Available online at www.sciencedirect.com
SCIENCE DIRECT®
PERGAMON
Radiation Physics and Chemistry 68 (2003) 199–203
Radiation Physics and Chemistry
www.elsevier.com/locate/radphyschem

Differential cross sections for positron impact excitation of hydrogen

L. Lugosi[a,*], B. Paripás[b], I.K. Gyémánt[c], K. Tőkèsi[a]

[a] *Institute of Nuclear Research, Hungarian Academy of Sciences (ATOMKI), P.O. Box 51, Debrecen H-4001, Hungary*
[b] *Department of Physics, University of Miskolc, Miskolc-Egyetemváros H-3515, Hungary*
[c] *Department of Theoretical Physics, University of Szeged, H-6720 Szeged, Tisza Lajos krt. 84-86, Hungary*

Abstract

A distorted wave polarized orbital model and a three-body classical trajectory Monte Carlo method are applied to study the excitation of hydrogen atom by positron impact. The total and differential cross section as a function of the scattering angle of the scattered positron are calculated at 54.4, 100 and 200 eV impact energies. Our results are compared with previous theoretical calculations.

PACS: 36.10.Dr; 34.80.−i; 34.90.+q

Keywords: Positron; Excitation; Cross section

1. Introduction

Positrons, since their discovery, have been extensively used as probes in different branches of physics as reviewed by Ghosh et al. (1982) and more recently by Drachman (1995). During the past few years great progress has been achieved in the experimental and theoretical study of positron-atom collisions (Charlton and Humberston, 2001). The collision process of a positron with a hydrogen atom attracts much attention as one of the simplest *three-body Coulomb system*. When a positron collides with a hydrogen atom the following reactions are possible

$$e^+ + H \rightarrow \begin{cases} e^+ + H & \text{elastic scattering} \\ p + Ps^* & \text{positronium formation} \\ e^+ + H^* & \text{excitation} \\ e^+ + e^- + p & \text{ionization} \\ p + \gamma & \text{annihilation.} \end{cases} \quad (1)$$

The study of the energy and angular distributions of the ejected electrons and scattering projectiles provides a sensitive test of various theories. Noteworthy contributions on the elastic scattering, positronium formation, discrete excitation and ionization processes in positron–hydrogen collisions can be found both theoretically and experimentally, for example, in works of Walters (1988), Kernoghan et al. (1996), Zhou et al. (1997) and Jones et al. (1993).

In this paper we present theoretical calculations for the angular differential and total 1s–2s excitation cross sections for collisions of positron with ground state hydrogen atom, using a distorted wave polarized orbital (DWPO) model and the classical trajectory Monte Carlo (CTMC) method Olson (1981). The CTMC method which is comprehensive used for the theoretical description of the ion–atom collision processes, it has also been successful for light mass projectile such as positron (Shultz and Olson, 1989; Tõkési and Kövér, 2000). The one of the main advantages of the CTMC method is that all reaction channels can be taken into account within the framework of the classical dynamics. In a complete treatment of the positron-hydrogen scattering, all the open channels are coupled together and the cross

*Corresponding author. Tel.: +36-52-417-266; fax: +36-52-416-181.
E-mail address: lugosi@atomki.hu (L. Lugosi).

0969-806X/03/$ - see front matter
doi:10.1016/S0969-806X(03)00280-9

sections for all various processes (1) are determined together. Such an approach has been made using the coupled-state method by Kernoghan et al. (1996) and Mitroy and Ratnavelu (1995).

2. Theory

Positron impact excitation of a hydrogen from an initial state with energy E_i to a final excited state with energy E_f is only possible if the energy of the positron exceeds the threshold value. Various theories have been applied for this fundamental problem as reviewed in the papers by Walters (1988), Kernoghan et al. (1996), Bubulev and Madison (1992), and Bransden et al. (1985). Unfortunately, experimental elastic and excitation cross sections do not exist for comparison with theoretical prediction in the literature.

2.1. DWPO model

Let us consider a transition from an initial ground state i to a final excited state f. The magnitudes of the initial and final momenta of the positron, k_i and k_f, respectively, are related through energy conservation by

$$E_i + \tfrac{1}{2}k_i^2 = E_f + \tfrac{1}{2}k_f^2. \tag{2}$$

In terms of the T-matrix element, the differential cross section for scattering through the angle Θ between k_i and k_f is

$$\frac{d\sigma_{fi}(E_i)}{d\Omega} = \frac{1}{4\pi^2}\frac{k_i}{k_f}|T_{fi}(E_i)|^2, \tag{3}$$

where $T_{fi} = \langle \Phi_f | V_f | \Psi_i^+ \rangle$. Here, Ψ_i^+ is the exact total scattering wave function in the initial channel, Φ_f is the unperturbed wave function in the final channel, the interaction potential in that channel being V_f. The total cross section can be derived by integration over all directions of k_f. A simple close-coupling approximation (Bransden, 1983) that describes this reaction is obtained if just two terms are retained in the expansion of the total wave functions of the system of the incident positron and hydrogen in terms of the target eigenfunctions. In this treatment, only two open channels are coupled together and all other transitions being ignored. In this work we have applied the polarized orbital model of Drachman and Temkin (1972), that describe the interaction between the positron projectile and the neutral polarizable hydrogen atom in multipole order, to evaluate the inelastic T-matrix element. This polarization potential incorporates for the static potential fields of the hydrogen in the initial and final states, respectively. In order to obtain the inelastic cross sections in the nonrelativistic treatment we have to solve the partial wave coupled radial Schrödinger equations numerically

$$\frac{1}{2}\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_i^2\right] u_i^l(r) = \sum_{j=1}^{2}[V_{ij}(r) + V_{pol}(r)\delta_{ij}]u_j^l(r) \quad i = 1, 2. \tag{4}$$

Here $u_i^l(r)$ radial wave function describes the continuum positron. The boundary conditions for $u_i^l(r)$ can be written as

$$u_i^l(r=0) = 0, \tag{5}$$

$$u_i^l(r\to\infty) = \frac{(2l+1)i^l}{k_i}\left[k_i r j_l(k_i r)\delta_{ij} + \sqrt{\frac{k_j}{k_i}}\exp\left[i\left(k_i r - \frac{l\pi}{2}\right)\right]T_{ij}^l\right], \tag{6}$$

where T_{ij}^l denote the partial transition matrix elements, $j_l(x)$ is the spherical Bessel functions, respectively. We have assumed that the target nucleus have infinite mass and the perturbation interaction between the incident positron and the hydrogen target can be written as

$$V_f(\mathbf{r},\mathbf{x}) = \frac{1}{r} - \left|\frac{1}{\mathbf{r}-\mathbf{x}}\right|, \tag{7}$$

where $\mathbf{r}$, $\mathbf{x}$ are the position vectors of the positron and the electron with respect to the proton. The repulsive static matrix potential is $V_{ij}(r) = \langle \varphi_i(\mathbf{x})|V_f(\mathbf{r},\mathbf{x})|\varphi_j(\mathbf{x})\rangle$, where i and j labels the 1s and 2s eigenfunctions of the H-atom, respectively. In Eq. (4) $V_{pol}(r)$ is the analytical Drachman–Temkin polarization potential function (see Drachman and Temkin, 1972). Further approximation is made in the distorted wave method of dropping the term $V_{12}u_2(r)$ on the right-hand side of (4) on the ground that the influence of the second channel can be neglected in the elastic scattering channel. Using the Green's function technique the inelastic partial transition matrix elements in the framework of the DWPO model can be expressed as

$$T_{2l}^l = -\frac{2}{\sqrt{k_1 k_2}}\exp\left[i\left(\delta_1^l + \delta_2^l\right)\right]\int_0^\infty g_2^l(r)V_{21}(r)u_1^l(r)\,dr \tag{8}$$

and

$$\frac{1}{2}\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V_{22}(r) - V_{pol}(r) + k_2^2\right]g_2^1(r) = 0, \tag{9}$$

where

$$g_2^1(r\to\infty) = \sin\left(k_2 r - \frac{l\pi}{2} + \delta_2^1\right). \tag{10}$$

Here $\delta_{1,2}^l$ are the partial wave phase shifts. Thus the differential cross section for excitation of hydrogen can

be expressed in the following form:

$$\frac{d\sigma_{21}}{d\Omega} = \frac{4}{k_1^3 k_2}\left|\sum_{l=0}^{\infty}(2l+1)\exp i(\delta_1^l+\delta_2^l) \times \int_0^{\infty} g_2^l(r)V_{21}(r)u_1^l(r)\,dr\,P_1(\cos\Theta)\right|^2, \quad (11)$$

where $P_1(x)$ denote Legendre's polinomal of the first kind and order of l. The angular integrated cross section for the excitation can be written as

$$\sigma_{21} = \frac{16\pi}{k_1^3 k_2}\sum_{l=0}^{\infty}(2l+1)\left[\int_0^{\infty} g_2^l(r)V_{21}(r)u_1^l(r)\,dr\right]^2. \quad (12)$$

From the DWPO equations the excitation cross sections can be calculated solving the elastic scattering problems using the polarization approximation. These functions are used to evaluate the T-matrix for the inelastic scattering. The $u_1^l(r)$ and $g_2^l(r)$ functions were propagated using a Numerov algorithm with energy-dependent radial mesh with step-size ranging from 10^{-3} to 10^{-2} atomic units. The converged values of the T-matrix were determined by summing a set of partial waves belonging to low values (usually up to $l_{max} = 10\ldots15$). For higher values the following effective range formulas were applied

$$\bar{\delta}_i^l = -2k_i\int_0^{\infty} r^2 j_l^2(k_i r)V_{ii}(r)\,dr,$$

$$\bar{T}_{21}^l = -2\sqrt{k_1 k_2}\int_0^{\infty} r^2 j_l(k_1 r)j_l(k_2 r)V_{21}(r)\,dr, \quad (13)$$

$$T_{21}^l = \bar{T}_{21}^l \exp\left[i\bar{\delta}_1^l + \bar{\delta}_2^l\right] \quad (14)$$

for the approximate determination of the partial phases shift and the inelastic transition matrix elements.

2.2. CTMC method

In the present nonperturbative CTMC approach, Newton's classical nonrelativistic equations of motions for a three-body system are solved numerically for a statistically large number of trajectories. The three-body, three-dimensional calculation was performed as described by Abrines and Percival (1966). The initial conditions of the individual collision system were selected at relatively large internuclear separation from the collision centre in such a way that the initial binding energy of the H(1s) level was constrained. The impact parameter of the projectile with respect to the target atom and the velocity vectors and the position of the electron moving around the target nucleus in Kepler orbits were randomly selected. The differential equations of motion were integrated with respect to time as an independent variable by the standard Runge–Kutta method. To distinguish between the various final states, the exit channels are tested at large distances from the collision centre. The differential and total cross sections for a specific event were computed using the following formulas:

$$\frac{d\sigma_{exc}}{d\Omega} = \frac{2\pi b_{max}\sum_j b_j^{(exc)}}{N\Delta\Omega}, \quad (15)$$

$$\sigma_{exc} = \frac{2\pi b_{max}\sum_j b_j^{(exc)}}{N}. \quad (16)$$

The standard deviation for a cross is given by

$$\Delta\sigma_{exc} = \sigma_{exc}\left(\frac{N-N_{exc}}{NN_{exc}}\right)^{1/2}. \quad (17)$$

In Eqs. (15)–(17) N is the total number of trajectories calculated for impact parameters less than b_{max}, N_{exc} is the number of trajectories that satisfies the criteria for excitation, $b_j^{(exc)}$ is the actual impact parameter when the criteria for excitation is fulfilled and $\Delta\Omega$ is the solid angle window.

In the CTMC calculations, the energy level of the electron after the excitation is determined simply by calculating its binding energy $U = -E$. A classical principal quantum number is assigned according to

$$n_c = 1/(2U)^{1/2}. \quad (18)$$

The classical values are then quantized to a specific level n if they satisfy the relation

$$\left[(n-1)\left(n-\frac{1}{2}\right)n\right]^{1/3} \leqslant n_c \leqslant \left[n\left(n-\frac{1}{2}\right)(n+1)\right]^{1/3}. \quad (19)$$

The classical orbital angular momentum is determined by

$$l_c = [(x\dot{y}-y\dot{x})^2 + (x\dot{z}-z\dot{x})^2 + (y\dot{z}-z\dot{y})^2]^{1/2}, \quad (20)$$

where x, y, z are the Cartesian coordinates of the electron relative to the proton. Since l_c^2 is uniformly distributed for a given n level, the quantal statistical weights are reproduced by choosing bin sizes such that

$$l \leqslant \frac{n}{n_c}l_c \leqslant l+1, \quad (21)$$

where l is the quantum mechanical orbital momentum value.

3. Results and discussions

We have performed DWPO and CTMC model calculations for the excitation process induced by positron impact on hydrogen at intermediate energies above the ionization threshold. Fig. 1 shows the angular distributions of scattered positrons at 54.4, 100 and 200 eV impact energies for 1s–2s excitation. Fig. 1 also shows results of Walters (1988), Bubulev and Madison (1992) as well as Bransden et al. (1985). The curves in each energy set are found to exhibit similar angular distribution. We find that the present CTMC results are very close to the second order distorted wave Born

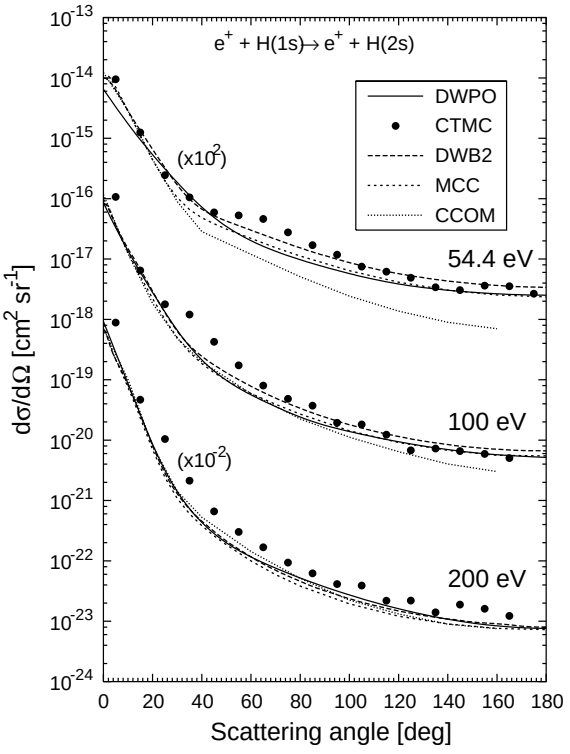

Fig. 1. Differential cross section for positron excitation of the 2s state of atomic hydrogen at 54.4, 100 and 200 eV bombardment energies. DWPO and CTMC: present calculations, DWB2: Bubulev and Madison (1992), CCOM: Bransden et al. (1985), MCC: Walters (1988). The 54.4 and 200 eV results have been multiplied by 10^2 and 10^{-2}, respectively.

(DWB2) data of Bubulev and Madison (1992) at 54.4 eV. For small scattering angles the various theoretical approximations give the same values except the data of present DWPO model. At large scattering angle the coupled channel optical model (CCOM) of Bransden et al. (1985) predicts smaller cross sections values than the other calculations. At 100 eV our data are in good agreement with the results obtained by the DWB2 approximation and the multi-state close coupling (MCC) calculation of Walters (1988). At 200 eV the CTMC data overestimate the results of previous and present quantum mechanical calculations.

Although the CTMC method directly includes the loss of particle flux from the incident channel to ionization and positronium formation channels, in general our results lie above the data of other authors. This is in contrast with our expectations but in accord with tests, carried out by Bubulev and Madison (1992) using the DWB2 approximation which indicate the inclusion of these channels raise the cross sections at large angles. The CTMC results are considerably above the CCOM method of Bransden et al., particularly at large angles and lower energies. This difference has already been noted by Bubulev and Madison (1992) and has been ascribed as an inadequate description of the continuum in the calculation of Bransden et al. (1985). For primary energies, 54.4 and 100 eV an enhancement in the distributions between the scattering angle from 40 to 100 and from 25 to 80° can be observed, respectively. To identify the origin of these peaks further test calculations within the framework of CTMC method have been performed. In the CTMC method, in principle, all interactions between the colliding partners can be taken into account exactly during the collision. On the other hand, in the classical picture it is also straightforward to switch on and off the interaction potentials between the individual particles. In this case the effects of particular interactions can be studied easily. According to our calculations the origin of the second peak is due to the ionization through double scattering, i.e. the projectile is scattered on both the target electron and target nucleus. Neglecting the scattering on the target nucleus the second peak is completely disappeared.

Table 1
Integrated 1s–2s excitation cross section in units of πa_0^2 for positron-hydrogen collision

E (eV)	DWPO	Kernoghan et al.	Walters	Bransden et al.
40	0.093	0.150	—	—
54.4	0.081	0.106	0.127	0.124
100	0.060	0.060	0.061	0.080
200	0.028	—	0.030	0.040
300	0.019	—	0.020	—

DWPO: present calculation, Kernoghan et al. (1996): 33-state approximation, Walters (1988): MCC model, Bransden et al. (1985): CCOM model.

In Table 1 our total cross section data are compared with those of Kernoghan et al. (1996), the MCC data of Walters (1988) and the CCOM data of Bransden et al. (1985). In the intermediate energy region, recently the most accurate results are probably those obtained by Kernoghan et al. (1996), using a 33-term expansion of the total wave function which included 3 positronium state and 30 hydrogen state, some of which were pseudostate. This model describes excellently all the experimental total cross sections for the positron–hydrogen collisions at low, medium and high energies. In our DWPO calculation we find that the values are almost identical with the data of Walters (1988) and Kernoghan et al. (1996) for higher energies, but underestimate the results of the latter calculation at lower energies. This discrepancies between the DWPO data and the results of the more sophisticated models is not surprising. It is due to that the simple DWPO model based on a two-state and one-centre approximation neglects the multi channel-coupling effects. For an adequate description of the positron–hydrogen scattering is especially important to take into consideration the

positronium formation channel which is a two-centre problem.

4. Conclusion

We have investigated the 1s–2s excitation cross sections for scattering of positrons from hydrogen atom at three incident energies using a distorted wave polarized orbital model and the classical trajectory Monte Carlo method. We found a reasonable agreement between our DWPO and CTMC results. Our data are also in agreement with the previous quantum mechanical calculations. Furthermore, our recent total cross sections are in good agreement with the results of Kernoghan et al. (1996) above 60 eV, where the multichannel and two-center effects seem to be unnoticeable. Further works is in progress to calculate the cross sections for higher excitation of hydrogen.

Acknowledgements

This work was supported by the Hungarian National Scientific Research Found: OTKA No. T032306, the grant "Bolyai" from the Hungarian Academy of Sciences, TéT A-19/2001, the Austrian Fonds zur Förderung der wissenschaftlichen Forschung, FWF (Austria) and EU under contract No. HPRI-CI-2001-50036.

References

Abrines, R., Percival, C., 1966. Classical theory of charge transfer and ionization of hydrogen atoms by protons. Proc. Phys. Soc. 88, 861–892.

Bransden, B.H., 1983. Atomic Collision Theory. The Benjamin Cummings Publishing Company. Durham, England.

Bransden, B.H., McCarty, I.E., Stelbovics, A.T., 1985. Coupled-channel optical model for positron-hydrogen scattering. J. Phys. B 18, 823–827.

Bubulev, V.E., Madison, D.H., 1992. Second-order distorted-wave calculation for elastic and inelastic positron-hydrogen scattering. J. Phys. B 25, 3229–3244.

Charlton, M., Humberston, J.W., 2001. Interaction of Positron Beams with Surfaces, Thin Films and Interfaces. Cambridge University Press, England.

Drachman, R.J., 1995. Why positron physics is fun. In: Dubé, L.J., Mitchell, J.B.A., McConkey, J.W., Brain, C.E. (Eds.), The physics of Electronic and Atomic Collisions, AIP Conference Proceedings. Woodbury, New York, pp. 369–383.

Drachman, R.J., Temkin, A., 1972. In: MacDanial, E.W., McDowell, M.R.C. (Eds.), Case Studies in Atomic Collisions Physics, Vol. II. North-Holland, Amsterdam, pp. 400.

Ghosh, A.S., Sil, N.C., Mandal, P., 1982. Positron–atom and positron–molecular collisions. Phys. Rep. 87, 313–406.

Jones, G.O., Charlton, M., Slevin, J., Laricchia, G., Kövér, Á., Poulsen, M.R., Nic Chormaic, S., 1993. Positron impact ionization of atomic hydrogen. J. Phys. B 26, L483–L488.

Kernoghan, A.A., Robinson, D.J.R., McAlinden, M.T., Walters, H.R.J., 1996. Positron scattering by atomic hydrogen. J. Phys. B 29, 2089–2102.

Mitroy, J., Ratnavelu, K., 1995. The positron-hydrogen system at low energies. J. Phys. B 28, 287–306.

Olson, R.E., 1981. n 1 distributions in $A^{q+}+H$ electron-capture collisions. Phys. Rev. A 24, 1726–1733.

Shultz, D.R., Reinhold, C.O., Olson, R.E., 1989. Large-angle scattering in positron-helium and positron-krypton collisions. Phys. Rev. A 40, 4947–4958.

Tõkési, K., Kövér, Á., 2000. Electron capture to the continuum at 54.4 eV positron-argon collisions. J. Phys. B 33, 3067–3077.

Walters, H.R.J., 1988. Positron scattering by atomic hydrogen at intermediate energies: 1s–1s–2s and 1s–2p transitions. J. Phys. B 21, 1893–1906.

Zhou, S., Li, H., Kaupilla, W.E., Kwan, C.K., Stein, T.S., 1997. Measurements of total and positronium formation cross section for positrons and electrons scattered by hydrogen atoms and molecules. Phys. Rev. A 55, 361–368.