f\varphi}\right|U\left|\varphi_i\right\rangle+\left\langle\chi_f^{(-)}\varphi_f\right|V-U\left|\chi_i^{(\pm)}\varphi_i\right\rangle \qquad (13)$$

The Integral Cross Section is obtained by integrating equation (3) for DCS to get

$$\sigma=\int\frac{d\sigma}{d\Omega}d\Omega \qquad (14)$$

The static potential V_{st} which will account for large-angle elastic scattering involving relatively small impact parameters takes the form given by [6];

$$V_{st}(r)=\frac{Z}{r}-\int_0^\infty\frac{\rho_0(r')d^3r'}{\left|r-r'\right|} \qquad (15)$$

where ρ_0 is the target unperturbed charge density.

The partial wave expansion of the distorted waves $\left|\chi_i^{(\pm)}\right\rangle$(with both outgoing and incoming boundary conditions) in terms of spherical harmonics is given by

$$\left|\chi^{(\pm)}\right\rangle=\sqrt{\frac{2}{\pi}}\frac{1}{kr}\sum_{lm}i^l\chi_l(k,r)Y_{lm}(\hat{r})Y^*_{lm}(\hat{k}) \qquad (16)$$

where Y_{lm} is a spherical harmonic and χ_l is the radial wave function corresponding to the angular quantum number *l*.

The radial distorted waves are solutions to the radial equation below

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-U(r)+k^2\right)\chi_l(r)=0 \qquad (17)$$

The Roothan-Hartree-Fock atomic wave functions of Clementi and Roetti (1974) are applied both for and the numerical values for the DCS and ICS for positron-helium scattering problem calculated using a modified form of computer program DWBA1 originally written by Madison and Bartschat (1996) for the electron-hydrogen scattering.

3. RESULTS AND DISCUSSIONS

The present calculated Differential Cross Sections for impact energy between 24eV and 500eV scattering angles up to 180^0 using the first order distorted wave method are discussed and the data compare well both qualitatively and quantitively with the available calculated results done using other approaches especially at higher energy range. These results are shown in figures 1-9, and they indicate a similar behaviour exhibited by the DCS at all the energies discussed. This clearly indicates the dependent of the DCS on the angle of the incident scatterer.

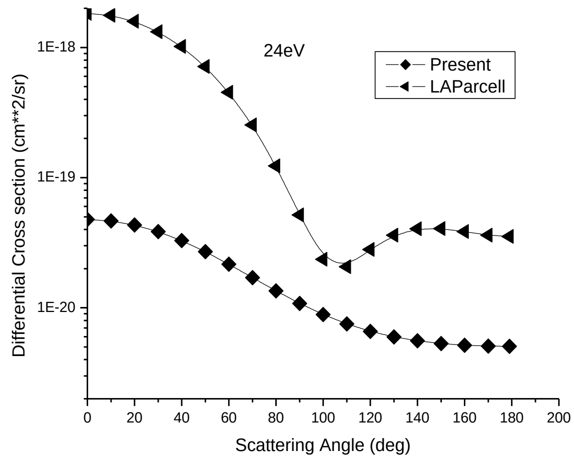
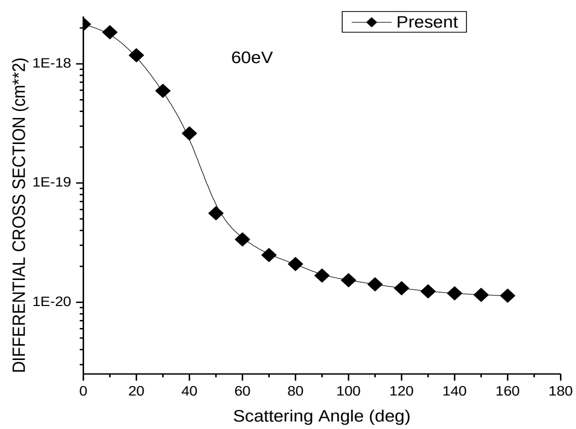


Fig 1. DCS for positron-helium scattering at impact energy of 24eV. Sharp decrease in DCS stop at a scattering angle of 110^0.



Present results compared to results of LaParcel [10]

Fig 2. DCS for positron-helium scattering at impact energy of 60eV. Sharp decrease in DCS stop at a scattering angle of 80^0.

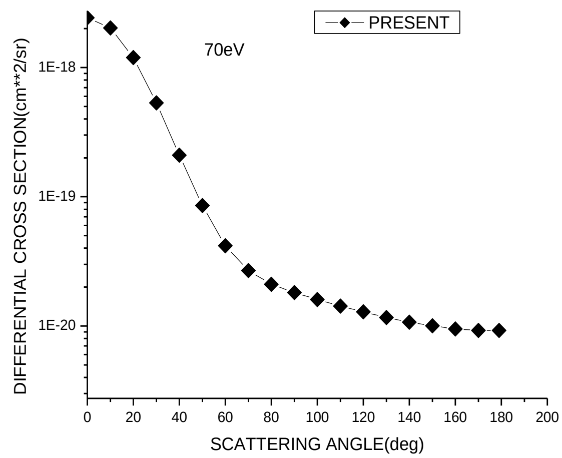


Fig 3. DCS for positron-helium scattering at impact energy of 70eV. Sharp decrease in DCS stop at a scattering angle of 110^0.

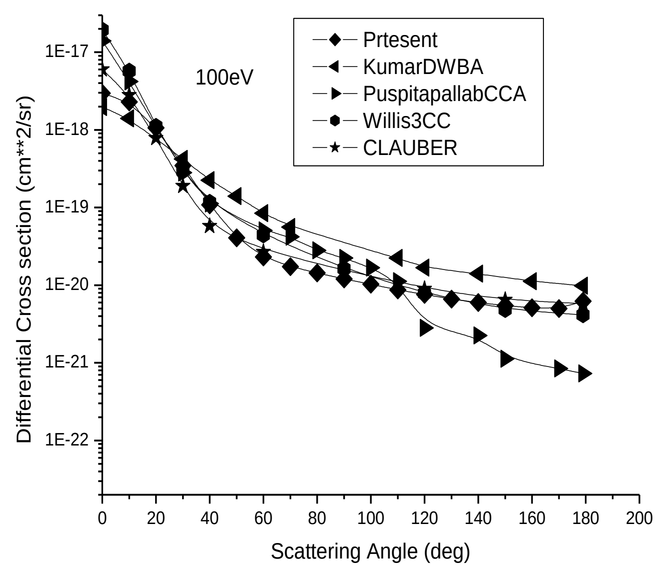


Fig 4. DCS for positron-helium scattering at impact energy of 100eV. Sharp decrease in DCS stop at a scattering angle of 70^0.

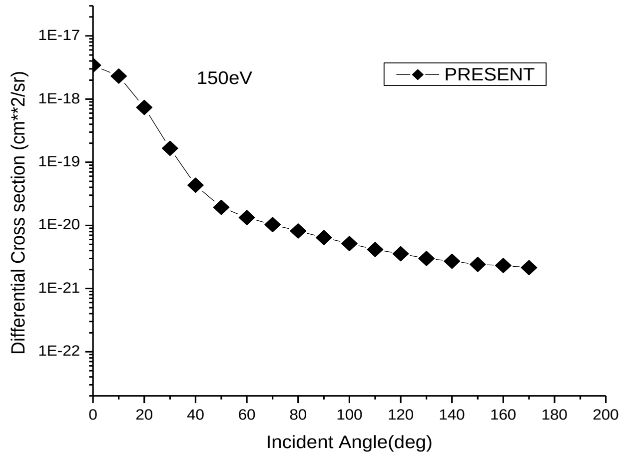


Fig 5. DCS for positron-helium scattering at impact energy of 150eV. Sharp decrease in DCS stop at a scattering angle of 55^0

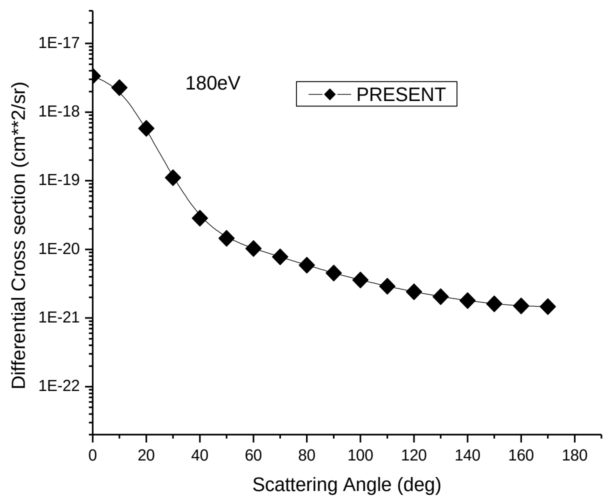


Fig 6. DCS for positron-helium scattering at impact energy of 180eV. Sharp decrease in DCS stop at a scattering angle of 42^0

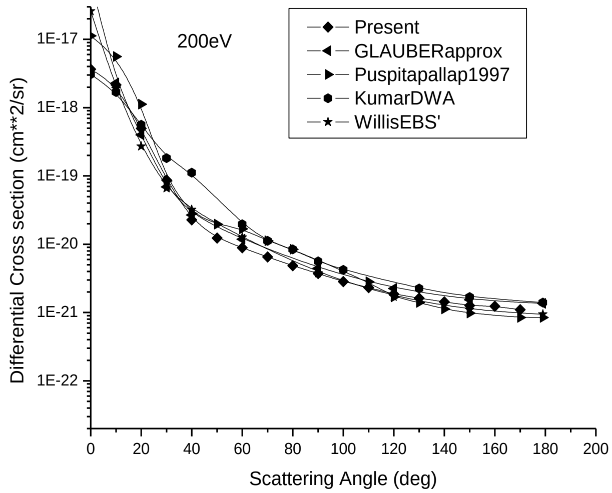


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Fig 7. DCS for positron-helium scattering at impact energy of 200eV. Sharp decrease in DCS stop at a scattering angle of 40^0.

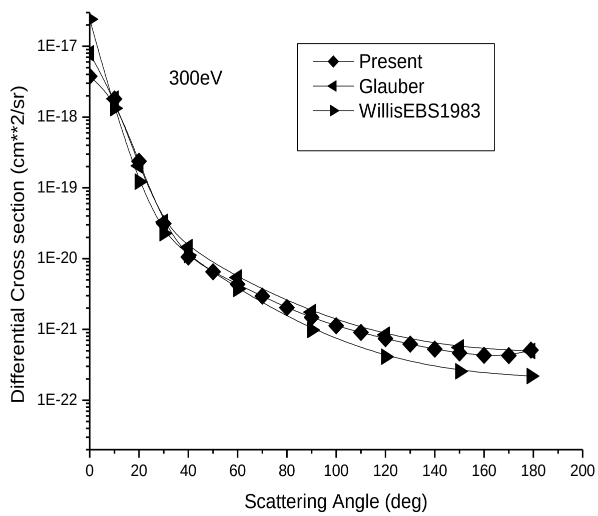

Fig 8. DCS for positron-helium scattering at impact of 300eV. Sharp decrease in DCS stop at a scattering angle of 38^0.

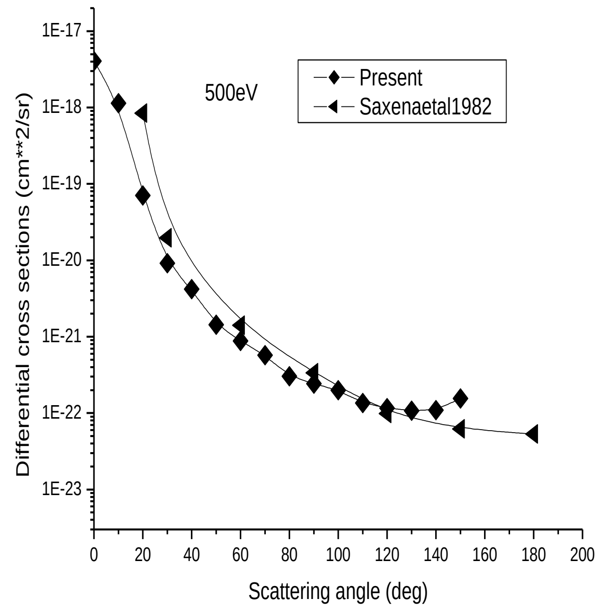

Fig 9. DCS for positron-helium scattering at impact energy of 500eV. Sharp decrease in DCS stop at a scattering angle of 35^0

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4. DISCUSSION

In the calculations analysed in this paper, there seems to be a systematic fall in the DCS as the scattering angle increases from the 0^0 up to some specific angle and then a slowed down/gradual decrease. This predicts a higher scattering at small angles as compared to larger angles.

Form the present calculations, there is an observed decrease in the angle at which the dip appears as the impact energy increases, for 24ev, the dip is at 110^0, for 60ev the dip is at an angle of 80^0, for 70ev at 75^0, for 110ev at 70^0, for 150ev at 55^0, for 180ev at 42^0, for 200ev at 40^0, for 300ev at 38^0, and for 500ev at a scattering angle of 35^0. These points indicate a decrease in the probability of scattering which may be attributed to the atomic structure of the target.

The observed "almost-uniform" DCS after the dip is an indication that at large scattering angles the probability of a scattering occurrence is not much dependent on the scattering angle

There is a qualitative agreement between the present results and those by LaParcel *et al.* 1983. However, the present calculation greatly underestimates those by LaParcel *et al.* 1983. Parcell *et al*. (1983) applied the distorted wave method taking the distortion potentials in respective atomic states, plus the corresponding polarization potentials.

5. CONCLUSION

The qualitative and quantitative agreement between our results and those done by other theoretical approaches show that the present formalism is reliable at intermediate impact energies and confirms that perturbation methods give better results at high impact energy.

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