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Scattering of protons and antiprotons by hydrogen atoms

Reda S. Tantawi and A.S.Sabbah

Department of Mathematics, Faculty of Science, Zagazig University, Zagazig, Egypt

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The two-, four-, five- and fourteen-state approximations of the impact parameter method have been applied to the excitation of hydrogen atoms by proton (p) and antiproton ($\overline{p}$) impact. The effect of both channel and back couplings on the $2s$ and $2p$ excitations are investigated. The total cross sections are calculated for incident energies ranging from 1 to 2500 keV. It is found that the effect of both channel and back couplings on the antiproton-induced reactions is greater than on that induced by protons. We compare the results with those of other theoretical and experimental works.

Keywords: impact parameter method, excitation cross sections, back coupling, sign of the projectile charge

PACC: 3410, 3450H

1. Introduction

Collisions of protons with atomic hydrogen have been extensively studied experimentally and theoretically. Because of its relative simplicity, this system has often been used as a testing ground for various models and approximations in the theory of heavy particle collisions. This work has now acquired a new aspect due to studies of the difference in cross sections for proton and antiproton interactions with matter. The application of the impact parameter method[1] to ion–atom collisions allows a simple account of the coupling with inelastic channels. This method assumes the classical motion of the projectile and applies an expansion of the total wavefunction 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 ion–atom collisions. Skinner[2] was probably the first to apply this approach to study the collisions of protons with ground-state hydrogen atoms. The approach has been already applied[3,4] to the interaction of protons and antiprotons with hydrogen atoms in the $1s$ and $2s$ states.

In the present work we have performed some routine calculations of cross sections for proton and antiproton hydrogen atom scatterings within the framework of the impact parameter method. We consider the two-, four-, five- and fourteen-state approximations. Our aim is to investigate the effect of back coupling, as well as that of the channel coupling, on both types of collision. Our main purpose is to compare the interaction of protons with that of antiprotons. We study only the direct excitations of the target electrons, and neglect the exchange effect in the proton-induced reactions, because the inclusion of the exchange effect will confuse the comparison. Many authors (see Refs.[5–8]) have considered the exchange effect in their calculations and have reported on the importance of this effect at low and intermediate energies.

2. Formulation of the problem

We consider the case when the target nucleus of the target atom is located at the origin of the coordinate system. The projectile affects the target atom by means of a perturbation interaction $V(\boldsymbol{r}, \boldsymbol{R}(t))$, which contains an implicit dependence on time t through its position vector $\boldsymbol{R}(t)$. In the impact parameter method, the relative motion of the projectile and the target nucleus is taken to be rectilinear $\boldsymbol{R}(t) = \boldsymbol{\rho} + \boldsymbol{\nu}t$, where $\boldsymbol{\rho}$ and $\boldsymbol{\nu}$ are the impact parameter and velocity of the projectile respectively. We then expand the wavefunction of the whole system in terms of the eigenstates of the target atom with time-dependent coefficients $a_{ij}(\rho, \nu; t)$

$$\Psi_i(\boldsymbol{r}, \boldsymbol{R}(t)) = \sum_j a_{ij}(\rho, \nu; t)\phi_j(\boldsymbol{r})\exp[-\mathrm{i}\varepsilon_j t], \quad (1)$$

where i indicates the state occupied initially, while $\phi_j(\boldsymbol{r})$ and ε_j are the eigenfunctions and eigenvalues of the hydrogen atom in state j, respectively. The vector $\boldsymbol{r} \equiv \{r, \vartheta, \varphi\}$ is the position vector of the electron of the hydrogen atom. In the general case, we have to solve a set of coupled differential equations

$$\mathrm{i}\frac{\partial}{\partial z}a_{if}(\rho,\nu;z) = \frac{1}{\nu}\sum_j a_{ij}(\rho,\nu,z)V_{fj}(\boldsymbol{R}) \times \exp\left[-\frac{i}{\nu}(\varepsilon_j - \varepsilon_f)z\right] \qquad (2)$$

for the transition amplitudes satisfying the initial conditions

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

with the matrix potential elements,

$$V_{fj}(\boldsymbol{R}) = \int \phi_f^*(\boldsymbol{r})V(\boldsymbol{r},\boldsymbol{R})\phi_j(\boldsymbol{r})\mathrm{d}\boldsymbol{r}, \qquad (4)$$

and $z = \nu t$. Here $V(\boldsymbol{r},\boldsymbol{R})$ is the interaction potential defined (in atomic units) as follows:
(i) in the case of proton–hydrogen atom collision,

$$V(\boldsymbol{r},\boldsymbol{R}) = \frac{1}{R} - \frac{1}{|\boldsymbol{R}-\boldsymbol{r}|}; \qquad (5a)$$

(ii) in the case of antiproton–hydrogen atom collision,

$$V(\boldsymbol{r},\boldsymbol{R}) = -\frac{-1}{R} + \frac{1}{|\boldsymbol{R}-\boldsymbol{r}|}. \qquad (5b)$$

Expanding Eqs.(5a) and (5b), the second term, in spherical harmonics, leads to the analytical expressions for the matrix potential elements.

We then express the probability for the $i \to f$ transition for a fixed impact parameter ρ as $|a_{if}(\rho,\nu;z\to+\infty)|^2$, and we obtain the cross section by integrating over the impact parameter, i.e.,

$$\sigma_{if}(\nu) = 2\pi\int_0^\infty |a_{if}(\rho,\nu;z\to+\infty)|^2\rho\mathrm{d}\rho. \qquad (5)$$

In the present work, we apply this method to calculate the $2s$ and $2p$ excitation cross sections of the hydrogen atom by the proton and antiproton. We truncate the series in Eq.(1) by involving only the ground state and excited states being investigated. Specifically, we consider the cases involving the two states $(1s, 2s)$, the four states $(1s, 2p_{+1}, 2p_0, 2p_{-1})$, the five states $(1s, 2s, 2p_{+1}, 2p_0, 2p_{-1})$, and the fourteen states (n=1,2,3). The $n = 2,3 \to 1s$ back couplings will be once ignored and once taken into account to investigate the effect of the back coupling. We obtain a set of equations equal to the number of states under consideration. It is convenient to separate the complex transition coefficients a_{ij} into real and imaginary parts and to obtain an enlarged set of coupled-differential equations for real unknown functions. We solve the set numerically using the fourth-order Rung–Kutta method. In what follows, we discuss our results and compare them with experimental results[9,10] as well as theoretical calculations.[5,11–14]

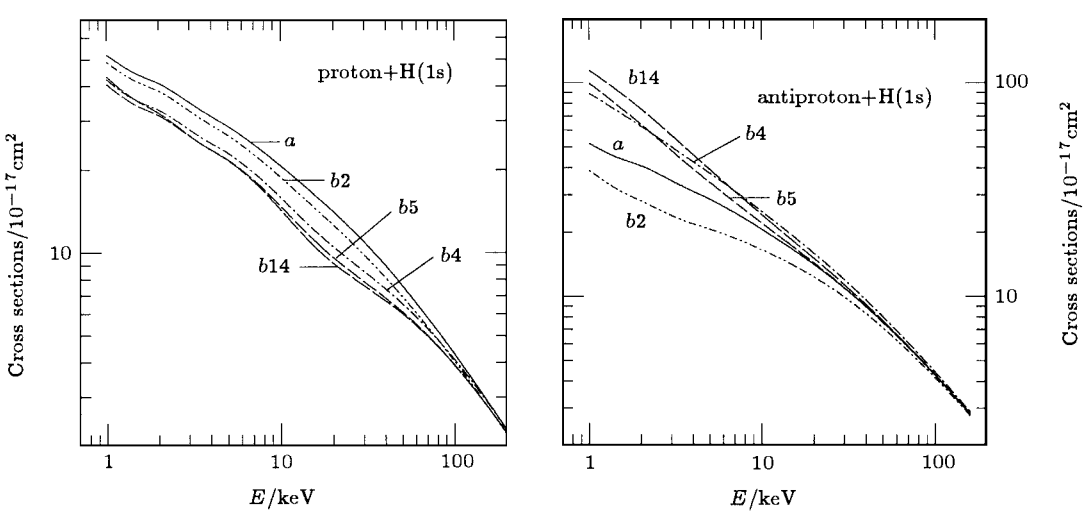


Fig.1. The cross sections of elastic scattering of the proton (on the left) and antiproton (on the right) hydrogen atom collisions. Curves $b2$, $b4$, $b5$ and $b14$ take the back coupling into account for the two-, four-, five- and fourteen-state approximations, respectively. Curve a does not allow for the back coupling.

Figure 1 compares the results of the calculation of the elastic scattering cross sections for cases when the back coupling is included (dotted and dashed curves), with the case when the back coupling is ignored (solid curve, a). We notice that allowing for the back coupling leads to a reduction of the proton scattering cross section. In the case of antiproton scattering, this effect reduces the cross section in the two-state approximation only. We also note that the effect of the channel coupling on the antiproton-induced reactions is greater than on the proton reactions.

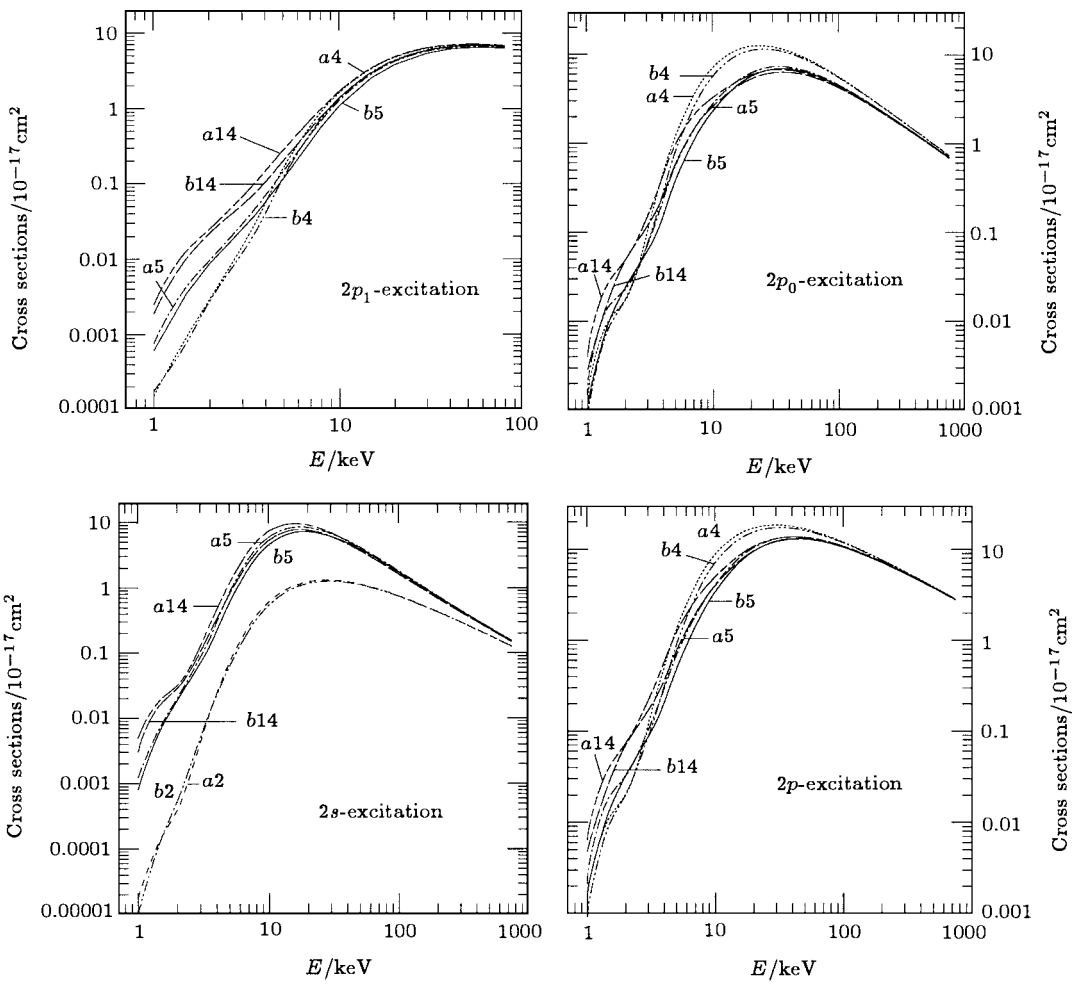


Fig.2. Cross sections for the $2s$ and $2p$ excitations of a hydrogen atom by protons. Curves $b2$, $b4$, $b5$ and $b14$ allow for the back coupling in the two-, four-, five- and fourteen-state approximations, respectively. Curves $a2$, $a4$, $a5$ and $a14$ do not allow for the back coupling in the two-, four-, five- and fourteen-state approximations, respectively.

In figure 2, we see that allowing for the back coupling leads to a small reduction of the $2s$ and $2p$ excitation cross sections. The effect of the channel coupling on the $2s$ excitation is more important than on the $2p$ excitation. Neglecting the coupling to the $2p$ state (curves $a2$ and $b2$) reduces the $2s$ cross section, while neglecting the coupling to the $2s$ state (curves $a4$ and $b4$) increases the $2p$ cross section at moderate and high energies. On the other hand, the fourteen-state approximation (curves $a14$ and $b14$) yields cross sections greater than those at low energies. The closeness of the results of the five- and fourteen-state approximations illustrates the convergence of the coupled channel approximation. We notice that the channel coupling plays a role more important for the $2p_0$ excitation than for the $2p_{\pm1}$ state at moderate and high energies. However, this coupling has a greater effect in the opposite direction in the case of the $2p_{\pm1}$ cross section at low energies. The contribution from the $2p_0$ cross section to the $2p$ cross section at low and

moderate energies is greater than from the $2p_{\pm1}$ cross section. At high energies, on the other hand, the $2p_{\pm1}$ cross section is greater than the $2p_0$ state. The effect of the back coupling falls off more rapidly than the channel coupling.

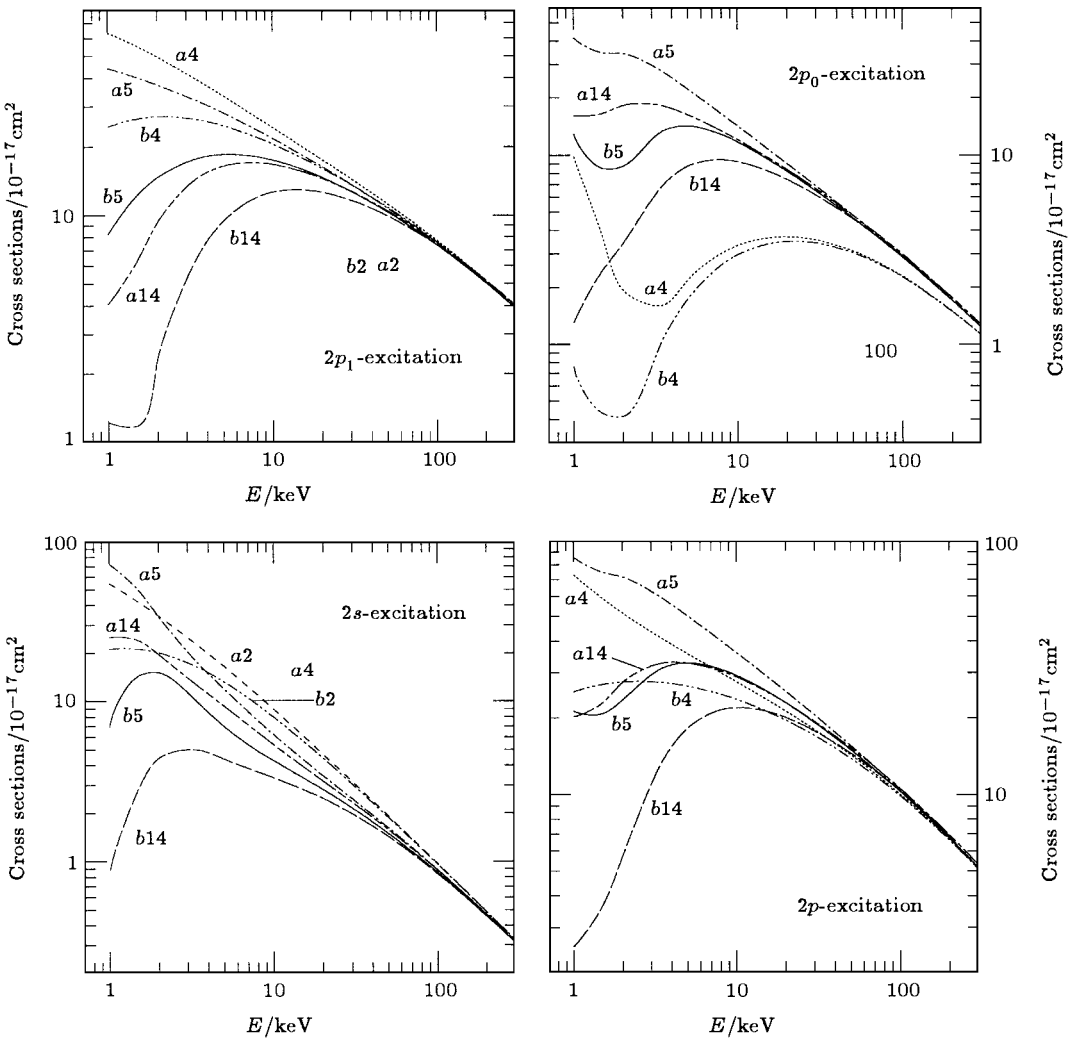


Fig.3. The same as Fig.2 but for hydrogen–antiproton collisions.

Figure 3 displays the effects of the channel coupling and the back coupling on the $2s$ and $2p$ excitations of a hydrogen atom by antiproton impact. We notice that these effects play more important roles in the antiproton-induced reactions than in the proton reactions, as illustrated in Fig.2. The effect of back coupling on the $2s$ state is greater than on $2p_0$ and $2p_{\pm1}$ states. When allowing for the back coupling, an increase of coupled channels corresponds to a reduction of $2s$ and $2p_{\pm1}$ excitation cross sections. A different situation occurs for the $2p_0$ state, where the four-state results are smaller than those of the others. The same applies for the calculations ignoring the back coupling, except for the $2s$ state at low energies. Therefore, in the case of the four-state approximation, the contribution of the excitation of the $2p_{\pm1}$ state to the $2p$ cross section is greater than that of the $2p_0$ state. However, for the five-state approximation, the contributions of both the $2p_{\pm1}$ and $2p_0$ states to the $2p$ cross section are of the same order of magnitude at low and moderate energies. The same applies for the fourteen-state approximation when taking the back coupling into account (curve $b14$). We note that, in general, the channel coupling effect is smaller at high energies. This is expected because all the methods of calculation of the reactions with hydrogen atoms converge to the first Born approximation.

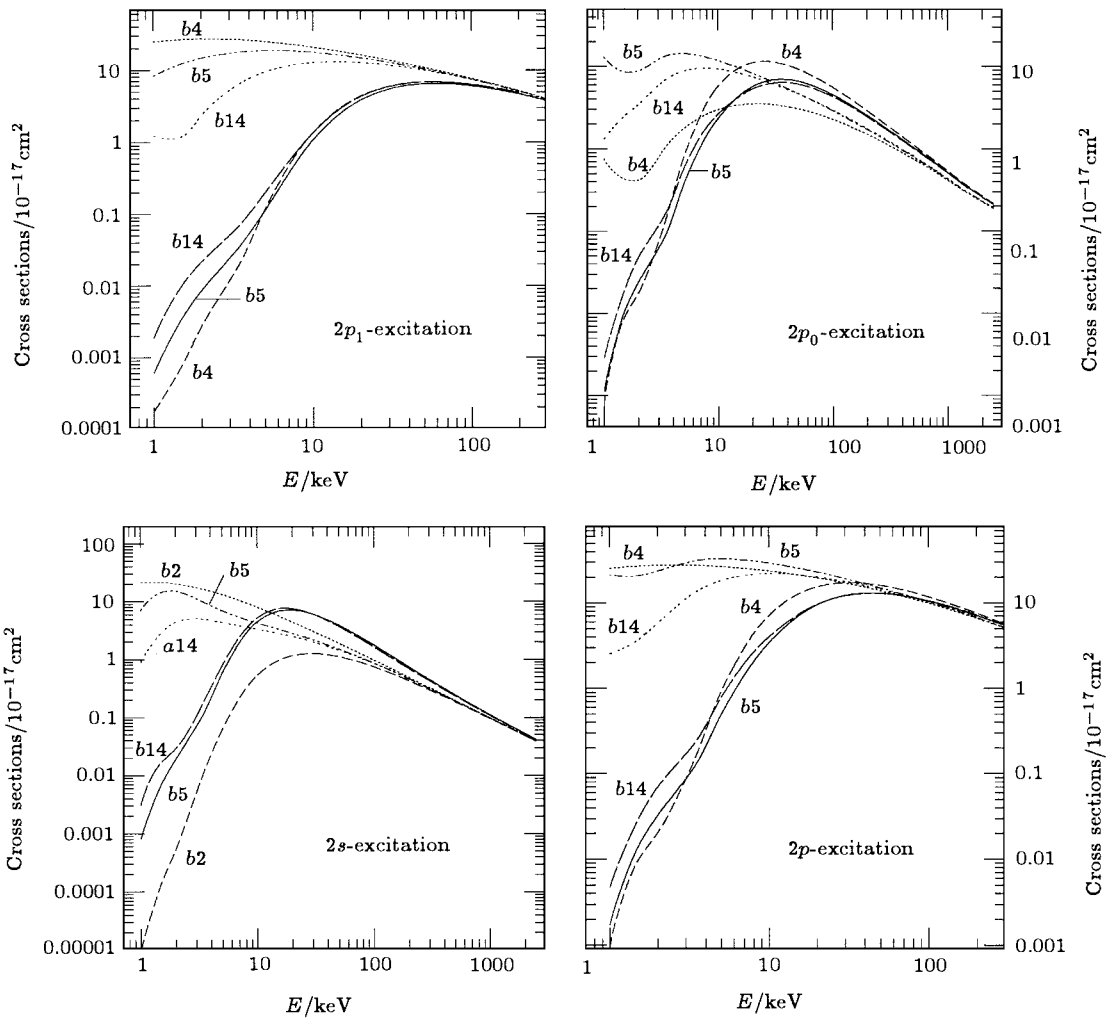


Fig.4. Cross sections for the $2s$ and $2p$ excitations of hydrogen by protons (long dashed and solid curves) and antiprotons (short dashed curves) taking the back coupling into account. Curves $b14$, $b5$, $b2$ and $b4$ represent the fourteen-, five-, two- and four-state approximations, respectively.

Figures 4 and 5 show that the low-energy dependent behaviours of the excitation cross sections of the proton-induced reactions are different from those of the antiproton-induced reactions. The effect of the sign of the projectile charge on the $2s$ and $2p$ excitation cross sections decreases as the number of coupled-channels increases, particularly at low energies. Moreover, the effects of the sign of the projectile charge on the $2s$ and $2p$ excitation cross sections when neglecting and allowing for the back coupling are approximately the same. The present calculations suggest that the effect due to the sign of the projectile charge can be neglected at high energies. The same conclusion has been made by Knudsen *et al*[15] in the investigation of the ionization of hydrogen atoms by protons and antiprotons. This insensitivity is expected because the calculations converge to the first Born approximation, which is independent of the sign of the projectile charge.

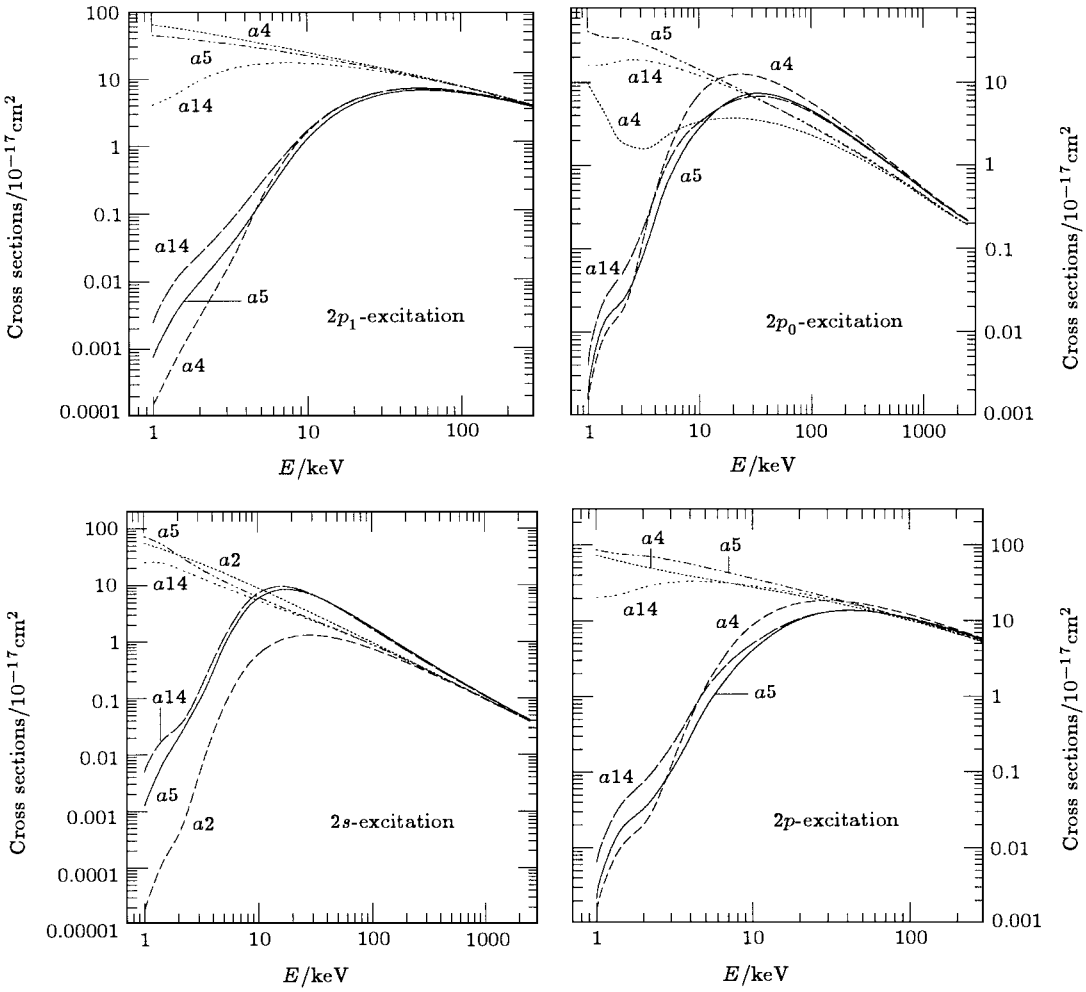


Fig.5. Cross sections for the $2s$ and $2p$ excitations of hydrogen by protons (long dashed and solid curves) and antiprotons (short dashed curves), neglecting the back couplings. Curves $a14$, $a5$, $a4$ and $a2$ represent the fourteen-, five-, four- and two-state approximations, respectively.

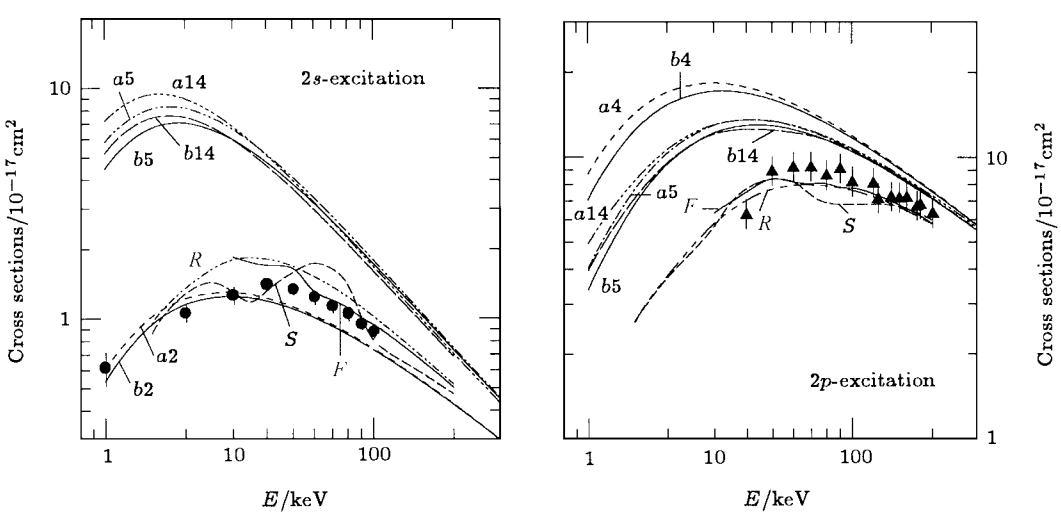


Fig.6. Cross sections for the $2s$ and $2p$ excitations of hydrogen by protons. For theory, the present curves $a2$, $a4$, $a5$, $a14$, $b2$, $b4$, $b5$ and $b14$ are from the present work (as in Fig.2); curve R is from Ref.[11]; curve S is taken from Ref.[5]; and curve F is from Ref.[12]. For experiment, the data for the $2s$ excitation are taken from Ref.[9] and those for $2p$ excitation are taken from Ref.[10].

In Fig.6, we compare our calculations for the $2s$ and $2p$ excitations of hydrogen atoms by protons with previous theoretical and experimental results. We notice that the result of the $2s$ excitation is in good agreement with the experimental work of Higgins *et al*[9] and the theoretical calculations.[5,11,12] The calculations of Ford *et al*[11] (curve R) address the problem of convergence of the cross section for a target centred basis. Slim and Ermolaev[5] (curve S) employed the semi-classical coupled channel method using an asymmetrical basis with only the $1s$ state of the projectile and a large set of 50 bound states and positive-energy pseudo states with $l \leq 3$ centred on the target. Martin[12] (curve F) performed large-scale close-coupling calculations for the excitation of atomic hydrogen by protons and multi-charged ions. The two-state results are in better agreement with the results obtained by these authors than what might have been expected to be more accurate five- and fourteen-state results. On the other hand, the calculations for the $2p$ excitation are comparable to the experimental work of Detleffsen *et al*[10] and theoretical calculations,[5,11,12] and the five- and fourteen-state calculations are in better agreement with these than the results of the four-state approximation.

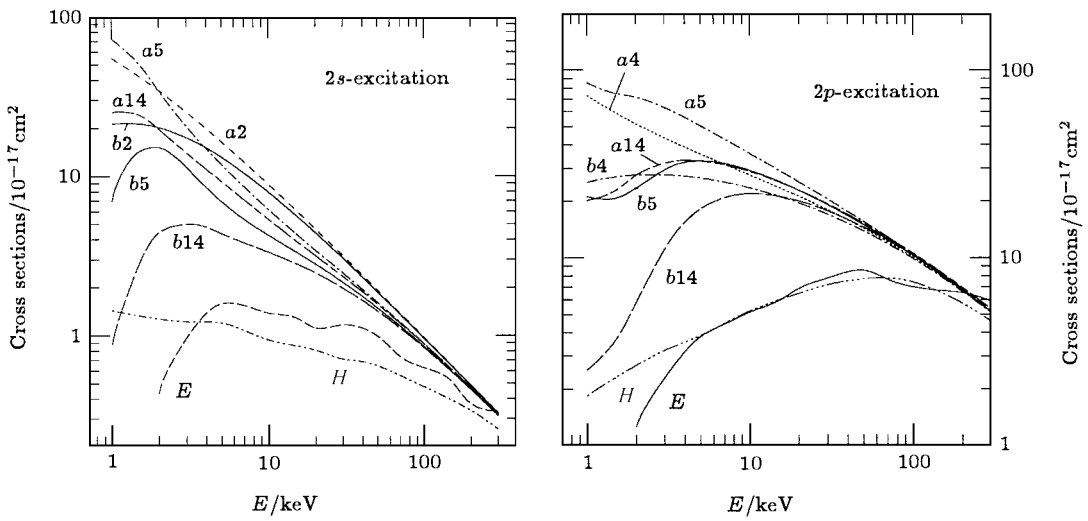


Fig.7. Cross sections for the $2s$ and $2p$ excitations of hydrogen atoms by antiprotons. For theory, the curves $a2$, $a4$, $a5$, $a14$, $b2$, $b4$, $b5$ and $b14$ are from the present work (as in Fig.2); curve E is taken from Ref.[13]; and curve H is from Ref.[14].

In Fig.7, we have compared our cross sections for the $2s$ and $2p$ excitations of hydrogen atoms by antiprotons with the calculations of Ermolaev[13] (curve E) and Hall *et al*[14] (curve H). The calculations by Ermolaev[13] presented two-centred expansion coupled-channel calculations using a symmetric large basis, involving a single pseudostate centred on the antiproton in addition to the 50 states centred at the hydrogen target. Hall *et al*[14] used the single-centred expansion in a finite Hilbert basis set method. The comparison in the case of the $2s$ excitation is seen to be better than in the $2p$ excitation. However, the fourteen-state approximation improves the situation over the other approximations, illustrating the importance of the channel coupling effect.

3. Conclusion

We have performed calculations of the $2s$ and $2p$ excitations of hydrogen atoms by proton and antiproton impact based on the two-, four-, five- and fourteen-state approximations of the impact parameter method. We have described the collisions in terms of a set of coupled differential equations, which allowed an account of the coupling between different channels. Also, we have investigated the effect of the $n = 2, 3 \rightarrow 1s$ back couplings, which is our main purpose, on the scattering cross sections. We found that the back coupling reduces the cross sections and plays an important role in the antiproton scattering, which is much greater than for proton scattering. We have demonstrated the importance of the back coupling, coupled channel, and the sign of the projectile charge, which varied from one channel to another. The differ-

ences between the results of the approximations under consideration for both $2s$ and $2p$ excitations illustrate that the couplings to higher excited states contribute significantly to the collision processes considered here, particularly in the proton-induced reactions. The coupling channel effect plays a more important role in the antiproton scattering process than in the proton scattering, particularly when allowing for the back coupling to the $1s$ state. Moreover, at low energies, the effect of the sign of the projectile charge on the $2s$ and $2p$ excitation cross sections decreases as the number of coupled channels increases. The present results are compared with some previous theoretical and experimental results. However, the agreement with the two-state results is better than the other approximations for the proton-induced reactions, while the fourteen-state approximation gives a better agreement for the antiproton scattering processes.

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