Indian J. Phys. **72B** (1), 11-17 (1998)

IJP B
— an international journal

Studies on positron-hydrogen ionization cross sections

A Bandyopadhyay[1], P K Dutta[2], K Roy[1], P Mandal[2] and N C Sil[1]

[1]Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta-700 032, India.

[2]Department of Mathematics, Visva Bharati University, Santiniketan-731235, West Bengal, India

Received 5 May 1997, accepted 17 November, 1997

Abstract : In this work, we report the results of the total ionization cross section of hydrogen atom by positron impact We also explore some interesting kinematical situations of the single and double differential cross sections for near future experiments In our calculation, we use the asymptotically correct final-state wave function which involves three apropriate confluent hypergeometric functions We compare our total cross section values with the available theoretical results and the existing experimental data.

Keywords . Ionization cross section, asymptotically correct final-state wave function, confluent hypergeometric functions

PACS Nos. 34 80 Dp, 34.50 Fa.

1. Introduction

The study of scattering by positron impact alone has its own beauty. A number of highly interesting phenomena occurs when a stream of positron passes through a gas. Moreover, the positron being positively charged is distinguishable from the atomic or molecular electron. There is no electron exchange analogue for positron scattering and as such the total wave function need not be antisymmetrized. In recent years, considerable developments are made in the experimental findings of positron-atom scattering due to the availability of intense positron beams of required energy and sensitive detectors. New fast-counting techniques have made it possible to enlarge much further the base already established and have brought into practical possibility of measurement that seemed unattainable before. So studies on positron collision have now become a very interesting field. A spurt of activities is also noticed in the positron-induced ionization studies, because of the recent observations in the laboratory. The points of contact between theory and experiment are thus becoming close.

Spicher *et al* [1] measured total ionization cross sections for atomic and molecular hydrogen targets upto incident positron energies of 600 eV and compared their results with the available theoretical predictions [2-5]. However, the agreement between these theoretical estimates and the observed data is reasonable upto 30 eV, the measured values become quite large at higher energies of impact.

Recently, Jones *et al* [6] have measured ionization cross section for positron impacting on atomic hydrogen for kinetic energies in the range of 15 to 700 eV. These results are found significantly lower than those obtained by Spicher *et al* [1] and show better agreement with the theoretical calculations [3, 4, 7, 8]. At present, the cause of discrepancy between two experiments is unknown and it demands more theoretical and experimental findings. In the above mentioned theoretical calculations, the final state wave function does not satisfy the asymptotic conditions. Garibotti and Miraglia [9] used a final state wave function consisting of the three Coulomb waves, each of which represents the two-body interactions between the final particles of the ion-atom collision processes. They applied this wave function in the case of ionization and electron capture to the continuum in the proton-hydrogen atom collision. Brauner et al [10] calculated Triple Differential Cross Section (TDCS) of electron and positron impact ionization considering this wave function in the final state which is asymptotically exact. Besides TDCS, Brauner, Briggs and co-workers [11-13] also calculated Double Differential Cross Section (DDCS) for incident energies upto 100 eV. To calculate DDCS, they have neglected projectile-electron interaction. Briggs and his group used the 3-Coulomb wave function in the final state for the calculation of ionization of atoms only for TDCS and DDCS. They never attempted to find out the total cross sectional values. We have developed the accurate numerical methods with proper consideration of phase factors arising in the numerical calculations and using these techniques calculated the TCS values. We have considered the 3-C wave function in the final state and performed the enormous numerical calculations to obtain the TCS values which we can claim as our originality and no one has attempted to do so. In the present work, we have calculated total cross section (TCS) values for incident energies upto 1000 eV. Here, we report our results of the total cross sections as well as the double differential cross sections (DDCS) and single differential cross sections (SDCS) in positron-hydrogen ionizing collisions. Recently, many groups [14-15] have reported DDCS data for different e^+-Atom systems. Due to the recent progress in experiments, now it is required to calculate theoretical values of the DDCS. Although there exist neither experimental nor theoretical results for single differential cross section (SDCS), we calculate those for the future experiments. In all the above calculations, we have considered all two-body interactions. The final-state wave function used in our calculation here involves the product of three appropriate confluent hypergeometric functions depending on the positron-proton, the electron-proton and the positron-electron interactions [10]. The contributions of these three interactions are equally significant as these are long range and Coulombic in nature. Although this final state wave function appears to be appropriate for intermediate and high energies of impact, its use at low energies may not be justified because of the negligence of short-range effects. Further, it is noticed that the results obtained by using three Coulomb wave function, the angular distributions are predicted very well whereas at lower energies total cross section values are not produced correctly. Our total cross section results are in good agreement with the data of University College London group [6] at high energies.

2. Theory

The DDCS for ionization, *i.e.* the integration over the angular variables of the scattered positron, can be expressed as (atomic units are used here) :

$$\frac{d^2\sigma}{dE_b d\Omega_b} = \frac{16\Pi^4 k_a k_b}{k_i} \int \left|T_{fi}\right|^2 d\Omega_a \tag{1a}$$

and the DDCS for secondary electron is obtained by

$$\frac{d^2\sigma}{dE_b d\Omega_a} = \frac{16\Pi^4 k_a k_b}{k_i} \int \left|T_{fi}\right|^2 d\Omega_b \tag{1b}$$

where T_{fi} corresponds to the scattering amplitude in the ionization process. In our calculation, the matrix element T_{fi} is taken as

$$T_{fi} = <\psi_f^-|V_i|\psi_i>, \tag{2}$$

where ψ_i is the initial state wave function given by

$$\psi_i = (2\Pi)^{-3/2} \exp[ik_i . r_a] \phi_i(r_b), \tag{3}$$

ϕ_i being the initial bound state wave function. In eq. (2), ψ_f^- is the solution of the three-body problem satisfying incoming-wave boundary conditions and is considered here is :

$$\psi_f^- = (2\Pi)^{-3} \exp[i\boldsymbol{k}_a . \boldsymbol{r}_a] \exp[i\boldsymbol{k}_b . \boldsymbol{r}_b]$$
$$\times \phi_{\boldsymbol{k}_a}(\alpha_a, r_a)\, \phi_{\boldsymbol{k}_b}(\alpha_b, r_b)\, \phi_q(\alpha_{ab}, r_{ab}), \tag{4}$$

where

$$\phi_{\boldsymbol{k}}(\alpha_i, r) = \Gamma(1+i\alpha_i) \exp[\pi\alpha_i/2]\ {}_1F_1[-i\alpha_i, 1, -i(kr + \boldsymbol{k}.\boldsymbol{r})] \tag{5}$$

and $\mathbf{q} = (\boldsymbol{k}_a - \boldsymbol{k}_b)/2$, $\boldsymbol{r}_{ab} = \boldsymbol{r}_a - \boldsymbol{r}_b$, $a_i = z_i / |\mathbf{k}|$;

$Z_i = -1, +1, 1/2$ as $i = 1, 2, 3$ respectively.

V_i is the perturbation interaction $(1/r_a - 1/r_{ab})$, (6)

k_i, k_a and k_b are the momenta of the incident, scattered positron and the ejectred electron respectively. Using eqs. (3) to (6) in eq. (2) we can write down the scattering amplitude as

$$T_{fi} = N^* \int \exp[i(\boldsymbol{k}_i - \boldsymbol{k}_a).\boldsymbol{r}_a]\ \exp[-i\boldsymbol{k}_b.\boldsymbol{r}_b]\ \exp[-\lambda_i r_b]$$
$$\times (1/r_a - 1/r_{ab})\ {}_1F_1[i\alpha_a, 1, i(k_a r_a + \boldsymbol{k}_a.\boldsymbol{r}_a)]$$
$$\times\ {}_1F_1[i\alpha_b, 1, i(k_b r_b + \boldsymbol{k}_b.\boldsymbol{r}_b)]\ {}_1F_1[i\alpha_{ab}, 1, i(qr_{ab} + \boldsymbol{q}.\boldsymbol{r}_{ab})] d\boldsymbol{r}_a . d\boldsymbol{r}_b\,, \tag{7}$$

where

$$N = \frac{1}{16(2^{1/2})\pi^5} \Gamma(1+i\alpha_a)\Gamma(1+i\alpha_b)\Gamma(1+i\alpha_{ab})\ \exp[(\alpha_a + \alpha_b + \alpha_{ab})/2].$$

The detailed evaluation of T_{fi} and the corresponding numerical techniques have been shown in our previous works [16-17], so there is no justification to discuss it here again. Brauner et al also followed the same method to calculate T_{fi} which has been applied first by Sil and co-workers [18]. The SDCS values can be obtained simply by performing the integrations of eq. (1a) or (1b) as follows :

$$\frac{d\sigma}{d\Omega_b} = \int \frac{d^2\sigma}{dE_b\, d\Omega_b} dE_b, \tag{8a}$$

$$\frac{d\sigma}{dE_b} = \int \frac{d^2\sigma}{dE_b\, d\Omega_b} d\Omega_b. \tag{8b}$$

Finally, one would obtain the TCS after carrying out the remaining integral in eq. (8a) or (8b).

3. Results and discussions

We have computed the results of the DDCS, SDCS and TCS for a wide range of incident energies and scattering parameters, as there is an obvious dearth of theoretical data for positron-impact ionizing collisions as opposed to (e-2e) collisions [1]. These are discussed separately and compared with the available theoretical and experimental values.

The results of the DDCS using formula (1a) as a function of the angle of ejection are plotted in Figure 1 for incident energies 200 and 500 eV respectively. The features of these results are distinctly different from those predicted by the first Born approximation which are

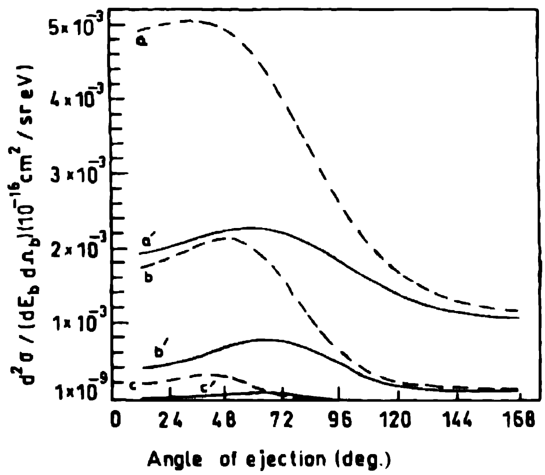

Figure 1. DDCS as a function of θ_b. Solid lines (——) E_i = 500 eV and Dashed lines (– –) E_i = 200 eV Curves a', b', c' correspond E_b = 1,10 and 50 eV. Curves a,b,c correspond E_b=2,10 and 50 eV respectively

displayed in Mott and Massey [19]. In our results, there is no sharp maximum in the angular distribution of the ejected electron for any incident energy, and for low energy of incidence, the DDCS falls off uniformly with angles of ejection, while for high energy, the DDCS falls off less rapidly and becomes almost flattened with a broad hump. Using formula (1b), we have also obtained values of the DDCS as functions of the angle of scattering and scattered energy. These results are again distinctly different from the first Born values [20] and are displayed in Figure 2 for an incident energy of 200 eV. The DDCS in this case falls off sharply from a maximum with the scattering angle at the scattered energy of 175 eV, while for lower energies of scattering at 145 eV, for instance, the angular distribution is quite uniform.

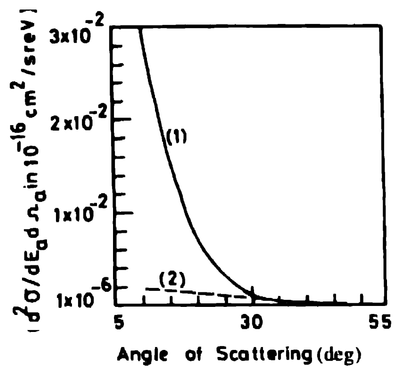

Figure 2. DDCS as a function of θ_a, E_i = 200 eV Curve 1 for E_a = 175 eV and Curve 2 for E_a = 145 eV

The angular distribution of the ejected electron for positron energies 100, 200, 300, 400 and 500 eV are displayed in Figure 3. The SDCS for 100 eV has a maximum at around 20° ejection angle and then falls off rather sharply. It is evident from Figure 3 that the results

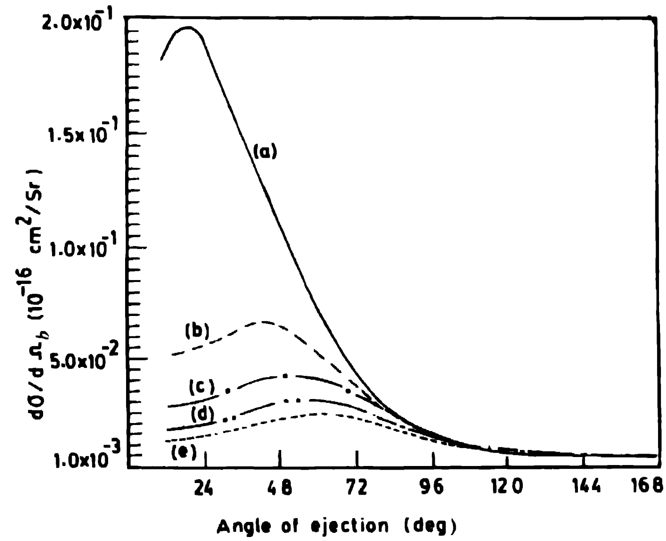

Figure 3. SDCS as a function of θ_b. Curves a,b,c,d,e represent for E_i = 100,200,300,400 and 500 eV respectively.

for the other higher incident energies manifest only broad maxima, and the values become more flat with increasing incident energies. The energy distribution of the ejected electron is depicted in Figure 4 for incident energies 75, 100 and 500 eV. These results show the same features as the first-Born results [20].

Recently, Spicher *et al* [1] and Jones *et al* [6] have performed experiments to obtain the total ionization cross sections for the above system. The results of Jones *et al* [6] for kinetic

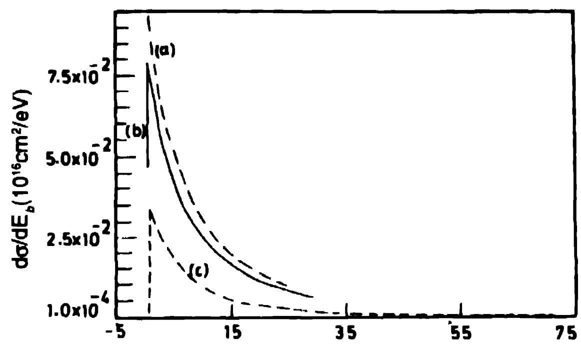

Figure 4. SDCS as a function of E_b. Curves a,b,c represent for E_i=75, 100 and 500 eV respectively

kinetic energies 15 to 700 eV. are found to be significantly lower than those obtained by Spicher *et al* [1]. The theoretical results of Acacia *et al* [21] using the distorted wave approximation and considering the improvements to the description of the interaction between the two outgoing particles, are in conformity with the experimental values of Spicher *et al* [1]. All other existing theoretical data for TCS confirm the experiment of Jones *et al* [6]. The values obtained by the continuum optical model calculation of Ratnavelu [7] and the first Born calculation of Peach [8] are available for a wide range of incident energies of positron. The other theoretical results of Golden and McGuire [22] using Glauber approximation, the Classical Trajectory Monte Carlo (CTMC) results of Ohsaki *et al* [4], the distorted wave polarised orbital values of Mukherjee *et al* [23] are available only for lower and intermediate energies. The results obtained by Glauber approximation [22] and by CTMC [4] almost coincide and underestimate the experimental values of Jones *et al* [6] whereas the values of Mukherjee *et al* [23] overestimate those values.

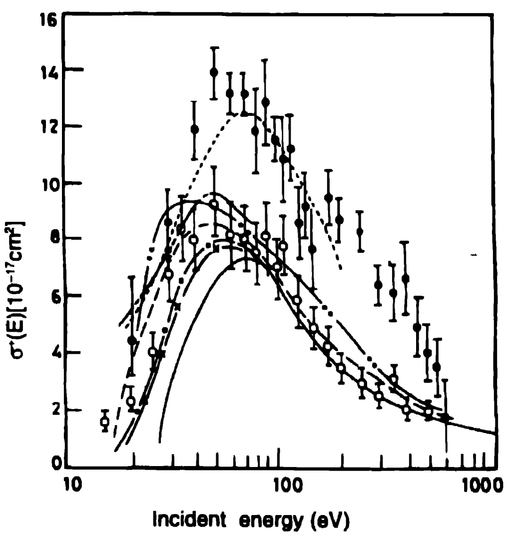

Figure 5. Total Cross Sections for different incident energies. (——) present results, (– x–x–) Golden and McGuire [22], (–•–•–) Ohsaki *et al* [4], (– – –)Peach [8], (– - - - -) Mukherjee *et al* [23], (–••–••–) Ratnavelu [7] and (------) Acacia [21], ϕ values of Jones *et al* [6] and Φ values of Spicher *et al* [1].

The values of Ratnavelu [7] overestimate the experimental values of Jones *et al* [6] except at a fewer energies. The Born results of Peach [8] overestimate the values of Jones *et al* [6] at lower energies and agree well at intermediate and high energies. It also agrees with the shape of the experimental curve of Jones *et al* [6] throughout the energy region. The present TCS results are also displayed with the above theoretical calculation and observed data [1,6]. As is evident from the Figure 5, the present TCS values are in conformity with the recent experimental data of Jones *et al* [6] and lie much below the observations of Spicher *et al* [1]. The agreement is much better beyond the incident energy of 75 eV where there is a peak in the cross section. The disagreement at lower energies may be due to the negligence of short range effects. Finally, we can conclude that our calculated values are in best agreement with the experimental values of Jones *et al* in comparison with other existing theoretical values except at lower energy region.

The present results for the DDCS, SDCS and TCS are yet to be verified experimentally We hope such an effort would be forthcoming soon.

References

[1] G Spicher, B Olson, W Raith, G Sinapiusand, W Sperber *Phys Rev. Lett* **64** 1019 (1990)

[2] A S Ghosh, P S Mazumdar and M Basu *Can J Phys* **63** 621 (1985)

[3] K K Mukherjee, N R Singh and P S Mazumdar *J Phys* **B22** 99 (1989)

[4] A Ohsaki, T Watanabe, K Nakanishi and K Iguchi *Phys Rev* **A32** 2640 (1985)

[5] A E Wetmore and R E Olson *Phys Rev* **34** 2282 (1986)

[6] G O Jones, M Charlton, J Slevin, G Lariccchia, A Kover, M R Poulsen and S Nic Chormaic *J Phys* **B26** L483 (1993)

[7] K Ratnavelu *Aust J Phys* **2** 265 (1991)

[8] G Peach (1986) *Private Communication* in M B Shah, D S Elliot and H B Gilbody *J Phys.* **B20** 3501 (1987)

[9] C R Garibotti and J E Miraglia *Phys Rev* **A21** 572 (1980)

[10] M Brauner, J S Briggs and H Klar *J Phys.* **B22** 2265 (1989)

[11] J Berakdar, J S Briggs and H Klar *Z Phys* **D24** 351 (1992)

[12] F Maulbetsch and J S Briggs *Phys Rev Lett* **68** 2004 (1992)

[13] J Berakdar and H Klar *J. Phys.* **B26** 39891 (1993)

[14] J Moxom, G Laricchia, M Charlton, G O Jones and A Kover *J Phys.* **B25** L613 (1992)

[15] A Kover, G Laricchia and M Charlton *J Phys.* **B26** L575 (1993)

[16] K Roy, P Mandal and N C Sil *Indian J Phys.* **68B** R1 (1994)

[17] A Bandyopadhyay, K Roy, P Mandal and N C Sil *J Phys* **B227** 4337 (1994)

[18] C Sinha and N C Sil *J Phys.* **B11** L333 (1978)

[19] N F Mott and H S W Massey *The Theory of Atomic Collisions*, 3rd ed (1965) p 490

[20] *ibid* p 492

[21] P Acacia, R I Campeanu, M Horbatsch, R P McEachran and A D Staufer *Phys. Lett* **A179** 205 (1993)

[22] J E Golden and J E McGuire *Phys Rev Lett* **32** 1218 (1974)

[23] K K Mukherjee, K B Chowdhury, N R Singh, P S Mazumdar and S Brajamani *Can J. Phys* **68** 249 (1990)