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Electron capture in proton collisions with alkali atoms as a three-body problem

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Abstract. *A previous paper of Avakov et al proposed an approach to the calculation of* electron transfer reactions in ion-atomic collisions based on the Faddeev three-body equations written in the Alt-Grassberger-Sandhas form. In the present work this approach is used to describe the electron capture in proton collisions with alkali atoms. The results of calculation of the total and partial cross sections for charge exchange in proton collisions with Li, Na, K and Rb atoms are presented. The calculated total cross sections are in good agreement with experiment for light target atoms. In going over to heavier targets, the theoretical total cross sections, while agreeing in form, tend to be larger than the experimental ones. The calculated partial cross sections for electron capture into the 2s state of the H atom are also in agreement with experiment. Some other partial cross sections were also calculated.

1. Introduction

In a recent paper (Avakov *et al* 1990a, hereafter referred to as I) we developed an approach to the calculation of electron transfer reactions in ion-atomic collisions based on the Faddeev three-body equations written in the Alt-Grassberger-Sandhas (AGS) form for the purely Coulomb interaction (Alt and Sandhas 1980) in the impact parameter representation (IPFA). In the following paper (Avakov *et al* 1990b, hereafter referred to as II) this approach was used to solve the purely three-body problem of collision of the fully stripped ions with hydrogen atoms.

The objective of the present paper is to check the applicability of the developed method to a description of electron capture in proton collisions with atoms of alkali metals when the problem can approximately be regarded as a three-body one in which the basic particles are the proton (α), the valence electron (e) and the inert core of an alkali atom (β):

$$\alpha + (\beta + e) \rightarrow (\alpha + e) + \beta$$

where $(\gamma + e)$ denotes the bound state of the particle γ and the electron.

The charge exchange reactions with protons and alkali atoms are rather important since alkali atoms are used as targets to obtain beams of polarized atoms and negative ions and are employed in thermonuclear fusion installations. On the other hand, at the present time there exist but a few theoretical investigations of these reactions which describe the experimental cross sections only in limited energy intervals. Therefore, we believe it is reasonable to develop a model which would describe the cross sections over a wide range of energies and target atoms.

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2. Calculation of total and partial cross sections

In the calculations of the total and partial cross sections for the processes under consideration we used equation (55) of I and equations (1) and (2) of II. For the effective potentials of equation (55) of I the hydrogen-like functions were taken as an approximation for a description of the state of the valence electron in an alkali atom. As the electron bound state energies we used the experimental values (Moore 1949, 1952), which are nl dependent. The dimension of the set of equations (55) of I used in the calculations depends on the maximum principal quantum number n_{max} in the set of quantum numbers (n, l, m) of the involved states for the target and atom formed by projectile, which ensures the required accuracy of the cross sections calculations.

Table 1 lists the values of the total cross section for the charge exchange in the proton collisions with the Na atom at different collision energies, E, calculated in IPFA at different n_{max}. One can see that an accuracy of the calculation better than 4% is ensured as the principal quantum number increases up to $n_{max} = 5$.

Table 2 gives the partial cross sections σ_{nl} for the electron capture in proton collisions with the Li atom in a wide energy range of 0.1–400 keV. It follows from this

Table 1. Total cross sections for reaction $H^+ + Na(3S) \rightarrow H + Na^+$, $\sigma(E)$ $(10^{-16}\,cm^2)$ calculated for different values of n_{max}.

	n_{max}			
E (keV)	3†	3	4	5
0.04	1.81	1.96−1	1.63−1	1.60−1
0.4	3.86+1	2.87+1	2.66+1	2.67+1
4	1.64+2	1.09+2	1.05+2	1.05+2
40	2.50	1.89	2.04	2.12

† Only the 3S state of the target is taken into account.

Table 2. Partial cross sections for reaction $H^+ + Li(2S) \rightarrow H + Li^+$, σ_{nl} $(10^{-16}\,cm^2)$.

		E (keV)							
n	l	0.1	0.4	1	4	10	40	100	400
1	0	6.78−5	2.87−2	2.35−1	1.09	2.62	7.14−1	1.08−1	3.58−4
2	0	2.20	6.01	1.48+1	2.35	2.10	4.73−2	1.67−2	5.42−5
2	1	3.22	6.61	3.18+1	3.72+1	9.48	9.38−2	1.70−2	1.20−5
3	0	1.37−3	2.53−2	1.60−1	4.37−1	1.14	1.53−2	5.09−3	1.67−5
3	1	1.01−3	1.01−1	6.28−1	1.73	5.47	4.31−2	5.87−3	4.34−6
3	2	1.72−3	2.56−1	1.53	8.49−1	1.81	1.26−2	7.17−4	1.37−7
4	0	8.45−5	6.29−3	1.34−1	5.01−2	5.03−1	7.05−3	2.17−3	7.12−6
4	1	2.98−4	1.97−2	6.86−1	4.76−1	2.57	2.34−2	2.59−3	1.95−6
4	2	2.00−4	1.95−2	5.64−1	4.19−1	1.17	9.37−3	4.19−4	8.29−8
4	3	5.78−5	8.40−2	2.55−1	1.94−1	1.76−1	8.22−4	1.63−5	8.85−10
5	0	5.01−6	2.14−2	5.66−1	3.32−2	2.50−1	3.80−3	1.11−3	3.67−6
5	1	2.63−4	4.49−2	6.85−1	3.23−1	1.34	1.36−2	1.35−3	1.03−6
5	2	4.26−4	7.26−2	2.48−1	4.69−1	7.16−1	6.11−3	2.43−4	4.88−8
5	3	1.89−4	1.76−1	4.38−1	1.69−1	1.64−1	7.80−4	1.37−5	7.61−10
5	4	1.42−4	3.58−2	6.88−2	5.86−2	1.57−2	2.94−5	2.40−7	3.74−12

table that the dominant transitions for all principal quantum numbers n of the captured electron at $E = 0.1$–40 keV are the transitions with the orbital quantum numbers $l > 0$ and we can say more definitely that the dominant transitions at $E = 1.0$–40 keV are those with $l = 1$ (an exception is $n = 5$ at $E = 4$ keV); at $E = 100$ keV the cross sections for transitions into the states with $l = 0$ and $l = 1$ are comparable and when E is as high as 400 keV the dominant transitions are those to the states with $l = 0$.

Figures 1–4 present the IPFA total cross sections for electron capture in proton collisions with Li, Na, K and Rb atoms and, for comparison, the available experimental data and other theoretical results. Note that the calculations included also all the states

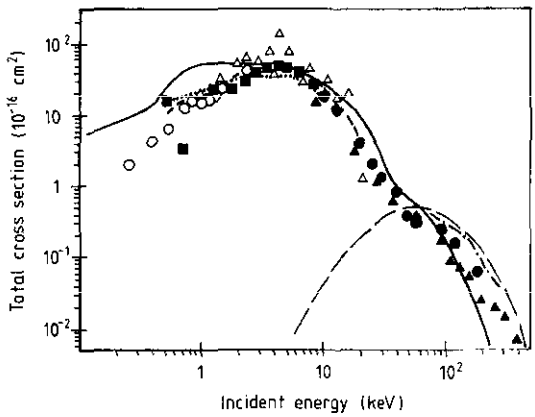

Figure 1. Total cross sections for the process $H^+ + Li(2s) \rightarrow H + Li^+$. Theory: full curve, IPFA (our results); long broken curve, IPFA for electron capture from the K shell; broken curve, Fritsch and Lin (1983) (atomic orbital method); chain curve, Olson (1982) (classical approach); dotted curve, Sato and Kimura (1983) (molecular treatment). Experiment: ●, Il'in *et al* (1966); ▲, Dyachkov (1969); △, ■ (data for D^+), Gruebler *et al* (1970); ○, Varghese *et al* (1984).

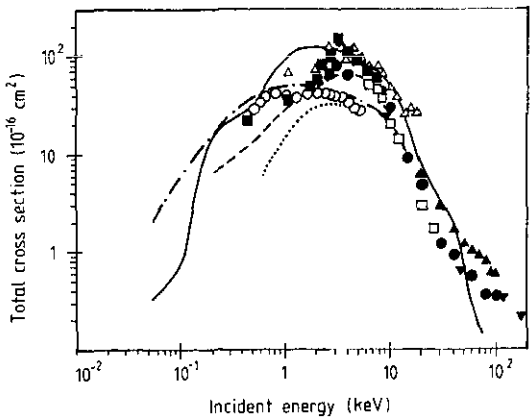

Figure 2. Total cross sections for the process $H^+ + Na(3s) \rightarrow H + Na^+$. Theory: full curve, IPFA; broken curve, Fritisch (1984) (atomic orbital method); chain curve, Kimura *et al* (1982b) (molecular treatment); dotted curve, Kubach and Sidis (1981) (projected valence bond method, $\sigma_{2s} + \sigma_{2p}$). Experiment: ▼, Il'in *et al* (1966); △, ■ (data for D^+), Gruebler *et al* (1970); ▲, O'Hare *et al* (1975); □, Anderson *et al* (1979); ○, Nagata (1982); ●, DuBois (1984).

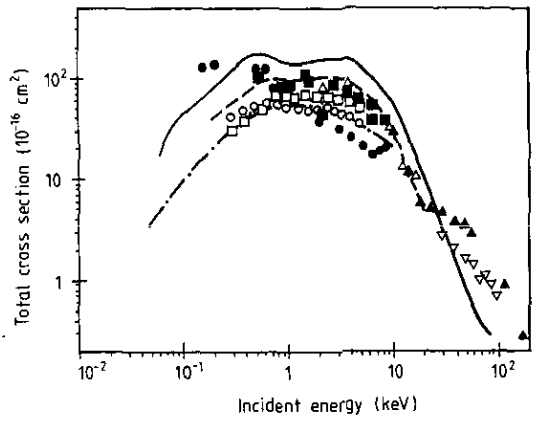

Figure 3. Total cross sections for the process $H^+ + K(4s) \rightarrow H + K^+$. Theory: full curve, IPFA; broken curve, Fritsch (1984) (atomic orbital method); chain curve, Kimura *et al* (1982b) (molecular treatment); dotted curve, Kubach and Sidis (1981) (projected valence bond method, $\sigma_{2s}+\sigma_{2p}$). Experiment: ▲, Il'in *et al* (1966); △, ■ (data for D^+), Gruebler *et al* (1970); ▽, O'Hare *et al* (1975); ●, Inoue (1972); ○, Nagata (1982); □, Ebel (1983).

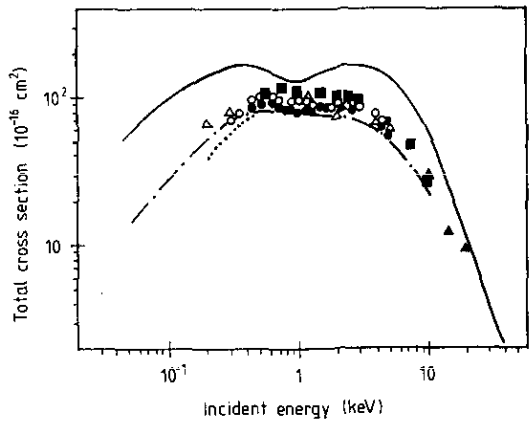

Figure 4. Total cross sections for the process $H^+ + Rb(5s) \rightarrow H + Rb^+$. Theory: full curve, IPFA; chain curve, Kimura *et al* (1982b) (molecular treatment); dotted curve, Kubach and Sidis (1981) (projected valence bond method, $\sigma_{2s}+\sigma_{2p}$). Experiment: ▲, ■ (data for D^+), Girnius *et al* (1977); ●, Nagata (1980); ○, Nagata (1982); △, Ebel (1983).

of the target atom with principal quantum numbers smaller than that of the valence electron in the ground state if these levels are above the ground state. Belonging to these levels are the 3d levels of the K atom, lying above the 4s level, and the 4d and 4f levels of the Rb atom, lying above the 5s level.

Figure 1 shows also the IPFA cross section with allowance for electron capture from the K shell of Li. The K-electron capture cross section at high energies is larger than the valence-electron capture cross section which increases the total cross section in the region of high energies. This conclusion seems also to be true for other reactions considered in the present paper, for which calculations of the capture of non-valence electrons have not been carried out.

On the whole, from comparison of the IPFA total electron capture cross sections with the experimental data we may conclude that there exists a good quantitative and qualitative agreement for light targets. At the same time, in going over to heavier targets the theoretical total cross sections tend to exceed the measured ones, agreeing with the latter in shape.

Figures 5–8 present the IPFA partial cross sections σ_{2s} and σ_{2p} and, for comparison, the experimental data and other theoretical results on σ_{2s}.

For the reaction $H^+ + Na(3s) \rightarrow H(2s) + Na^+$ with the formation of atomic hydrogen in the excited state there are sets of experimental data and theoretical calculations which display discrepancies between them (see figure 6). The previous measurements by Nagata (1980) agree with molecular orbital calculations of Kimura *et al* (1982a), and the data of Berkowitz and Zorn (1984) agree with the calculations of Kubach and Sidis (1981). In the papers by Shingal *et al* (1986) and Fritsch (1984) it was supposed

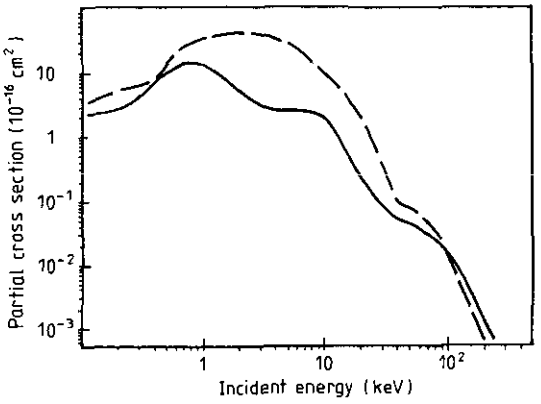

Figure 5. Partial cross sections for the process $H^+ + Li(2s) \rightarrow H + Li^+$. IPFA; full curve, σ_{2s}; long broken curve, σ_{2p}.

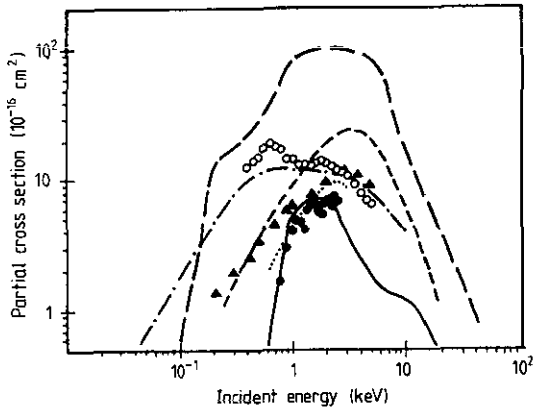

Figure 6. Partial cross sections for the process $H^+ + Na(3s) \rightarrow H + Na^+$. Theory for σ_{2s}: full curve, IPFA; broken curve, Fritsch (1984) (atomic orbital method); chain curve, Kimura *et al* (1982a) (molecular treatment); dotted curve, Kubach and Sidis (1981) (projected valence bond method). Theory for σ_{2p}: long broken curve, IPFA. Experiment for σ_{2s}: ○, Nagata (1982); ●, Berkowitz and Zorn (1984), ▲, Nagata and Kuribara (1986).

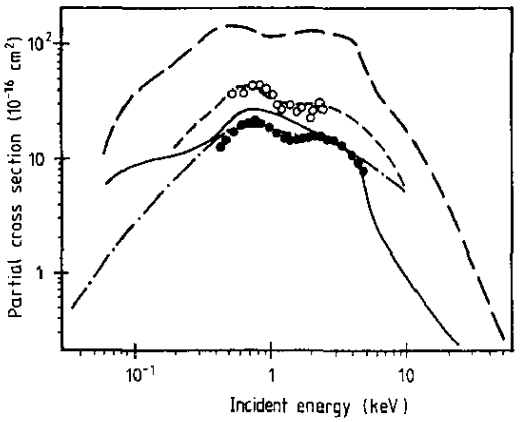

Figure 7. Partial cross sections for the process $H^+ + K(4s) \rightarrow H + K^+$. Theory for σ_{2s}: full curve, IPFA; broken curve, Fritsch (1984) (atomic orbital method); chain curve, Kimura *et al* (1982b) (molecular treatment). Theory for σ_{2p}: long broken curve, IPFA. Experiment for σ_{2s}: ○, Nagata (1980); ●, Berkowitz and Zorn (1984).

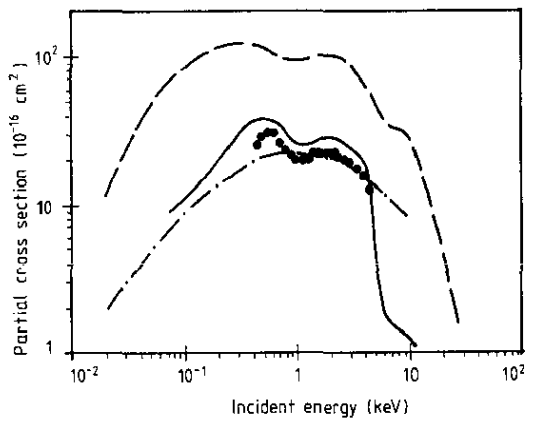

Figure 8. Partial cross sections for the process $H^+ + Rb(5s) \rightarrow H + Rb^+$. Theory for σ_{2s}: full curve, IPFA; chain curve, Kimura *et al* (1982b) (molecular treatment); theory for σ_{2p}: long broken curve, IPFA. Experiment for σ_{2s}: ●, Nagata (1980).

that the measurements by Nagata (1980) were not correct and the calculations by Kimura *et al* (1982a) did not have sufficient accuracy. It seems to be true since the latest measurements of Nagata and Kuribara (1986) are closer to the experimental data of Berkowitz and Zorn (1984) than the previous results. Figure 6 shows that our IPFA calculations are close to those of Kubach and Sidis (1981) and are in good agreement with the data by Berkowitz and Zorn (1984).

Figure 7 represents the situation with partial 2s cross sections for the reaction $H^+ + K(4s) \rightarrow H(2s) + K^+$. There are also two sets of experimental data by Nagata (1980) and Berkowitz and Zorn (1984) which are distinguished by the absolute value but have identical shape. Two theoretical curves by Kimura (1982b) and Fritsch (1984) describe the first and the second sets of data correspondingly. Our calculations in this case, as in the case of Na, agree with the measurements by Berkowitz and Zorn (1984).

Such discrepancies are absent for the heavier targets.

3. Conclusion

In I the AGS three-body equations in the impact parameter representation were written in a convenient form to calculate the electron transfer reactions in ion–atom collisions. In the present paper the developed approach is employed to calculate the electron capture in proton collisions with atoms of alkali metals which are considered as an inert core plus a valence electron. For the effective potential we use the lowest approximation corresponding to the pole amplitude. The calculated total (σ) and partial (σ_{2s}) cross sections for electron capture in the proton collisions with the Li, Na, K and Rb alkali atoms are, on the whole, in good qualitative and quantitative agreement with the experiment throughout the energy interval under study. The partial (σ_{2s}) cross sections obtained for the electron capture from Na and K give additional information for clearing the situation with some discrepancies between the sets of experimental data and theoretical calculations. It can be supposed that the inclusion of higher-order terms of the quasi-Born expansion for the effective potential would lead to improved theoretical results.

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