Effect of couplings of the n=2 states on excitation processes by protons and anti-protons impact on H(2s) atoms

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Effect of couplings of the n = 2 states on the n = 3 excitation cross-sections in scattering of protons and antiprotons by hydrogen atoms being initially in the 2s state has been investigated by means of the impact parameter approximation. The calculations take into account the n = 1, 2, 3, and 4 states of the target and cover energy range from 3 - 2500 keV. The study of the influence of the electric charge of the projectile is a target of this investigation. Therefore, the exchange effects in the case of proton-induced reactions are ignored. The results of calculations for protons are in reasonable agreement with a previous work.

[Keywords: Coupling, Proton scattering, Anti-proton scattering, Impact parameter approximation]

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1 Introduction

Collision processes involving excited atomic states have become subject of considerable interest in relation to injection of energetic neutral beams into high-density fusion plasma\(^1,2\). Collision processes of protons and antiprotons on hydrogen atoms are one of the most important and the simplest cases of atomic collision research. The comparison of the two processes will give detailed information on the fundamental mechanism of the few-particle dynamic processes. Hydrogen atoms are of fundamental interest for testing theoretical methods and models in ion-atom collisions, and have been of considerable interest, both theoretically and experimentally for a long time\(^3,4\). Approximations are needed only to describe dynamical aspects of the problem. Besides the traditional Born approximation method in high energy collisions for excitation process by proton impact, there is also the close-coupling method. The close-coupling approximation shows great success in investigating the impact excitation in atom-ion collisions\(^3,4\). In the close-coupling method, we have to choose a basis of orbitals. Such orbitals could be one-atomic-center orbitals\(^5\), two-atomic-center orbitals\(^6-8\) or molecular orbitals\(^9,10\). The choice of orbitals depends on the physical process as well as the computational effort, convergence and so on. If a complete basis set of orbitals could be included, the collision process could be studied with any kind of basis set. In practice, it is very difficult to include a complete basis set, as discussed by Kuang and Lin\(^11\).

The impact parameter method\(^12\), assumes a classical motion of the projectile and applies an expansion of the total wave-function in terms of the various states of the target atom, with time dependent coefficients. It has been widely used to study the ion-atom collision particularly ground-state atom\(^13,14\). In contrast, there are few theoretical works concerning the inelastic collisions with excited hydrogen atoms. Ionization of hydrogen atoms in the 2S state by various multiply charged ions is studied by Sahoo et al.\(^15\). Reinhold et al.\(^16\) used the symmetrized eikonal approximation to calculate cross-sections for the \(n = 2(3) \rightarrow n' = 3, 4 (4)\) transitions. Janev and Krstic\(^17\) used the asymptotic adiabatic method and the concept of hidden crossings of adiabatic potential energy surfaces in the complex plane of internuclear distance to carry similar calculations. Ford et al.\(^18\) reported cross-sections for the individual 2s and 2p initial states as well as the cross-sections averaged over all \(n = 2\) initial state sub-levels for the \(p+H (n = 2)\) collision system. They used a single-centered expansion method based on the ability of the target-centered basis to present projectile centered orbitals for a sufficient range of projectile-target separations. The method represents the wave function of the system in the interaction picture. The transition amplitudes are calculated by a time-development operator where the basis states are the matrix eigenvectors of the target Hamiltonian and are obtained by diagonalizing this Hamiltonian on an underlying basis. These states yield an accurate
representation of the low-lying bound states and also produce pseudo-states, which provide a discrete representation of the ionization continuum. Two-state model applicable to top-of-barrier processes in ion-atom collisions at low velocity has been investigated by Tantawi et al.\textsuperscript{19}. An expression for the Massey parameter of the transition $n \rightarrow n+1$ was derived and used it to compute ionization, capture, and excitation from states of high principal quantum number in proton-hydrogen atom collisions. Recently, an impact parameter approach, based on one-center expansion in atomic orbitals, is applied to study impact excitations of protons and antiprotons on H(2s, 2p) collisions\textsuperscript{20-23}.

In the present work, we apply the impact parameter method to investigate the effect of couplings of the $n=2$ states on the $n=3$ excitation cross-sections in excitation processes by protons and antiprotons impact on H(2s) atoms. We also aim to investigate the effect of the electric charge of the projectile on the collision. For this purpose, the interaction of protons is compared to that of antiprotons.

\section{2 Formulation of the Problem}

We consider the collision of protons and antiprotons with hydrogen atoms in the impact parameter representation. Because of the large mass of the projectile we suppose that it is moving with constant velocity $\nu$ parallel to the $Z$ axis of a rectangular Cartesian frame of reference. The nucleus of the target hydrogen atom is located at the origin. The projectile affects the target atom by means of an interaction $V(r, R(t))$, which implicitly depends on time $t$ through the position vector $R(t)=\rho+\nu t$, where $\rho$ is the impact parameter of the projectile. Since we aim to compare the interaction of proton and antiproton with hydrogen atoms, it is appropriate to use an expansion of atomic orbitals around the target only. One then expands the wavefunction of the total system in terms of the eigenstates of the target atom with time dependent coefficients $a_{if}(\rho, \nu; t)$ (atomic units are considered throughout):

$$\Psi_i(r, R(t)) = \sum_{f} a_{if}(\rho, \nu; t) \phi_f(r) \exp\left[-i\epsilon_f t\right] \quad \ldots(1)$$

where $i$ indicates the state occupied initially, while $\phi_f(r)$ and $\epsilon_f$ are the eigenfunctions and eigenvalues of the hydrogen atom in state $j$, respectively. The vector $r \equiv \{r, \theta, \phi\}$ is the position vector of the electron of the hydrogen atom. In the general case, one has to solve a set of coupled differential equations:

$$i \frac{\partial}{\partial z} a_{if}(\rho, \nu; z) = \frac{1}{\nu} \sum_{j} a_{if}(\rho, \nu, z)$$

$$\sum_{j} V_{ij}(R) \exp \left[-\frac{i}{\nu} (\epsilon_j - \epsilon_f) z\right] \quad \ldots(2)$$

for the transition amplitudes satisfying the initial conditions

$$a_{if}(\rho, \nu; z \rightarrow -\infty) = \delta_{if} \quad \ldots(3)$$

with the matrix potential elements,

$$V_{ij}(R) = \int \phi_i^*(r) V(r, R) \phi_j(r) \, dr \quad \ldots(4)$$

One then expresses the probability for the $i \rightarrow f$ transition for a fixed impact parameter $\rho$ as

$$\sigma_{if}(\nu) = \int \frac{2 \pi}{\nu} \left| a_{if}(\rho, \nu; z \rightarrow +\infty) \right|^2 \rho \, d\rho \quad \ldots(5)$$

Clearly, in a coupled-channel expansion of the total wave function in terms of the various states of the target atom there is coupling between all the states of the target and not just between the initial and particular excited state being investigated. Any modification of the full expansion is therefore an additional approximation, which should be clearly specified.

In the present work, we apply this method to calculate the $n=3$ excitation cross-sections of hydrogen atoms being initially in the 2s states by interacting with protons and antiprotons. In practical calculations it is better to pull out the oscillating factor $\exp[-i(\epsilon_f-\epsilon_i)z/\nu]$ from the coupled-differential Eq.(2), using a suitable substitution. The new form of the system of equations is quicker to solve and enhances the accuracy of calculations. The series in Eq. (1) is truncated by involving only a finite number of states of the target, the $n = 1, 2, 3$ and 4 states of H-atom. It is convenient to separate the complex transition coefficients $a_{if}$ into real and imaginary parts and obtain an enlarged set of coupled-differential equations for real unknown functions. The resulting integral curves of these equations oscillate rapidly
around $z=0$. Therefore, the step of integration has to be decreased near this point particularly at low impact parameters. We solve the set of coupled-differential equations numerically using the Bulirsch-Stoer method\textsuperscript{24}, which automatically adjusts the smallest step size of integration and save the time of calculations. It is found that, the integration over the impact parameter, Eq. (5) converges slowly as the energy of the incident projectile increases.

In the next section, we present our results and compare the interaction of protons with that of antiprotons. Finally we compare with a previous calculations by Ford et al.\textsuperscript{18} for the proton-induced reactions. They reported cross-sections in the higher energy region, $15 \leq E \leq 300$ keV, the method provides a discrete representation of the ionization continuum which is not included in the present work. So far, there are no impact excitation measurements for proton, (antiproton) on H (2s) collisions to compare with.

Cross-sections for H (2s) excitation to the 3s state are plotted in Fig. 1 for protons (curves a, c, e, g, i, and m) and antiprotons (curves b, d, f, h, j, and n). The curves show that the low and intermediate energy behaviour of the cross-sections in the case of proton-induced reaction is different from the antiproton ones. At low energy, cross-sections due to the interaction with protons are above those due to the interaction with protons. The effect of neglecting the 2s-2s coupling only, corresponding to distortion of the atomic wave function in the initial state due to the presence of the projectiles (curves c and d) is the smallest. In the case of proton-induced reactions, neglecting the 2s-2s coupling (curve c) gives a minimum above that provides couplings to all of the $n = 1, 2, 3,$ and 4 states (curve a). On the other hand, calculations neglect couplings to the 2p state and the 2s-2s coupling (curve e); couplings of the n=2 states (curve g); the 2s-2s and 2s-2p couplings (curve i); and the 2s-2p couplings (curve m) enhance the effect of the projectile electric charge and hold large minima with different factors at higher energies. In the case of antiproton scattering, the effect of the channel coupling is much smaller than in the protons. The results of calculations neglect couplings to the 2p state and the 2s-2s coupling (curve f) and the 2s-2p couplings (curve n) are close; curve f represents both of them. Also, curve h represents both of the calculations neglect the 2s-2s, 2s-2p couplings (curve j) and couplings of the n=2 states (curve h).

Figure 2 displays the 3p-excitation cross-sections of H(2s) by protons and antiprotons. The effect of neglecting the 2s-2s coupling on $^3p_1$ state, for protons, is negligible. For antiproton reactions, calculations neglect both the 2s-2s and 2s-2p couplings is close to that neglects couplings of the n=2 states, and are represented by curve h. The effect of the projectile electric charge, particularly for the calculations takes into account the coupling of all the states (curves a and b) and that neglects the 2s-2s coupling (curves c and d). It is much greater than in the case of the 3s state. The same applies for the channel coupling effect on the antiproton scattering processes. The approximations neglect any of the couplings of the n=2 states and increase the minima with different order, but without shift. In case of antiproton reactions, the Fig. 2 shows that the $^3p_1$ cross-section due to allowing couplings to all states (curve b) and neglects the 2s-2s coupling (curve d), are above the others and have different behaviour at low energies. In case of the $^3p_0$ state, the curves b and d are always below the others. The effects of both of the projectile charge and the channel coupling in the case of the $^3p_0$
From Figs 1 and 2, it is seen that the 3s and 3p excitation cross-sections for antiprotons cross those for protons at low energies. This may be attributed to the so-called binding/antibinding effect in the close collisions that dominate excitation at low velocities. However, the cross-sections for antiproton impact do not show the typical peaks of proton. This may be understood if we take into account the fact that no electron capture is feasible by antiprotons and therefore there is no depletion of probability due to exchange for the lower energies.

The curves in Fig. 3 show that the 3d cross-sections for protons and antiprotons are similar in shape, which is different from the 3s and 3p cross-sections. In case of proton-induced reactions, neglecting any/all couplings of n = 2 states hold an increment, in contrast to Figs 1 and 2, of the total 3d cross-sections. The situation is changed for antiprotons. The projectile electric charge and channel coupling effects in the $^3d_0$ state is stronger than the $^3d_1$ and $^3d_2$ states.

In the proton scattering processes, calculations neglect the 2s-2s coupling are close to those allow coupling to all states under consideration (curve a), except for $^3d_0$ state. The cross-sections do not allow couplings of n=2 states and that neglects both of the 2s-2s and 2s-2p couplings are close, and antiprotons in the case of $^3d_0$ and 3d excitations (curve h), and for protons in the case of $^3d_0$ excitation (curves g). The same happens for the $^3d_0$ and $^3d_0$ states, in addition to the calculations neglect the 2s-2p couplings for proton and antiproton respectively. Moreover, the results for 3d excitation represented by curves e, i, and m are close.

For antiproton scattering, the low-energy behaviour of the $^3d_0$ cross-section due to allowing couplings to all states (curve b) and that neglects the 2s-2s coupling (curve d) is different from the others. At low energies, the contribution of the $^3d_2$ state to the total 3d cross-section is less than the others particularly for the proton-induced reaction. An opposite situation takes place at high energies. However, adding the contribution of the $^3d_2$, $^3d_1$, and $^3d_0$ states reduces the effect of the projectile charge on the total 3d cross-section.

Finally, the cross-sections of the 3d excitation do not show the peaks appear in the 3s and 3p states, for protons. This may be interpreted by the weak influence of the electron capture on the 3d excitation, which is less important at energies above 30 keV as
shown by Olson. Moreover, neglecting couplings of the \( n = 2 \) states yield a very good agreement with the calculations by Ford et al., particularly in the cases of the 3s and 3p cross-sections.

In general, the channel coupling effect on the protons and antiprotons scattering processes is different from one channel to another. The projectile electric charge plays a more important role than the channel coupling. However, both of these effects are small at high energies. This insensitivity is expected as the calculations converge to 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 energies. The same conclusion is made by Knudsen et al., for ionization of hydrogen atoms by protons and antiprotons, and by Watanabe et al., for excitation of \( \text{H}(1s) \) by proton and antiproton using direct solution for Schrödinger equation with the split-operator method and a generalized pseudo-spectral in energy representation.

3 Conclusion
An impact parameter approach, based on a one-center expansion in atomic orbitals, is applied on the impact excitation of hydrogen atoms, being initially in the 2s states, impact by protons and antiprotons. We have presented calculations of \( n = 3 \) excitation cross-sections at energies ranging from 3 to 2500 keV. We have found that the effect of couplings of the \( n = 2 \) states in the proton-induced reactions is stronger than in the antiproton scattering. However, the 2s-2p coupling has the greatest effect. By comparing the cross-sections calculated for protons and antiprotons, it seems that by neglecting the couplings of \( n = 2 \)
states enhance the influence of the electron capture which seems to be very weak in the case of the 3d excitation. As the energy increases, the effect of both the electric charge of the projectile and the channel-coupling decrease, as predicted by the first Born approximation. The agreement with a previous calculation\textsuperscript{17} is satisfactory.

References