Scattering of protons and antiprotons by hydrogen-like atoms

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The impact parameter method is applied to the excitation of hydrogen-like atoms in the 2s-state. Cross-sections for the n=3 excitation of H(2s) atoms and H'(2s), Li'(2s) ions, by colliding with protons (p) and antiprotons (bar p) are evaluated for incident energies, ranging from 1.5 KeV to 2500 KeV. The results of calculations for hydrogen atoms are compared with a previous work.

1 Introduction

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. Approximations are needed only to describe dynamical aspects of the problem. For one-electron systems, the close-coupling approximation shows great success in investigating the impact excitation in atom–ion collisions. In the close-coupling method, a basis of orbitals have to be chosen. Such orbitals could be one-atomic-center orbitals, two-atomic-center orbitals or molecular orbitals. The choice of orbitals depends on the physical process we are interested in, 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 & Lin.

Collisions of protons with atomic hydrogen have been extensively studied, experimentally and theoretically. This work has now acquired a new aspect due to studies of the difference in cross-sections for proton and antiproton interactions with matter [see, e.g. Ref. (10) and references therein]. The application of the impact parameter method to ion-atom collisions allows a simple account of the coupling with inelastic channels. The method 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. A set of simple-coupled differential equations for the elastic and inelastic collisions are obtained. This method has been widely used to study the ion-atom collision. Skiner was, probably, the first to apply this approach to study the collisions of protons with ground-state hydrogen atoms. In contrast, there are a few theoretical works concerning the inelastic collisions with excited hydrogen atoms. Reinhold et al. used the symmetrized eikonal approximation, to calculate cross-sections for the n=2(3)→n'=3,4(4) transitions. Janev & Krstic used the asymptotic adiabatic method and the concept of hidden crossings of adiabatic potential energy surfaces in the complex plane of inter-nuclear distance, to carry similar calculations. Ford et al. reported coupled-state calculations for the p+H(n=2) collision. A time-dependent operator, connecting the wave-function at different time in the interaction picture calculated the transition amplitudes. The basis states are matrix eigenvectors of the target Hamiltonian and are obtained by diagonalizing this Hamiltonian on an underlying basis of specific form. Ionization of hydrogen atom in 2s-state by various multiply-charged ions is studied by Sahoo et al. A two-state model applicable to top-of-barrier processes in ion-atom collisions at low velocity is investigated in Ref. 16. An expression for the Massey parameter of the transition n→n+1 was derived and used to compute ionization, capture, and excitation from states of high principal quantum number in proton-hydrogen atom collisions.

The excitation process of proton on H'(1s) ion has been a subject of interest for a long time, but there is no much theoretical work on it. Kimura & Thorson, Winter et al. applied close-coupling calculations, based on molecular basis to the n=2
excitation of $H'(1s)$ ions, by protons. Grozdanov & Solov'ev performed calculations within the framework of the asymptotic theory of non-adiabatic transitions. Krsic & Janev employed the method in Ref. 13, to study the collisional dynamics in the system $P+He^+(n), n \leq 6$. Errea & Sanchez applied a one-centre atomic expansion with regularization of the coulomb potential interactions, using projection technique, to study the $P+He^+(2s)$ system. Tong et al. studied the problem, by solving the time-depending Schrödinger equation with the split-operator method and a generalized pseudospectral method in the energy representation, based on the impact parameter method. So far, to the best of our knowledge, there are no impact excitation investigations for the $p(\bar{p})+He^+(2s)$ and $p(\bar{p})+Li^+(2s)$ collisions.

Recently, the authors have applied an impact parameter approach, based on a one-centre expansion in atomic orbitals, to study impact excitation of protons and antiprotons on $H(1s,2p)$ collisions. Their calculated cross-sections are in reasonable agreement with previous theoretical and experimental investigations.

The present work is devoted to provide theoretical data for inelastic scattering cross-sections of protons and antiprotons by $H$ atoms and $He^+, Li^+$ ions, being initially, in the excited 2s states, within the framework of the impact parameter method. Also, it is aimed to investigate the effect of the electric charge of the projectile on the collisions under consideration. For this purpose, the interaction of the protons was compared with the target ions to that of the antiprotons. The authors shall, therefore, study only direct excitations of the target electrons, and shall not consider the exchange effect in the proton induced-reactions. The inclusion of exchange effect will confuse the comparison with the antiproton reactions. Many articles (e. g. Refs. 4,5,24) are devoted to the study of the exchange effect in the scattering of protons by hydrogen atoms. They agreed on the importance of this effect at low and intermediate energies. However, the exchange effect is less important energies above 30 KeV as shown by Olson.  

2 Formulation of Problem

Consider the case when the nucleus of the target atom is located at the origin of coordinates. The projectile affects the target atom by means of a perturbation interaction $V(r,R(t))$, which implicitly depends on time $t$, through the position vector $R(t)$. In the impact parameter method, the relative motion of the projectile and the target nucleus is taken to be rectilinear $R(t)=\rho+u t$, where $\rho$ and $u$ are the impact parameter and velocity of the projectile, respectively. In cases where a collision causes predominantly direct excitation of the target electrons, it is appropriate to use an expansion of atomic orbitals around the target only. One then expands the wave-function of the total system in terms of the eigenstates of the target:

$$\Psi_r(r,R(t))=\sum_j a_j(\rho,v,z)\phi_j(r) \exp\left[-i\epsilon_j t \right]$$  \hspace{2cm} (1)

where $a_j(\rho,v,z)$ are time-dependent coefficients. Here, $i$ indicates the state occupied initially, while $\phi_j(r)$ and $\epsilon_j$ are the eigenfunctions and eigenvalues of the hydrogen atom in state $j$, respectively. The vector $r=\{r,\rho,\phi\}$ is the position vector of the electron of the hydrogen atom. In the general case, one has to solve an infinite set of coupled differential equations:

$$\frac{1}{v} \frac{\partial}{\partial z} a_j(\rho,v,z) = \frac{1}{v}$$

$$\sum_j a_j(\rho,v,z) V_{ij}(R) \exp\left[-i(\epsilon_i - \epsilon_j) z \right]$$

for the transition amplitudes satisfying the initial conditions:

$$a_j(\rho,v,z=-\infty) = \delta_{ij}$$

with the matrix potential elements:

$$V_{ij}(R)=\left|\phi_i(r) \psi_j(r) \right| dr$$

and $z=ut$. One then expresses the probability for the $i\rightarrow j$ transition with an impact parameter $\rho$ as

$$\sigma_{ij}(\rho) = \left| \frac{\rho}{v} \int a_j(\rho,v,z\rightarrow +\infty) a_j(\rho,v,z\rightarrow -\infty) \right|^2$$

In the present work, the series in Eq. (1) shall be truncated, by involving only the $n=1,2,3$ states of the targets, to calculate the cross-sections for
excitation of each of the $\text{H}(2s)$, $\text{He}^+(2s)$, and $\text{Li}^+(2s)$ to the $n=3$ state by interacting with protons and antiprotons. A set consisting of number of equations are obtained equal to the number of states taken into account. The complex transition coefficients $a_i$ are separated into real and imaginary parts to obtain an enlarged set of coupled-differential equations for real, unknown functions. The set is solved numerically, using the fourth-order Rung-Kutta method. 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. The integration over the impact parameter (5) converges slowly, as the charge of the target nucleus decreases and as the energy of the incident projectile increases. In what follows, results are discussed by comparing them with the calculations by Ford et al.\textsuperscript{14} for the $p+\text{H}(2s)$ collision system.

Fig. 1 shows the results of calculation of $3s$ and $3p$ excitation cross-sections, for the processes under consideration. It is seen from the figure that, the effect of the sign of the projectile charge plays a role in the case of $p(\bar{p})+\text{H}(2s)$, different from $p(\bar{p})+\text{He}^+(2s)$ and $p(\bar{p})+\text{Li}^+(2s)$ collisions. The effect increases as the charge of the target nucleus increases, particularly, at low energies. The curves show that, the low-energy dependence behavior of the cross-sections in the case of the $\text{H}(2s)$ target is different from the other targets. In the case of scattering by hydrogen atoms, the sign of the projectile charge affects the cases of the excitation $3p_0$ and $3p_\pi$, in the opposite direction. Therefore, the effect of the projectile electric charge on the total $3p$ cross-section is reduced by cancellation between these contributions. In the interactions with the $\text{He}^+(2s)$ and $\text{Li}^+(2s)$ ions, it is observed that, the effect of the sign of the projectile charge on the $3p_\pi$ cross-section is stronger than on the $3p_0$ and $3s$ ones. The $3p_0$ and $3s$ cross-sections of the antiproton-induced reactions are larger than for the proton-induced reactions. The same situation takes place

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Cross-sections for the $3s$ and $3p$ excitations of $\text{H}(2s)$ atoms and $\text{He}^+(2s)$, $\text{Li}^+(2s)$ ions by protons ($p$) and antiprotons($\bar{p}$). Curves a(b) are for $p(\bar{p})+\text{H}$ collision; curves c(d), $p(\bar{p})+\text{He}^+$; and curves e(f), for $p(\bar{p})+\text{Li}^+$. The short curves with triangles represent data from Ref. 14.}
\end{figure}
for the $3p_h$ cross-section at energies, less than about 50 KeV, in the case of scattering by He$^+$(2s) and 150 KeV for the Li$^+$(2s) target. The contribution of the $3p_i$ state to the total $3p$ is greater than the $3p_h$ one. The total effect of the projectile charge on the excitation of $3p$ states is reduced at high energies due to the opposite sense effect on both $3p_i$ and $3p_h$ states. However, The effect of the sign of the projectile charge on $3s$ state is approximately greater than on $3p$, in the case of H(2s), but an opposite situation takes place in other cases.

In Fig. 2, the curves show that, the high-energy dependence behavior of $3p_h$ cross-section, in the case of H(2s) target, is different from He$^+$(2s) and Li$^+$(2s) targets. The $3p_h$ cross-section in antiproton scattering processes lies above that of the proton. The same applies for $3p_h$ at both the low and high-energy domains but with different orders of magnitude. An opposite situation takes place in the $3p_i$ state at energies larger than about 8 KeV for H(2s), 7 KeV for He$^+$(2s), and at energies larger than about 55 KeV in the case of Li$^+$(2s). However, the contribution of $3p_i$ state to the $3d$ cross-section can be approximately neglected at high energies, and has a small effect at intermediate energies in the case of scattering by hydrogen atoms. On the other hand, the contribution of $3p_h$ state to the $3d$ cross-section is considerably greater than $3p_i$ and $3p_h$ states at low energies except for $p$+Li$^+$(2s) collision.

Figs 1 and 2 also illustrate that, at low energies, the difference between the cross-sections of the processes $p$($\bar{p}$)+H(2s) and $p$($\bar{p}$)+He$^+$(2s) is smaller than that between $p$($\bar{p}$)+He$^+$(2s) and $p$($\bar{p}$)+Li$^{2+}$(2s) collisions, but the situation changes at high energies. The effect of the projectile charge increases as the charge of the target nucleus increases, particularly, at low energies. The present calculations are in good agreement with the calculations by Ford et al.34.

It is finally noted that, the low-energy dependence behavior of cross-sections in the proton-
induced reactions is different from the antiproton ones. Reduction of the effect of the sign of the projectile charge on 3p and 3d states by cancellation due to adding the degenerate sub-level cross-sections in the case of H(2s) is greater than in other cases. This effect can be neglected at high energies, particularly in the case of scattering of hydrogen atoms where the calculations converge to the first Born approximation which is independent on the sign of the projectile charge.

3 Conclusion

Coupled-state calculations based on a single-centre expansion in atomic orbitals have been carried out for protons and antiprotons colliding with H(2s), He(2s), and Li(2s), in the impact energy range 1.5-2500 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 allow an account of the coupling between different channels. The n=1,2,3 states are taken into account. The importance of the sign of the projectile charge is demonstrated, which varied from one channel to another. The effect of the charge of the target nucleus in proton-induced reactions is found to be considerably greater than the reactions of antiprotons. On the other hand, the difference between the cross-sections of the processes $p(\bar p)+H(2s)$ and $p(\bar p)+He^+(2s)$ is smaller than that between $p(\bar p)+He^+(2s)$ and $p(\bar p)+Li^{+7}(2s)$, particularly, at low energies. These results are in reasonably good agreement with that obtained by Ford et al. for the $p+H(2s)$ collision system. Finally, it is found that, the greater the charge of the target nucleus, the greater the effect of the sign of the projectile charge on the excitation cross-sections. However, the effect becomes smaller as the incident energy increases and may be neglected in the case of excitation of the hydrogen atom earlier than in other reactions.

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References