DIRECT EXCITATION OF H(2P) ATOMS DUE TO COLLISIONS WITH PROTONS AND ANTIPROTONS

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Abstract: Excitation of hydrogen atoms, being initially in the excited 2p state by colliding with protons (p) and antiprotons (\overline{p}) is investigated within the impact parameter method. The calculation involves the n = 1,2,3,4 states of the target in addition to considers previously, in an incident energy range from 3 keV to 1000 keV. The effect of the electric charge of the projectile on the collision is discussed.

Keywords: Impact parameter approach, Excitation cross-sections, Protons and antiprotons, Channel-coupling effect

1. INTRODUCTION

Over the years many theoretical approaches have been formulated and implemented in detail to study ion-atom collisions. The most important is the direct solution of the time-dependent Schrödinger equation technique using atomic [1] and molecular basis function [2], close-coupling methods [3,4], and classic trajectory or "impact parameter" methods [5]. The close-coupling method has the advantage of allowing one to choose physically important configurations as the basis and study the specified process with a reasonable computational effort. The disadvantage of the method is that the computational effort increases dramatically if we want to study many-electron process in ion-atom collisions.

The proton-hydrogen atom collisions have been of considerable interest both theoretically and experimentally for a long time [3, 6]. Despite the simple nature of this three-body collision, there are still discrepancies between theory and experiment, and differences among the results of various theoretical approaches. On the computational side, there is no general approach that gives accurate inelastic cross sections at all energies. At high collision energies, Born approximation works well, but it does not predict the correct energy dependence for the inelastic cross sections at lower energies.

For electron excitation at intermediate impact energies, close-coupling [7, 8] and distorted wave [9] methods have been widely applied. The close-coupling approximation shows great success in investigating the impact excitation in atom-ion collisions [10]. In the close-coupling method, one has to choose a basis of orbitals. Such orbitals may be one-atomic-center orbitals [11], two atomic- center orbitals [12-14], or molecular orbitals [15,16]. The choice of orbitals depends on the physical process of interest, as well as on the computational effort, convergence, and so on. If one can include a complete basis set of orbitals, one might study the collision process with any kind of basis set. In practice, it is very difficult to include a complete basis set, as discussed by Kuang and Lin [17].

There are many calculations for the collisions of proton (p) and antiproton (\overline{p}) with hydrogen atom in the ground state [18-22].The collision of protons with excited hydrogen atoms is considered in a limited number of theoretical papers. Reinhold *et al.* [23] employed the symmetrized eikonal approximation to calculate cross sections for

the $n=2(3) \rightarrow n'=3, 4(4)$ transitions. Janev and Krstic [24] carried out similar calculations using the asymptotic adiabatic method and the concept of hidden crossings of adiabatic potential energy surfaces in the complex plane of the internuclear distance. Ford *et al.* [3] studied the excitation of H (2s, 2p) atoms by protons using coupled-state calculations.

Heavy projectiles, as p and \overline{p} , allow the theoretical simplification of a straight-line, constant-velocity projectile path. The application of the impact parameter method [25] to ion-atom collisions allows a simple account of the coupling with inelastic channels. The total wave function of the system is expanded in terms of the target eigenstates with time-dependent coefficients. A set of simple coupled differential equations for the elastic and inelastic collisions is obtained. The approach has been already applied in the proton (antiproton)-hydrogen collisions (e.g., Ref. [26]). Inelastic scattering of protons and antiprotons with excited hydrogen atoms was studied in Ref. [26,27]. The cross sections of the n = 3 excitations of hydrogen atoms being initially in the 2p and 2s states was considered by taking into account the coupling with all of the n = 1, 2, and 3 states. It was found that the effect of the projectile electric charge on the cross sections becomes smaller as the incident energy increases and may ultimately be neglected. This was expected, since the calculations converge to the first Born approximation. Our previous results, for H (2p) target, were not consistent with other calculations [3] in the low-energy domain. We tried to take care of this discrepancy by including transitions to higher excited states.

In the present work, we investigate the effect of the coupling to higher excited states in the interaction of protons and antiprotons with hydrogen atoms being initially in the excited 2p states. The calculation involves the n = 1, 2, 3, and 4 states of the target in an incident energy range from 3 keV to 1000 keV within the framework of the impact parameter method. We also aim to study the effect of the projectile electric charge on the collisions.

2. THEORY

The impact parameter approach [25] defines the coordinate system so that the nucleus of the target atom is located at the origin. The projectile affects the target atom by means of a perturbation interaction $V(\mathbf{r}, \mathbf{R}(t))$, which contains an implicit dependence on time t through the position vector $\mathbf{R}(t)$. The vector $\mathbf{r} = \{r, \vartheta, \varphi\}$ is the position vector of the electron of the hydrogen atom. In the impact parameter method, the relative motion of the projectile and the target nucleus is taken to be rectilinear $\mathbf{R}(t) = \mathbf{\rho} + \mathbf{v}t$, where $\mathbf{\rho}$ and \mathbf{v} are the impact parameter and velocity of the projectile, respectively. One then expands the wavefunction of the total system in terms of the eigenstates of the target atom with time dependent coefficients $a_{ij}(\rho, v; t)$ (atomic units are considered throughout):

$$\Psi_{i}(\mathbf{r}, \mathbf{R}(t)) = \sum_{j} a_{ij}(\rho, v; t) \phi_{j}(\mathbf{r}) \exp\left[-i\varepsilon_{j} t\right],$$
(1)

where *i* indicates the state occupied initially, while $\phi_j(\mathbf{r})$ and ε_j are the eigenfunctions and eigenvalues of the hydrogen atom in state *j*, respectively, and a_{ij} are

time dependent coefficients. In the general case, one has to solve a set of coupled differential equations:

$$i\frac{\partial}{\partial z}a_{if}(\rho,v;z) = \frac{1}{v}\sum_{j}a_{ij}(\rho,v,z)V_{fj}(\mathbf{R})\exp\left[-\frac{i}{v}(\varepsilon_{j}-\varepsilon_{f})z\right]$$
(2)

for the coefficients a_{ii} satisfying the initial conditions

$$a_{ij}(\rho, v; z \to -\infty) = \delta_{ij} \tag{3}$$

Here the V_{ii} are the matrix potential elements, defined by

$$V_{fj}(\mathbf{R}) = \int \phi_{f}^{*}(\mathbf{r}) V(\mathbf{r}, \mathbf{R}) \phi_{j}(\mathbf{r}) d\mathbf{r}, \qquad (4)$$

and z = vt. One then expresses the probability for the $i \to f$ transition for a fixed impact parameter ρ as $|a_{if}(\rho, v; z \to +\infty)|^2$, and finally obtains the cross section by an integration over the impact parameter, i.e.,

$$\sigma_{if}(v) = 2\pi \int_{0}^{\infty} \left| a_{if}(\rho, v; z \to +\infty) \right|^{2} \rho \, d\rho \,.$$
⁽⁵⁾

In the present work, we apply this method to calculate the n=3 excitation cross sections of hydrogen atoms initially in the 2p state by interacting with protons and antiprotons taking into account n = 1,2,3,4 states. We shall truncate the series in equation (1) by involving only a finite number of states of the target. We obtain a set of equations equal the number of states under consideration. It is convenient to separate the complex transition coefficients a_{ij} into real and imaginary parts and obtain an enlarged set of coupled-differential equations for real unknown functions. We solve the set numerically using the fourth-order Rung-Kutta method [28]. The resulting integral curves of these equations oscillate rapidly around z=0 so that the step of integration has to be decreased near this point particularly at low impact parameters.

3. RESULTS AND DISCUSSION

Figure 1 presents the result of calculation of the cross sections for excitation of the individual $2p_{0,1}$ - 3s states as well as averaged 2p-3s excitation of hydrogen atoms by protons and antiprotons. It is shown that the effect of the sign of the projectile charge for the $2p_0$ -3s transition (curves a and b) is much greater than for the $2p_1$ -3s one (curves c and d). As can be seen, for $2p_0$ -3s transition, the calculated cross sections in the proton induced reaction (curve a) are higher than those of the antiproton (curve b), the difference increase as the incident energy decrease. The ratio of the proton and antiproton cross sections reaches its maximum at incident energy of 5 keV, and then appears to be smaller at the higher incident energies.



Fig .1 The 3s cross sections for direct excitation of H (2p) atoms by protons and antiprotons. For proton (antiproton): curve a (b) for $2p_0$ -3s; curve c (d) for $2p_1$ -3s; curve q(r) for 2p-3s; curve s (t) for 2p-3s from Ref. [26] and the short solid curve, u, represents data from Ford *et al* [3].

There is an indication that for $2p_{+1}$ -3s transition, the excitation cross section in the proton induced reaction (curve c) lies above that of the antiproton (curve d), except at energy range 5<E<13 keV. Furthermore, the antiproton cross section crosses the proton at impact energies E=5keV and E=13 keV. Then the effect of the projectile charge for $2p_1$ -3s transition decreases gradually and can be ignored at energies more than 105 keV. In the case of antiproton scattering, the $2p_1$ -3s excitation cross section lies above that of $2p_0$ -3s one. An opposite situation takes place in the case of proton-induced reactions except at energies above 115 keV. We observe that, the channel coupling plays a role more important in proton scattering process than in the antiproton one except at low energies. Furthermore, considering coupling to n = 4 states gives an increament in the projectile electric change effect.



Fig. 2 The 3p cross sections for direct excitation of H (2p) atoms by protons and antiprotons. For proton (antiproton): curve a (b) for $2p_0 - 3p_0$; curve c (d) for $2p_0 - 3p_1$; curve e (f) for $2p_{-1} - 3p_{-1}$; curve g (h) for $2p_{-1} - 3p_0$; curve i (j) for $2p_{-1} - 3p_{+1}$; curve q (r) for 2p-3p; curve s (t) for 2p-3p from Ref. [26] and the short solid curve, u, represents data from Ford et al [3].

In figure 2, the curves show that the $2p_0-3p_0$ excitation cross section in the proton-induced reaction is always greater than for the antiproton. The same applies for both $2p_{-1}$ - $3p_0$ (curve g and h) and $2p_0$ - $3p_{+1}$ (curve c and d) transitions except at energies less than 6.5 keV. An opposite situation takes place for $2p_{-1}$ - $3p_{-1}$ (curve e and f) transitions and $2p_{-1}$ - $3p_{+1}$ (curves i and j) transition except at energy E<10 keV. The figures again show that, the effect of the electric charge of the projectile on $2p_0-3p_0$ cross section (curves a and b) is the greatest at low energy and intermediate energies. Even the electric charge of the projectile still effects on the individual $2p_0-3p_{+1}$ cross section at higher energies, the contribution to the total 2p-3p cross section can be ignored. As can be seen the proton cross section crosses that of the antiproton at energies E=12 keV and E=70 keV for $2p_{-1}$ - $3p_{+1}$ transition and at energy E=6.5keV for $2p_0-3p_{+1}$ transition. At low and intermediate energies, it is found that the $2p_0-3p_0$ excitation (curve a) yields highest values of cross sections than the others. It can be noted that, all curves have the same behavior except (curves i and j) they have more than one critical point. We note also that, the $2p_{-1}$ - $3p_0$ excitation cross section (curves g and h) falls down rapidly as the incident energy increases. However, in all over the present work the total 3p excitation cross section for protons is always greater than that for antiprotons. On the other hand, neglecting the coupling to n=4 states (curves s and t) changes the situation at energies less than 5.8 keV.



Fig. 3 The 3d cross sections for direct excitation of H (2p) atoms by protons and antiprotons. For proton (antiproton): curve a (b) for $2p_{-1}-3d_{-2}$; curve c (d) for $2p_{-1}-3d_{-1}$; curve e (f) for $2p_{-1}-3d_{0}$; curve g (h) for $2p_{-1}-3d_{+2}$; curve i(j) for $2p_{-1}-3d_{+1}$; curve k (l) for $2p_{0}-3d_{0}$; curve m (n) for $2p_{0}-3d_{+1}$; curve o (p) for $2p_{0}-3d_{+2}$; curve q (r) for $2p-3d_{0}$; curve s (t) for $2p-3d_{0}$ from Ref. [26] and the short solid curve, u, represents data from Ford et al [3].

The curves in figure 3 illustrate the effect of the sign of the projectile charge on the 3d excitation cross sections. It is seen that, the effect of the electric charge of the projectile on the individual $2p_{-1}$ - $3d_{-2}$ cross section is the smallest, but the effect on the $2p_{-1}$ - $3d_0$ cross section is the greatest at intermediate energies. The intermediate energy behavior of the $2p_{-1}$ - $3d_0$ is different from the others. the $2p_{-1}$ - $3d_{1,2}$ cross sections falls down more rapidly than the $2p_{-1}$ - $3d_{-2,-1,0}$ as the energy increases, hence their contributions to the total cross section may be ignored. The effect of the sing of the projectile charge in the case of $2p_{0}$ - $3d_{+1}$ disappears eariliar than in the cases of $2p_{0}$ - $3d_{0,+2}$. This also achieved for $2p_{-1}$ - $3d_{-2}$ transition. In contrast, the effect of the projectile charge for $2p_{-1}$ - $3d_{+2}$ transition at low energy have values higher than this effect at intermediate energy. The same situation takes place in the case of $2p_{-1}$ - $3d_{+2}$ transition. Furthermore, for $2p_{-1}$ - $3d_{-1}$ transitions the effect of the projectile charge reaches its

maximum at low energy. A similar situation applies for $2p_{-1}$ -3d₀ but at intermediate energy. It can be noted that curves (curves k and o) have two critical points at different places; the same applies for (curve f) but are shifted at higher energies. As can be seen, the calculated cross sections in (curve 1) for antiproton induced reaction have the greatest values than the others. Furthermore, the antiproton cross section have the same value as that of the proton at impact energies E=22keV for 2p₋₁-3d₋₁ transition, at E=4keV for 2p₋₁-3d₊₁ transition and for 2p₀-3d₀ transitions at two impact energies E=3keV and E=18 keV. It is observed that, the $2p_{-1}$ -3d $_{+1}$ (curve j) cross section for the antiproton interaction falls more rapidly than the others as the incident energy increases. The $2p_0-3d_{+2,+1}$ and $2p_{-1}-3d_{+2,-2}$ excitation cross sections in the antiproton induced reactions are greater than those of the protons. The same applies for both $2p_0-3d_0$ state at energies below 18 keV, and for the $2p_{-1}$ -3d_1 state at energies below 23 keV. An opposite situation occurs in the cases of $2p_{-1}$ -3d₀ and applies also for $2p_{-1}$ -3d₊₁ transitions except at energy less than 4 keV. Even the difference between the proton and antiproton scattering cross sections in the $2p_{-1}$ - $3d_{+1}$ and $2p_0$ - $3d_{+2}$ cases does not fade out at high energies, they do not affect on the total cross sections. Therefore, the total effect on the 2p-3d cross section is reduced due to the cancellation between these contributions. It is seen that, the excitation cross sections for proton induced reaction (curve q) have values less than those of antiproton (curve r) except at energies less than 32keV. The effect of the projectile charge can be ignored at energies higher than 100keV. For 2p-3d transitions we clearly observed that our calculated cross sections for proton and antiproton induced reactions have values less than that in Ref [26], which does not consider the effect of the n=4 channel. Furthermore, for the proton induced reactions the difference between our results and the results in Ref [26] at low energy appears to be smaller than this difference at intermediate energy. An opposite situation takes place in the case of the antiproton. Comparing our results for 2p-3d transition with results in Ref [26], we can observe that, at low energy, the effect of the projectile charge in our results is less than that effect in Ref [26]. The effect of the inclusion of n=4 states on the proton-induced reaction is smaller than the effect of the antiproton, and reduces the cross sections of both of them. Furthermore, the present calculations reduce the effect of the projectile electric charge, and shift the crossing point of the proton and antiproton scattering cross sections at higher energy.

In general, the effect of the projectile charge on the 3d transition is greater than this effect on the 3p transition. Furthermore, the same effect on the 3p transition is greater than that effect on the 3s one. At high impact energies, the calculated cross sections for excitation of hydrogen by protons and antiprotons are almost equal. This is expected from the first Born approximation, which scales as the square of the projectile charge, and which is usually assumed to be valid at asymptotically high impact velocities. The comparison between the present results and previous results of Tantawi [26] and Ford et al [3] that, including the n=4 states (curves q and r) reduces the cross sections and improves the situation compared with the results of Ref [26].

4. CONCLUSION

Coupled-state calculations based on a single-center expansion in atomic orbitals have been carried out for protons and antiprotons colliding with H(2p), in the impact energy range 3–1000 KeV. Cross-sections for excitation to the level n = 3 are presented. The collisions are described in terms of a set of coupled-differential equations, which allows an account of the coupling between different channels. The n = 1,2,3,4 states are taking into account. The importance of the sign of the projectile charge is demonstrated, which varied from one channel to another. We observed that the effect of the sign of the projectile charge on 3d excitation cross-sections is greater than this effect on 3s and 3p ones. However, the effect becomes smaller as the incident energy increases and may be neglected as expected, where the calculations converge to the first Born approximation. Comparing our results with previous works which considered only n = 1,2,3 states; It is shown that, including the n=4 states reduces the cross sections and improves the results.

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