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Distorted Wave Method Calculation of Positron Impact Excitation of 2^1s State of Helium Atom

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Abstract
We have calculated the differential and integral cross-section for positron-helium scattering for the excitation of 1^1S to 2^1S state at impact energy range of 22-200eV using a distorted wave method. The results are compared with the available experimental and theoretical results. It is observed that at higher energies present results are in good agreement with other theoretical results.

INTRODUCTION

The studies of positron as a projectile in atomic collision processes have drawn more interest in the past decades. This is because positron presents most of the possible outcomes of scattering processes such as target excitation, positronium formation, ionization and annihilation and because of the availability of positron beams now. Positron impact eliminates the possibility of the exchange processes with the target.

Numerous theoretical methods have been applied to study positron-helium scattering. These includes; close coupling approximation (CCA) Puspitapallab *et al*.(1997), Hewitt *et al.*(1991) and Wu *et al*.(2004), first Born approximation (FBA) Willis *et al*.(1981), two potential modified born approximation (TPMBA) Saxena *et al*. (1985), 3 state convergent close coupling method (3CCC) Willis *et al*.(1981), distorted wave method (DWA) Mukesh *et al*.(1985), Parcel *et al*. (1983), Eikonal born series (EBS)Willis *et al*.(1981), and convergent close coupling method (CCC) Utamuratov *et al*.(2010).

The distorted wave method applied by Saxena *et al*. (1981), employed distortion in both channels by the coulomb potential, Willis *et al.* (1981) used a distorted wave Born model where by the distortions in both channels were taken in the field of static and polarization potentials of the target ground state while Parcel *et al.*(1983), used distortions by static potential incorporating various polarization potentials in the final channel, (Mukesh *et al,* 1985).

Measurements of the integral cross section have been done by Sueoka *et al.*(1982) and More and Sueoka (1994) in which the time-of-flight technique was applied. This method has a weakness in that it has the inability to distinguish between energy loss and angular deflection, which means it cannot uniquely identify particular transitions (Hewitt *et al,* 1991).

In the distorted wave method used in this work 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. The reason for this choice is as follows. 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. When the energy from the positron is transferred to the target atom, the atom takes time (relaxation time) to go to its final state. That is, there is a time lag between the time of transfer of energy and the instant when 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. Hence the final state distortion is taken as the sum of one-half of the initial state static potential and one-half of the final state static potential of the helium atom. (Singh, 2004)

By the time of this work, no experimental results, known to us, for the differential cross section for 1^1S -2^1S excitation of helium atom by positron impact were available.

THEORY

In the two potential scattering model, the interaction potential V is broken into two parts as

$$V = U + W \tag{1}$$

and the first order distorted wave transition from the initial state to the final excited state of the target can be written as (Madison and Bartschat, 1996)

$$T_{if} = \left\langle \chi_f^- \psi_f \middle| U \middle| \phi \psi_i \right\rangle + \left\langle \chi_f^- \psi_f \middle| W \middle| \Psi_i^+ \right\rangle \tag{2}$$

where ψ_i and ψ_f are the initial and final states of the target respectively, ϕ is the initial state plane wave of the projectile and Ψ_i^+ is the total wave function.

Choosing U as linear combination of static potential of target states, the T-matrix element (2) reduces to

$$T_{if} = \left\langle \chi_f^- \psi_f \left| W \right| \Psi_i^+ \right\rangle \quad (3)$$

The first term in (2) vanishes because of the orthogonality of the atomic wave functions. In the first order distorted wave approximation Ψ_i^+ is replaced by $\psi_i \chi_i^+$ where χ_i^+ is the distorted wave function representing the projectile positron in the initial state and is a solution to the wave equation

$$\left(\nabla_i^2 - U_i + k_i^2\right)\chi_i^+ = 0 \quad (4)$$

Where U_i is an arbitrary potential chosen for the distortion of the initial state projectile positron wave function, and $\mathbf{k}_i$ is the initial wave vector of the projectile positron. Similarly, the final state projectile distorted wave function satisfies the equation

$$\left(\nabla_f^2 - U_f + k_f^2\right)\chi_f^- = 0 \quad (5)$$

where the subscript f denotes the final channel.

Before we evaluate the T-matrix, we first mention the atomic wave functions used and the choice of the distortion potentials.

Atomic wave functions

For ground state (1^1S) of helium atom, we used the Hatree-fock wave function of Byron and Joachain (1966) given by

$$\Psi_i(r_1, r_2) = \phi_0(r_1)\phi_0(r_2) \quad (6)$$

where

$$\phi_0(r) = \frac{N_1}{4\pi}\{\exp(-pr) + C\exp(-qr)\} \quad (7)$$

where N_1, p, q, and C are constants whose values are;
N_1 =2.60505, p =1.41, q=2.61 and C =0.799 (Byron and Joachain, 1966).

For the excited state (2^1S) we used the wave function of Van den Bos, (1969) given as

$$\Psi_f(r_1, r_2) = \left(2 + 2\Delta^2\right)^{-1/2}\{\varphi_{1S}(2, r_1)\chi_{2S}(r_2) + \varphi_{1S}(2, r_2)\chi_{2S}(r_1)\} \quad (8)$$

where $\varphi_{1S}(z, r)$ is the ground state hydrogenic orbital for nuclear charge Z given by

$$\varphi_{1S}(Z,r) = Z^{3/2} \cdot 2 \cdot e^{-Zr} \cdot Y_{00} \tag{9}$$

and

$$\chi_{2S}(r) = \frac{N}{\sqrt{4\pi}} \left\{ e^{-\beta r} + \eta r \; e^{-\gamma r} \right\} \tag{10}$$

with

N=0.6451, $\beta = 1.136$, $\gamma = 0.464$, $\eta = -0.2806$ and $\Delta = \int \varphi_{1S}(2,r)\chi_{2S}(r)dr = 0.06996$

Distortion potentials

The distortion potentials U_i and U_f could be arbitrarily picked but they are usually chosen as the static potentials of the target atom in its initial or final state or any linear combination of the two. The distortion potentials used here are those suggested by Singh (2004) where the initial distortion potential is taken as the static potential of the target atom in the initial state and the final state distorted wave is generated by a potential taken as the sum of one-half of the initial state static potential and one-half of the final states static potential of helium atom (Singh, 2004). This is because there is a time lag between the time of transfer of energy and the instant when the atom reaches the final excited state. That is;

$$U_i = \left\langle \Psi_i \middle| V \middle| \Psi_i \right\rangle \tag{11}$$

and the final distortion potential taken as

$$U_f = \frac{1}{2}\left\langle \Psi_i \middle| V \middle| \Psi_i \right\rangle + \frac{1}{2}\left\langle \Psi_f \middle| V \middle| \Psi_f \right\rangle \tag{12}$$

where Ψ_i and Ψ_f are the initial and final states of helium atom.

Evaluation of the T-matrix

We only evaluate the direct transition matrix for the 1^1S to 2^1S transition by positron impact because positron will not exchange with the target electron. Thus (using equation (3) and writing $W = V - U_f$ and replacing ψ_i^+ as $\psi_i \chi_i$

$$T_{if}^d = \left\langle \chi_f^-(0)\psi_f(1,2) \middle| V \middle| \psi_i(1,2)\chi_i^+(0) \right\rangle$$
$$- \left\langle \chi_f(0)\psi_f(1,2) \middle| U_f(0) \middle| \psi_i(1,2)\chi_i^+(0) \right\rangle \tag{13}$$

The second term will vanish because of the orthogonality of the atomic wave functions. Substituting the value of V as given in the equation below

$$V = -\frac{2Z_P}{r_{01}} - \frac{2Z_P}{r_{02}} + \frac{2Z_P Z_N}{r_0}$$

Where Z_P and Z_N are the positron charge and nuclear charge of the helium atom respectively and taking Z_P=1 and Z_N=2 in atomic units, we get

$$T_{if}^{d} = -2Z_p \left\langle \chi_f^{-}(0)\psi_f(1,2)\left|\frac{1}{r_{01}}\right|\psi_i(1,2)\chi_i^{+}(0)\right\rangle$$

$$-2Z_p \left\langle \chi_f^{-}(0)\psi_f(1,2)\left|\frac{1}{r_{02}}\right|\psi_i(1,2)\chi_i^{+}(0)\right\rangle \qquad (14)$$

The term associated with $\frac{1}{r_0}$ vanishes because of the orthogonality of the atomic wave functions. Because of the symmetrical nature of both the initial $\{\psi_i(r_1,r_2)\}$ and final $\{\psi_f(r_1,r_2)\}$ wave functions of helium atom, given by equations (2.5) and (2.6), with respect to $\mathbf{r_1}$ and $\mathbf{r_2}$, the two terms in equation (2.13) will be equal. We calculate the first term which, after substituting for $\psi_i(r_1,r_2)$ and $\psi_f(r_1,r_2)$ from equation (2.5) and (2.6), can be written as the sum of the following terms,

$$\frac{2}{(2+2\Delta^2)^{1/2}}\left\langle \chi_f^{-}(r_0)\varphi_{1S}(2,r_1)\chi_{2S}(r_2)\left|\frac{1}{r_{01}}\right|\phi_0(r_1)\phi_0(r_2)\chi_i^{+}(r_0)\right\rangle$$

$$+\frac{2}{(2+2\Delta^2)^{1/2}}\left\langle \chi_f^{-}(r_0)\varphi_{1S}(2,r_2)\chi_{2S}(r_1)\left|\frac{1}{r_{01}}\right|\phi_0(r_1)\phi_0(r_2)\chi_i^{+}(r_0)\right\rangle \qquad (15)$$

In both the terms of the above equations the $\mathbf{r_2}$ integral can be performed analytically to give, say K_1 for the first term and K_2 for the second term. Then the direct scattering amplitude can be written as

$$T_{if}^{d} = \frac{4}{(2+2\Delta^2)^{1/2}}K_1\left\langle \chi_f^{-}(r_0)\varphi_{1S}(2,r_1)\left|\frac{1}{r_{01}}\right|\phi_0(r_1)\chi_i^{+}(r_0)\right\rangle$$

$$+\frac{4}{(2+2\Delta^2)^{1/2}}K_2\left\langle \chi_f^{-}(r_0)\chi_{2S}(r_1)\left|\frac{1}{r_{01}}\right|\phi_0(r_1)\chi_i^{+}(r_0)\right\rangle \qquad (16)$$

To evaluate the direct scattering amplitude [equation (2.15)], the distorted waves χ_i^{+} and χ_f^{-} are expanded in terms of the partial waves as (Singh, 2004, Madison and Bartschat, 1996)

$$\left|\chi_i^{+}\right\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{k_i r}\sum_{l_i m_i} i^{l_i}\chi_{l_i}(k_i,r)Y_{l_i m_i}(r)Y^{*}_{l_i m_i}(k_i) \qquad (17)$$

and

$$\left|\chi_f^-\right\rangle = \sqrt{\frac{2}{\pi}}\frac{1}{k_f r}\sum_{l_f,m_f} i^{l_f}\chi_{l_f}^*(k_f,r)Y_{l_f m_f}(r)Y_{l_f m_f}^*(k_f) \tag{18}$$

where Y_{lm} is a spherical harmonic. In the expansion of χ_f^- the complex conjugate of the radial part χ_{l_f} is taken so that it satisfies the incoming boundary conditions. Substituting the above partial wave expansions of the distorted waves in equations (2.3) and (2.4) we find that the radial distorted waves are solutions of the following equation

$$\left(\frac{d^2}{dr^2} - \frac{l_S(l_S+1)}{r^2} - U_S(r) + k_S^2\right)\chi_l(r) = 0 \tag{19}$$

with s=*i* for the initial state and s=*f* for the final state distorted waves. The asymptotic boundary condition is given as

$$\lim_{r\to\infty}\chi_l(k_i,r) = j_{l_s} + B_{l_s}\left(-\eta_{l_s} + ij_{l_s}\right)$$

where j_l and η_l are regular and irregular Ricatti-Bessel functions, and B_l is given by

$$B_l = \exp(i\delta_l)\sin\delta_l$$

Where δ_l is the elastic scattering phase shift.

The radial distorted wave equation (18) for initial and final states is solved by using Numerov method.

The differential cross section $\left(\frac{d\sigma}{d\Omega}\right)$ for helium excitation from ground state to the 2^1S state by positron impact using the distorted wave method, was evaluated using the relation

$$\frac{d\sigma}{d\Omega} = 4\pi^4\left|T^d\right|^2 \tag{20}$$

For total cross section (σ), equation (2.19) is integrated to give the relations as shown below,

$$\sigma = \int \frac{d\sigma}{d\Omega}d\Omega$$
$$= 2\pi \int_0^\pi \frac{d\sigma}{d\Omega}\sin\theta d\theta \tag{21}$$

The modified form of computer program DWBA1 written by Madison and Bartschat (1996) was used to evaluate the matrix elements and the cross sections. The original program is written for the electron-hydrogen scattering. It was modified for our positron-helium scattering problem.

RESULTS AND DISCUSSIONS

We have calculated the differential and integral cross sections for 2^1S excitation of helium atom by positron impact for incidence energies ranging from 22-200eV and compared them with available theoretical and experimental results.

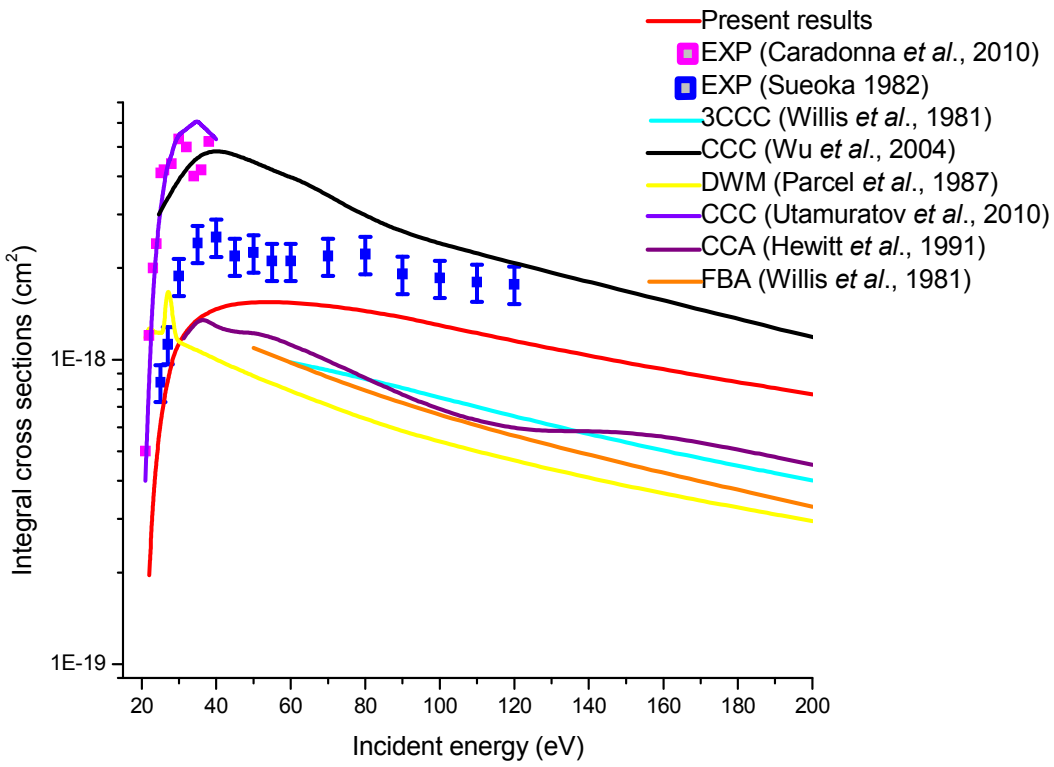

Figure 1.Integral cross-section for 1^1S-2^1S excitation of helium by positron impact.

We find that the integral cross-section results of the present work are reasonably close and in good qualitative agreement with the experimental results of Sueoka (1982). The CCC results of Wu *et al.* (2004) and the present results seem to agree better with results of Sueoka (1982) than the FBA results of Willis *et al*. (1981), the DWBA results of Parcel *et al*. (1987), the three-states CCC results of Willis *et al*. (1981), the CCA results of Hewitt *et al*. (1991) and the two-centre CCC results of Utamuratov*et al*. (2010). Though the Wu's results over estimate and the present results under estimate Sueoka's experimental results.

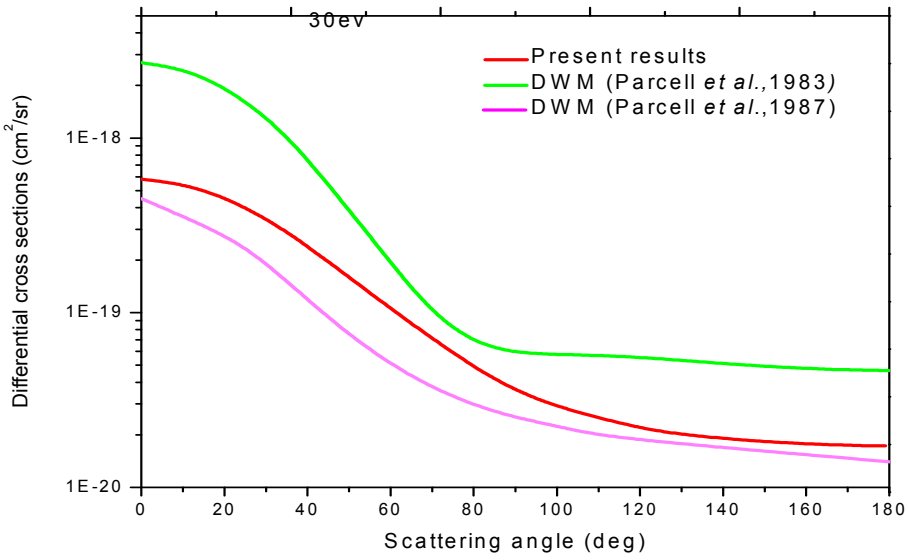

Fig.2. Differential cross-section for 1^1S-2^1S excitation of helium by positron impact at 30eV impact energy.

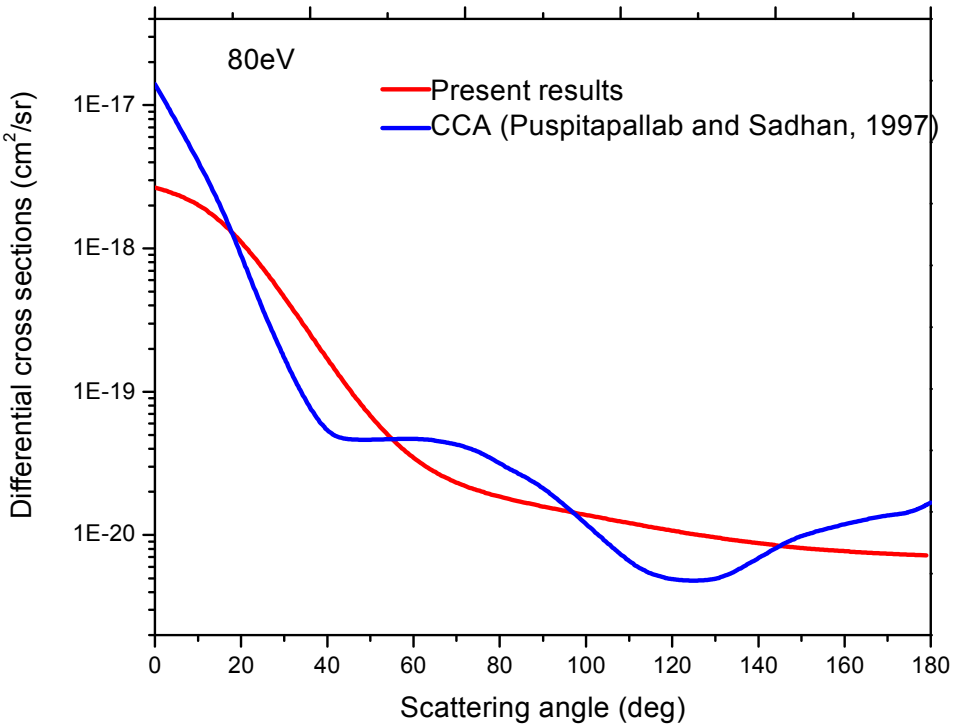

Fig.3. Differential cross-section for 1^1S-2^1S excitation of helium atom by positron impact at 80eV impact energy

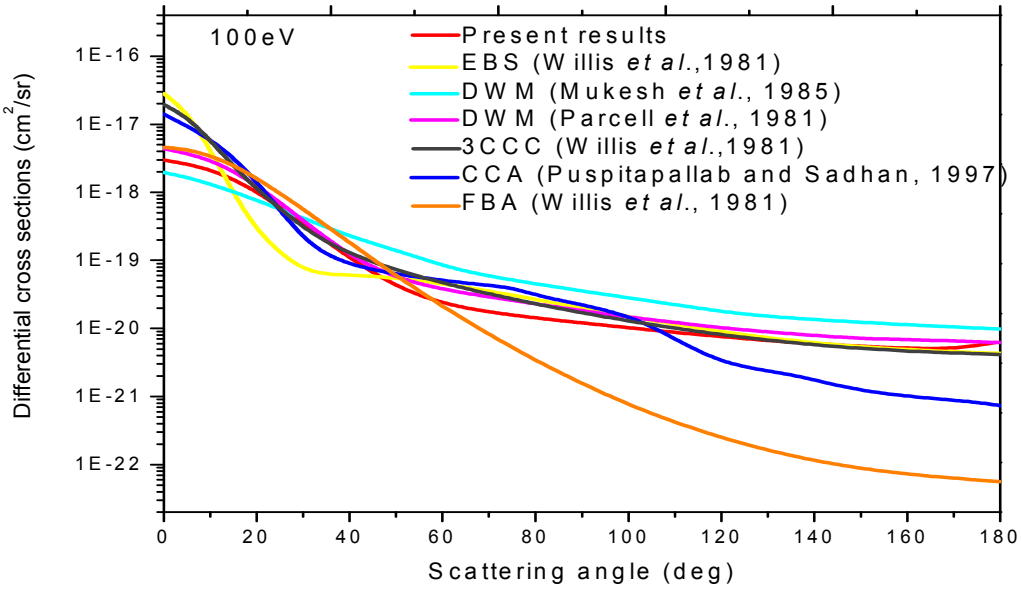

Fig 4. Differential cross-section for 1^1S-2^1S excitation of helium atom by positron impactat 100eV impact energy.

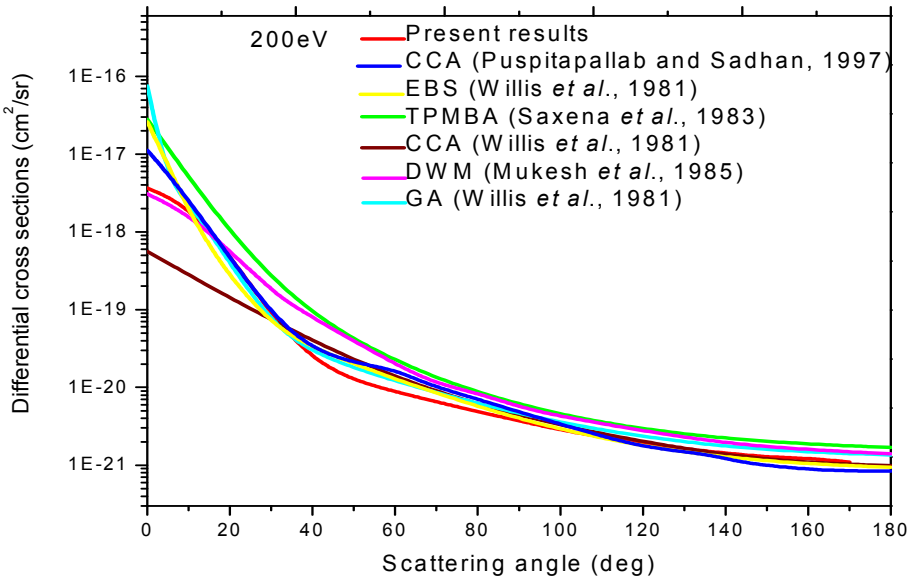

Fig 5. Differential cross-section for for 1^1S-2^1S excitation of helium atom by positron impact at 200eV impact energy.

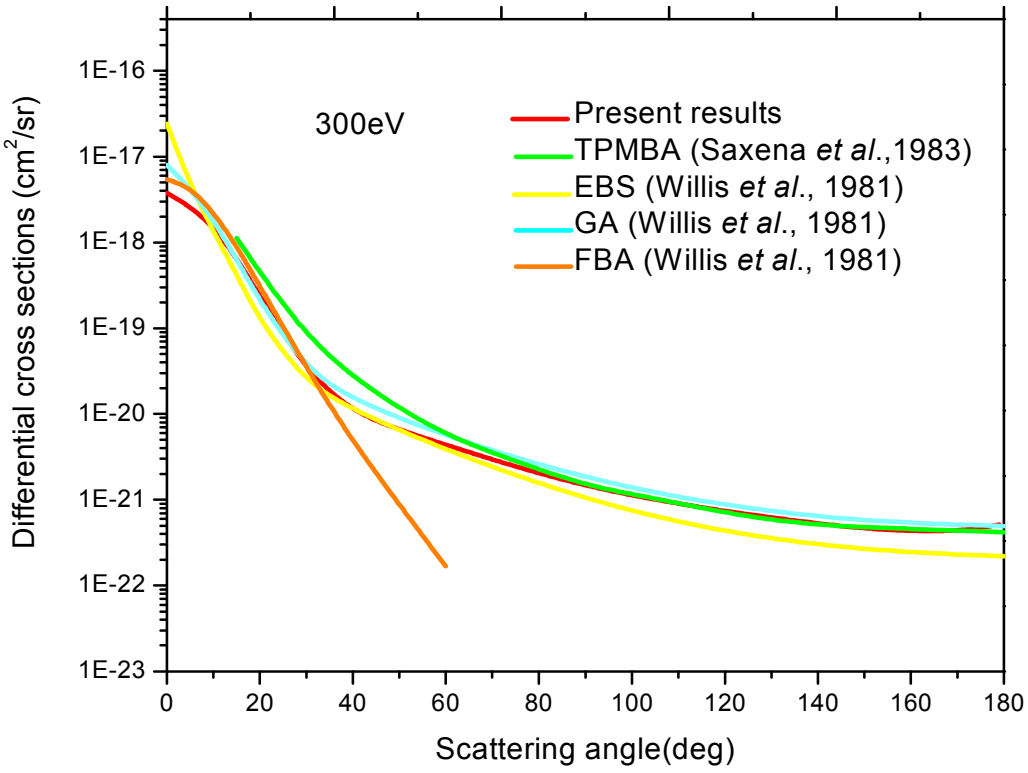

Fig 6.Differential cross-section for 1^1S-2^1S excitation of helium atom by positron impact at 300eV impact energy.

Differential cross section results are compared in figs 2-6. We find that at the impact energies of 100, 200, and 300eV the differential cross section results for the present distorted wave method are in good agreement with the results of Willis *et al*. (1981) and also with the results of Saxena *et al*. (1983) calculated in the framework of the two-potential Modified Born approximation. The present results seem to be in improved agreement with results of Puspitapallab and Sadhan (1997) at impact energies of 100eV and 200eV compared to their mismatch at 80ev though their results still show oscillatory character whereas no other results show this behavior. The observed qualitative and quantitative agreement between present results and those calculated using other methods at 100eV, 200eV and 300eV confirms that perturbation methods give better results at high impact energy. It is seen that the plane wave results of first order Born approximation greatly under estimate the cross sections at 100eV and 300eV at high scattering angles as compared to other calculated results.

Conclusion

It is interesting to note that at impact energies of 100, 200 and 300eV the present distorted wave method give results that are in good agreement with those obtained through other theoretical methods like the EBS, GA, CCA and 3CCC. Thus the present method is reliable for intermediate and high energies.

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