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Electron capture, ionization and n-shell distributions in collisions of Ar^{q+} ions with hydrogen

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Abstract. Collisions between multicharged Ar^{q+} ions and atomic hydrogen are considered. In this paper, the classical trajectory Monte Carlo (CTMC) method is employed to calculate cross sections for charge transfer and ionization. For multicharged Ar^{q+} ions, a q-scaled curve for the transfer cross sections is obtained. We have also calculated the n-shell distributions for capture.

1. Introduction

Charge transfer and ionization in collisions of ions with atomic hydrogen play an important role in research on fusion plasmas (Phaneuf *et al* 1987, Phaneuf 1992, Barnett 1990). The classical trajectory Monte-Carlo (CTMC) method is employed to calculate cross sections for charge transfer and ionization in the intermediate impact-energy range. We have calculated the cross sections for charge transfer and ionization in Ar^{q+} collisions with atomic hydrogen. The q-scaled cross sections are obtained. At the same time, the n-shell distributions of capture electrons are calculated. The impact energy is limited to a range of 20–300 kev amu^{-1} for charge-transfer processes, which corresponds to a relative velocity of 0.89–3.46. The impact energy is limited to a range of 100–1000 kev amu^{-1} for the ionization processes, corresponding to a relative velocity of 2.0–6.3. Atomic units will be used throughout this paper.

The CTMC method, used in the present work to calculate the cross sections for charge transfer and ionization, is described in detail elsewhere (Peach *et al* 1985, Olson and Salop 1977, Olson 1981, Abrines and Percival 1966). We outline the essentials in the next section. In section 3, we give some typical results and discuss them. In section 4, we give a summary.

2. Theory and some remarks

The system consists of three particles, i.e. the projectile Ar^{q+}, the core H^+ of the target and the active electron e. Initially, the electron is moving about the H^+ ion and is in the ground state. The three-body problem is decomposed into two two-body problems. Peach *et al* (1985) have given Hamilton's equations of motion.

Following the previous work of Peach *et al* (1985) (see also McDowell and Janev 1984, Janev and McDowell 1984), the interaction of the 'active' atomic electron with the incompletely stripped ions is represented in the form

$$V_{\mathrm{ac}}(r) = -\frac{q}{r} - \frac{N_c}{r}(1 + \alpha r + \beta r^2)\mathrm{e}^{-z_e r} \qquad (1)$$

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Table 1. Parameters for the potential $V_{ac}(r)$ for the Ar^{q+} + H system.

q	Z_e	α	β
17	17.03	2.446	164.0
16	16.62	4.618	157.0
15	16.02	8.340	25.55
14	14.96	7.072	38.16
13	14.23	6.721	44.90
12	13.43	6.334	43.51
11	12.62	5.938	38.77
10	11.74	5.489	31.75
9	10.80	4.987	23.86
8	10.40	4.318	33.29
7	9.387	3.386	31.18
6	8.052	2.394	23.32

where N_c is the number of bound electrons of the Ar^{q+} ion, the parameters α and β are fitting parameters which are obtained from the self-consistent potential of the $Ar^{(q-1)+}$ ion and Z_e is the effective nuclear charge obtained from the ionization energy of the $Ar^{(q-1)+}$ ion (Desclaux 1969). The fitting parameters α and β are listed in table 1. The RMS relative errors of fit are, in general, within 1%. Potential (1) has the proper asymptotic limit. The full three-body potential is neglected, the other two potentials are Coulombic.

The maximum impact parameters, B_{max}, depend on the nuclear charge and impact energy of the projectile. No analytic formula is available for B_{max}. The values of B_{max} are different for charge transfer and ionization. Charge transfer occurs at small impact parameters, while ionization occurs at larger impact parameters. With our experience, we choose an appropriate B_{max} for a given system and repeat the calculations until convergence is obtained. For charge transfer a rough estimate of B_{max} is given by $B_{max} \propto (Z/E)^{1/2}$.

The 12 Hamilton's equations are numerically integrated by the Runge–Kutta–Gill method. Six random variables are needed to completely describe the initial conditions. After integrating the equations one can sort the reaction types according to whether the active electron is bound to Ar^{q+} or H^+. If the active electron is neither bound to the Ar^{q+} nor H^+, then ionization has occurred. Cross sections depend upon the values of q. Janev and Winter (1985) have introduced reduced variables $\bar{E}$ and $\bar{\sigma}_{tr}$ for charge transfer: $\bar{E} = E/q^{0.5}$, $\bar{\sigma}_{tr} = \sigma_{tr}/q$. For ionization, they introduced the reduced variables $\tilde{E} = E/q$ and $\tilde{\sigma}_{ion} = \sigma_{ion}/q$.

To make a correspondence between classical binding states and quantum levels, we use the quantization rules derived by Becker and MacKellar (1984) (see also Meng *et al* 1990). The classical principal quantum number, n_c, is obtained by the formula

$$E = -\frac{q^2}{2n_c^2}. \tag{2}$$

The quantum number, n, is then obtained by the following inequality:

$$[(n-1)(n-\tfrac{1}{2})n]^{\frac{1}{3}} \leqslant n_c \leqslant [n(n+\tfrac{1}{2})(n+1)]^{\frac{1}{3}}. \tag{3}$$

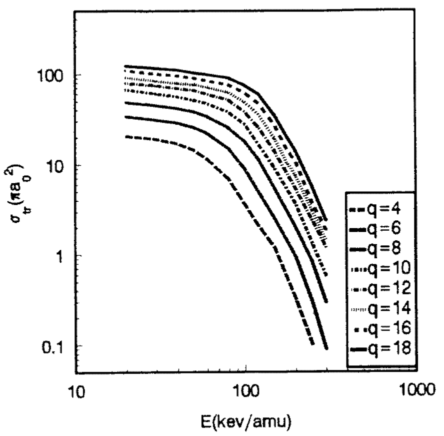

Figure 1. Charge transfer total cross sections for $Ar^{q+} + H$ collisions ($q = 4$–18).

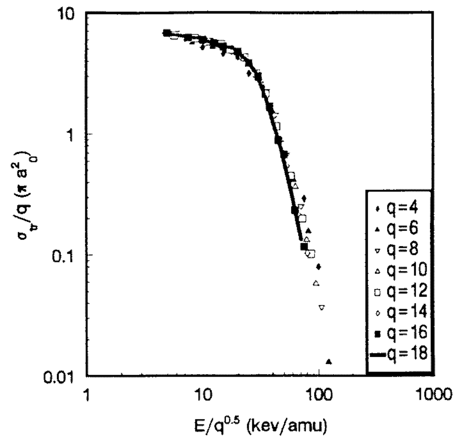

Figure 2. q-scaled charge transfer total cross section for $Ar^{q+} + H$ collisions ($q = 4$–18).

3. Results and discussion

3.1. Cross sections for charge transfer

We have calculated cross sections for the collision of Ar^{q+} ions with atomic hydrogen in the ground state, where the values of q are from 6–18. Figure 1 shows the cross sections of charge transfer versus incident energy. Only the cross sections with even values of q are shown; the cross sections with odd values of q are similar. The cross sections decrease with increasing energy. For different values of q, the cross sections for charge transfer versus energy have a similar behaviour, so a q-scaled cross section is adequate. For the fully stripped ion collisions, the potential between projectile and the active electron is simply Coulombic. With reduced variables, we have plotted the curve of $\bar{\sigma}_{\rm tr}$ versus $\bar{E}$ as shown in figure 2. For incompletely ionized argon, the results are indicated using symbols (see figure for explanation). It is seen that all the cross section data are grouped around the curve for Ar^{18+}. As the value of q decreases, the deviation from the curve increases. As the energy increases, the deviation from the curve increases because the probabilities of ionization increase with increasing energy. At $q = 6$, the q scaling is broken, the reason might be the complicated structure of the projectile ion and thus the complicated potentials between the particles. The data points for the q-scaled universal curve can be fitted to the analytic expression,

$$\bar{\sigma} = \frac{A \ln(B/\bar{E})}{1 + C\bar{E}^2 + D\bar{E}^{4,5}} \tag{4}$$

by an RMS relative error of fit of about 2%, with the following values of fitting parameters

$$A = 0.9534 \qquad B = 5.752 \times 10^3 \qquad C = 1.130 \times 10^{-4} \qquad D = 1.428 \times 10^{-7}.$$

3.2. n-shell distributions

If the inequality (3) is satisfied, we say that the electron is captured into the n shell. In the work of Maynard *et al* (1992), the probabilities for the population of ionic n shells by $Ne^{q+} + H$ electron-capture collision are obtained. The probability for the population of

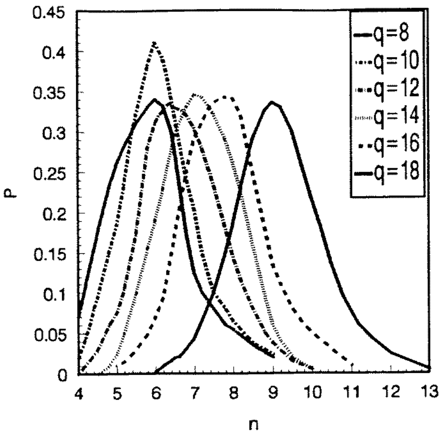

Figure 3. n-shell distributions for $Ar^{q+} + H$ collisions ($q = 8$–18) at $E = 25$ keV amu^{-1}.

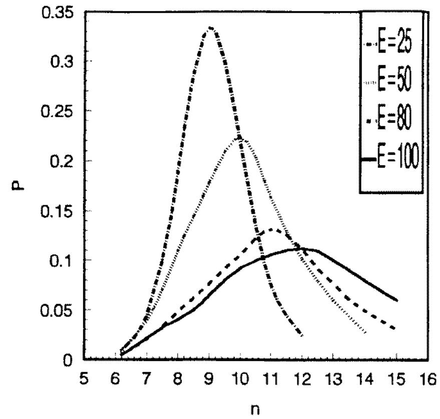

Figure 4. n-shell distributions for $Ar^{18+} + H$ collisions at $E = 25, 50, 80, 100$ keV amu^{-1}.

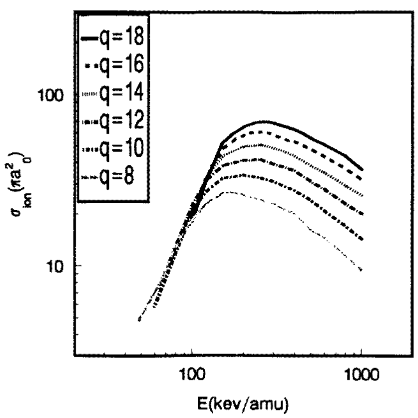

Figure 5. Ionization cross sections for $Ar^{q+} + H$ collisions ($q = 10$–18).

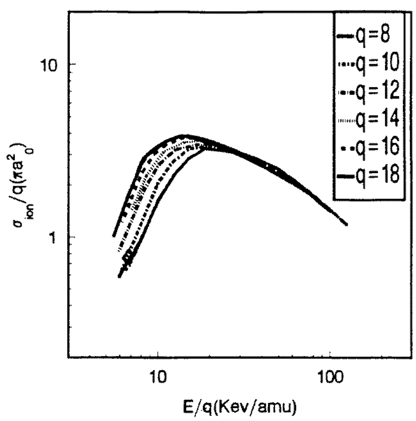

Figure 6. q-scaled ionization cross section for $Ar^{q+}+H$ collisions ($q = 8$–18).

ionic n shells is defined as

$$P_n = \sigma_{tr}(n)/\sigma_{tr}. \tag{5}$$

In the present paper, we have calculated the probabilities of an electron captured into specific n shells of the Ar^{q+} ions with $q = 8$, 10, 12, 14, 16 and 18 at an incident energy of 25 keV amu^{-1}. The results are shown in figure 3. It is seen that the most probable value, n_m, increases with increasing q. The n shell distributions are very similar to those of Maynard *et al* (1992). With increasing collision velocity, the value of n_m increases and the width of the n-distribution becomes larger. For the fully stripped Ar^{18+} ion, we have calculated the n-distribution with different collision velocities. The results are shown in figure 4.

Table 2. Cross sections of σ_{tr} (in units of πa_0^2) for electron capture by the Ar^{6+} ion.

Energy (keV amu^{-1})	σ_{tr} (experimental)	σ_{tr} (this paper)
20.0	43.2 ± 1.7	34.0
30.0	36.7 ± 1.4	31.0
40.0	33.8 ± 1.3	28.5
45.0	30.0 ± 1.4	27.2
60.1	17.7 ± 0.8	22.2
80.1	10.32 ± 0.53	14.8
100.0	6.17 ± 0.38	8.83

Table 3. Cross sections of σ_{ion} (in units of πa_0^2) for ionization of H atoms by the Ar^{8+} ion.

Energy (keV amu^{-1})	σ_{ion} (experimental)	σ_{ion} (this paper)
75.1	13.41 ± 0.83	12.0
112.6	20.80 ± 1.03	21.0
169.0	24.1 ± 0.9	26.2
244.2	21.4 ± 0.8	24.5

3.3. Ionization cross sections

Ionization cross sections increase with increasing collision velocity. After reaching maximum, the ionization cross sections decrease slowly. The ionization cross sections are calculated in the energy range from 100 to 1000 keV amu^{-1}. Below this energy range, the ionization cross sections are much smaller than those for charge transfer. The results are shown in figure 5. The cross sections for different ions show similar energy behaviour. The cross section maximum, $\sigma_{ion,m}^{(q)}$, and the energy, $E_m^{(q)}$, at which it appears are approximately given by

$$E_m^{(q)} \cong E_m^{(1)} q^{0.60} \tag{6}$$

and

$$\sigma_{ion,m}^{(q)} \cong \sigma_{ion,m}^{(1)} q^{1.30} \tag{7}$$

where $E_m^{(1)} = 45$ keV amu^{-1} and $\sigma_{ion,m}^{(1)} = 1.60\pi a_0^2$ are the corresponding values of the proton impact ionization of the hydrogen atom. Figure 6 shows the curves of reduced variable $\tilde{E}$ versus $\tilde{\sigma}_{ion}$. It is seen that a simple q-scaling is not available. At energies above $E_m^{(q)}$, the classical behaviour $\sigma_{ion}^{(q)} \approx q^2/E$ is quite evident. Our results are very similar to those of Maynard *et al* (1992).

3.4. Comparison with experimental results

Shah and Gilbody (1983) presented the measured cross sections for ionization of atomic hydrogen by Ar^{q+} for $3 \leqslant q \leqslant 9$ and measured cross sections σ_{tr} for electron capture by Ar^{q+} for $3 \leqslant q \leqslant 6$. Some of the results are listed in tables 2 and 3. Our results are also listed for comparison. The present results are in reasonable agreement with those of Shah and Gilbody (1983).

4. Summary

We have employed the CTMC method to calculate charge transfer and ionization cross sections for the $Ar^{q+} + H$ collision system. The results are in reasonable agreement with experimental measured results. The CTMC method is adequate for the intermediate energy range.

The potentials between Ar^{q+} ions and the active electron are assumed to be the self-consistent potentials calculated from $Ar^{(q-1)+}$ ions. The potentials are fitted to an analytical form (Peach's form) to save the computer time. In general, the fitting errors are within 1%.

In order to reduce the statistical errors, 2000–4000 trajectories are necessary in our calculations so as to keep the statistical errors of the results below 10%.

Competition between charge transfer and impact ionization varies with energy and charge of Ar^{q+}. For the collision system Ar^{q+}+H, charge transfer dominates at low energies. Impact ionization increases with increasing energy. At energies below E_1 ($E_1 = 80q^{0.5}$) ($q = 8$–18), the cross sections for charge transfer can be scaled with respect to q. At energies above E_2 ($E_2 = 20q$) ($q = 8$–18) the ionization cross sections can be scaled with respect to q.

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