EVALUATION OF CROSS SECTIONS AT INTERMEDIATE COLLISION ENERGY (1-1000 keV/amu) USING THE CLASSICAL TRAJECTORY MONTE CARLO (CTMC) METHOD

K. Katsonis, G. Maynard

► To cite this version:

K. Katsonis, G. Maynard. EVALUATION OF CROSS SECTIONS AT INTERMEDIATE COLLISION ENERGY (1-1000 keV/amu) USING THE CLASSICAL TRAJECTORY MONTE CARLO (CTMC) METHOD. Journal de Physique IV Proceedings, 1991, 01 (C1), pp.C1-313-C1-337. 10.1051/jp4:1991129 . jpa-00249767

HAL Id: jpa-00249767

<https://hal.science/jpa-00249767>

Submitted on 1 Jan 1991

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

**EVALUATION OF CROSS SECTIONS AT INTERMEDIATE COLLISION ENERGY
(1-1000 keV/amu) USING THE CLASSICAL TRAJECTORY MONTE CARLO (CTMC) METHOD**

K. KATSONIS and G. MAYNARD

*Laboratoire de Physique des Gaz et des Plasmas, CNRS UA-73, Bat. 512,
Université de Paris-Sud, F-91405 Orsay Cedex, France*

Résumé - On décrit les activités récentes de l'opération scientifique du laboratoire sur l'évaluation de données atomiques; un choix des résultats obtenus avec la méthode Monte Carlo de trajectoires classiques (CTMC) est présenté. Malgré que la plupart des résultats concerne des plasmas confinés par dispositifs magnétiques, des résultats relatifs aux plasmas de fusion inertielle ont été aussi évalués par la même méthode.

Abstract - Recent activities of the Atomic Data Evaluation unit of this Laboratory are described and selected results obtained using the CTMC method are presented. Although most of these results are relevant to the magnetically confined plasmas, results relevant to inertially confined plasmas have been also evaluated with the same method.

1 - INTRODUCTION

Evaluation of atomic data relevant to plasma physics are needed for diagnostics and modeling of nature (astrophysics), laboratory (arcs, experimental devices) and industrial (Tokomaks, lasers, ion beams) plasmas. The development of the research on these fields is leading to concrete data needs which, being outside the frame of common atomic experiments results and theoretical studies, are often difficult to evaluate. We therefore have constituted in this Laboratory a theoretical group (Atomic Data Evaluation unit) in collaboration with scientists from the Laboratory and from abroad, in order to promote the evaluation of the most urgently needed data. Data needs for each field can be quite different but the evaluation of a part of them is easing the evaluation of the rest. Problems arising in atomic data evaluations were thoroughly discussed in an 'ad hoc' workshop sponsored by CODATA and NIST on 'Atomic Data Management' organized by the Atomic Data Centre GAPHYOR in August 1987 at Abingdon, UK.

Our project has first addressed atomic data needs relevant to magnetic fusion, as evaluated following a Coordinated Research Programme of the International Atomic Energy Agency initiated by one of us (KK) for magnet fusion plasma diagnostics (see the review paper "Recent Progress in Production and Evaluation of Atomic Data for Fusion", /1/). It clearly appears that it is practically impossible to consider an experimental measurement of the needed data. Experimental results are practically used only as benchmarks in order to verify the theoretical results. Moreover, universal theoretical methods are to be developed in order to evaluate collision cross sections in a large domain of energy. We have therefore chosen the CTMC method, initiated in the field of intermediate energy atomic collisions by Olson and collaborators /2,3/, as developed at Royal Holloway College, Egham, UK, for calculation of cross sections of iron and gold ions colliding with hydrogen or helium atoms /4,5/. After modifying the used code and applying conveniently chosen potentials, we have been able to obtain a wide number of results /6,7,8/, some of which will be presented in this paper, after a summary description of the CTMC method as used at Orsay. Prospects of further activities and conclusions relevant to this work are also included.

2 - THE CTMC METHOD; CALCULATION OF TOTAL CROSS SECTIONS

We describe here only the general principles of the method. Details concerning the potentials and the calculation of n -resolved cross sections are given in §6.

The CTMC method is based on the numerical solution of the canonical equations of Hamilton

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad (1)$$

In this formulation the generalized coordinates q_i and the canonical momentums p_i are the independent variables describing the particle movement in the general n -body problem and H is the Hamiltonian of the system. It is possible to consider an ion - atom collision as a three body problem, the ion, the core consisting of the atom minus an electron, and the removed electron being the three potential centers. Analytic solution of this system is theoretically possible, as deterministic arguments valid in classical mechanics imply. Nevertheless, the delicate problem of the initial conditions is prohibiting a satisfactory solution even if an approximate third integral of motion (in addition of these of momentum and of angular momentum, arising from the space isotropy and from the space homogeneity correspondingly) could sometimes be found; note that for a closed system an energy integral is obtained due to the time uniformity. On the contrary, a numerical solution for a limited time interval is always possible whenever the initial and boundary conditions are given. The Monte Carlo method takes advantage of this fact, and examines statistically a sufficiently big number of trajectories resolved numerically. The initial conditions are determined from a set of random values covering all the spectrum of the possible initial conditions of the given physical problem. In the present case, if the electron of which we calculate the trajectory is found in the vicinity of the remaining core after the collision, only an excitation of the atom was possible. If, on the contrary, it is found near the ion, it is a capture case and if it is far from both the atom and the ion it is an ionization.

It is evident that, simply using a coulomb potential in the canonical equations (1), we cannot obtain any quantum effect. But it is possible to use other kinds of potentials (e.g. model potentials) in order to improve the CTMC method. The results obtained this way are analogous to those resulting from various approximate solutions of the differential equations set corresponding to a rigorous quantum formulation (for a detailed review of the most common quantum methods see /9/. Actually, in order to resolve such a set it is obligatory to reduce the possible states and/or simplify otherwise the system through various approximations (e.g. semi-classical approximation, perturbation methods, etc.). The implications of these artifacts are often delicate to evaluate; hence the results are valid in a more or less narrow domain.

We have applied the CTMC method in a big number of colliding species of various positive ionization stages and for a wide energy domain. This paper is restricted to evaluation of charge transfer (σ_c) and ionization (σ_i) cross sections in collisions of 1 to 1000 keV/amu ions with neutral hydrogen. For the highly ionized species we used the coulomb potential, our calculations demonstrating that the use of an improved potential in this case is redundant. This illustrates the well known hydrogen-like properties of such ions. In all other cases a Tomas - Fermi (T-F) potential was used for the ion, as defined in the previously mentioned publication of M.R.C. McDowell and R.K. Janev /4/ concerning collisions of iron ions with neutral hydrogen in the ground state.

This potential has the form

$$V(r) = -\epsilon(r)/r \quad (2)$$

with a apparent charge defined by

$$\epsilon(r) = q[1 - (a_0 + a_1 r) \exp(-Z_1 r)] \quad (3)$$

For a multiply charged ion and for $r \geq R_N$ the value of $\epsilon(r)$ given from (3) be-

comes $q[1-\exp(1-\Gamma r)]$ with $\Gamma = -\ln(1-Z_{\text{eff}}/q)/R_N$; for $r = R_N$ it is equal to Z_{eff} . Evaluation of the effective charge Z_{eff} of the ion after one electron was removed is based to Hartree - Fock binding energies with relativistic corrections calculated by Carlson et al. /10/. Table 1 is giving the values of Z_{eff} , a_0 and a_1 used for the ions of neon ($q = 1$ to 8), titanium ($q = 3$ to 11), chromium ($q = 3$ to 15) and iron ($q = 3$ to 20).

Table 1. Parameters a_0 and a_1 and the effective charge Z_{eff} of selected Ne, Ti, Cr and Fe ions.

NEON								
q	1	2	3	4	5	6	7	8
Z_{eff}	1.302	1.941	2.416	2.812	3.16	3.473	4.038	4.307
a_0	-9	-4	-2.33	-1.5	-1	-0.667	-0.429	-0.25
a_1	6.771	4.031	4.49	5.645	6.714	7.33	7.8	7.26

TITANIUM									
q	3	4	5	6	7	8	9	10	11
Z_{eff}	1.368	1.792	2.697	3.018	3.307	3.573	3.851	4.083	4.536
a_0	-6.33	-4.5	-3.4	-2.667	-2.143	-1.75	-1.44	-1.2	-1
a_1	9.513	8.423	9.21	9.967	10.95	12.0	13.168	14.05	16.13

CHROMIUM							
q	3	4	5	6	7	8	9
Z_{eff}	1.603	2.0	2.331	2.62	3.42	3.71	3.98
a_0	-7	-5	-3.8	-3	-2.429	-2	-1.667
a_1	10.545	9.32	9.092	9.359	11.734	13.01	14.301

CHROMIUM						
q	10	11	12	13	14	15
Z_{eff}	4.227	4.509	4.732	5.172	5.382	8.29
a_0	-1.4	-1.182	-1	-0.846	-0.714	-0.6
a_1	15.498	16.826	17.628	19.783	19.991	48.785

Table 1. Parameters a_0 and a_1 and the effective charge Z_{eff} of selected Ne, Ti, Cr and Fe ions (continued).

IRON									
q	3	4	5	6	7	8	9	10	11
Z_{eff}	1.55	2.054	2.47	2.819	3.13	3.412	4.203	4.47	4.721
a_0	-7.667	-5.5	-4.2	-3.333	-2.7143	-2.25	-1.889	-1.6	-1.364
a_1	11.502	10.073	9.862	10.28	11.06	12.04	16.0	17.6	19.05

IRON									
q	12	13	14	15	16	17	18	19	20
Z_{eff}	4.96	5.231	5.45	5.894	6.1	9.267	9.713	10.142	10.551
a_0	-1.667	-1	-0.857	-0.733	-0.625	-0.5294	-0.444	-0.368	-0.3
a_1	20.278	21.582	22.202	24.469	24.29	60.578	58.434	54.255	48.46

Let Z be the nuclear charge and N the number of the ion electrons; the radius R_N can then be simply expressed by:

$$R_N = \frac{(3\sqrt{2}N)^{2/3}}{Z} \tag{4}$$

For the derivation of this expression see /7/.
The chosen limit conditions are giving:

$$a_0 = 1 - Z/q \tag{5} \quad \text{and} \quad a_1 = [-a_0 + (1 - z_{\text{eff}}/q)\exp(Z_{\text{eff}}r_0)]/r_0 \tag{6}$$

Evidently, whenever a_0 , a_1 are zero, this potential becomes a coulomb one with $\epsilon(r) = q$. The values of the apparent charge $\epsilon(r) = -V(r).r$ for some ionization stages are given by the curves shown in Fig. 1 for neon, in Fig. 2 for titanium and in Fig. 3 for iron.

Fig. 1. Apparent charges $\epsilon(r) = -V(r).r$ for neon ions

Fig. 1. Apparent charges $\epsilon(r) = -V(r) \cdot r$ for neon ions (continued)

Fig. 2. Apparent charges $\epsilon(r) = -V(r) \cdot r$ for titanium ions

Fig. 3. Apparent charges $\epsilon(r) = -V(r) \cdot r$ for iron ions

Fig. 3. Apparent charges $\epsilon(r) = -V(r) \cdot r$ for iron ions (continued)

Once the interaction potential is defined, the canonical equations are leading to a set of twelve coupled differential equations which describe the movement of the three particles in the center of mass. This system is transformed in elliptic coordinates according to the problem of Kepler and subsequently resolved numerically with random initial values defining the initial values of the momentum in a microcanonical distribution, the target orientation and the impact parameter stratified in M layers.

In using the numerical code a convenient adjustment of the parameter "factog" (which is related with the impact parameter b_0 and the number of layers M by $b_0 = \sqrt{M} \cdot \text{"factog"}$) it is essential both for the economy of the calculation time and for the achievement of the chosen approximation. This parameter has to be obtained initially by empirical formulas and/or evaluated by extra- and interpolation over a set of curves giving its variation as a function of the filled layers M' over a total number of layers M . In our calculations M was mostly chosen between 19 and 21. In fact, once the total number of layers M is fixed (e.g. $M = 19$), one has to make sure that for this M value the parameter "factog" has such a value that at least 90% of the used layers (i.e. about $M' = 17$ in this case) contain at least one event. Choosing the trial impact parameter too small means neglecting a region where the particles are probably reacting. Inversely, trying to calculate a set of trajectories using a trial impact parameter which is too big (i.e. $M' \ll M$), even if the total number of layers M was sufficient, the number of the used layers M' is too small for evaluating the shape of the potential in its region of variation as a function of r with a satisfactory precision.

After optimizing the parameter "factog", the total number of trajectories to be calculated for each energy varies as a function of the process studied (ionization, charge transfer) and of the energy itself. With a satisfactory random number generator, 600 trajectories are sufficient for 'easy' regions (energies about 80 to 400 keV/amu, cross sections greater than 1 a.u.) but for 'difficult' regions, and also for calculating the n distribution of the captured electrons, more than 10000 trajectories are necessary for each energy point.

3 - STUDY OF THE $\text{Ne}^{q+} - \text{H}$ COLLISIONS

For the neon case the cross sections for collisions involving the higher ionization stages $q = 9$ and 10 have been calculated with a pure Coulomb potential. On the other side the low ionization stages ($q = 1$ and 2) may not be treated successfully in the frame of classical trajectories. The values obtained by the CTMC method in this case are only given here for completeness; we are now calculating improved values for these cases using the Landau - Zener approximation.

In general, according to the description of the CTMC method given in §2, the energy range of its validity is not clearly defined. It has to be kept in mind that molecular effects are to be expected at the lower energy region and tunneling effect at the higher. It is also to be noted that the expression (4) given for the T-F radius is only valid for $Z \gg N$. Moreover, the validity region is depending on the form of the used model potential.

Our calculations for Ne have been extended from 0.1 keV/amu for σ_c up to 10 MeV/uma pour σ_i . For low energies the time needed for the calculation of one trajectory grows very fast. For high energies, the number of trajectories needed in order to obtain a satisfactory statistics becomes excessive.

The obtained charge transfer and ionization cross sections are presented schematically in atomic units (πa_0^2) versus energy in keV/amu .

3.1 - Charge transfer

The curves of the Fig. 4 giving the calculated charge transfer cross sections (σ_c) are showing a plateau for lower energies and an exponential decay for higher energies. This well known asymptotic behavior is in agreement with the experimental and theoretical results discussed elsewhere [11/].

Fig. 4. Charge transfer cross sections in $\text{Ne}^{q+} - \text{H}$ collisions.

The numerical values obtained for the charge transfer (σ_c) cross sections are also shown in mao^2 units in the Fig. 5, but expressed in reduced coordinates (σ_c/q versus $E/q^{0.5}$). As expected, the results follow the universal curve proposed by Janev and Hvelplund /12/, except for $q = 1$ and $q = 2$. The included continuous curve constitutes a parametrization of the the form

$$y = 3.91 \cdot 10^7 / (a + x^b)^{1.4}$$

with the reduced energy and the reduced cross section as coordinates x , y and with the numerical values of the parameters $a = 7.3648 \cdot 10^4$ and $b = 3.142857$. This parametrisation allows a straightforward evaluation of the corresponding rate coefficients which are necessary in the construction of plasma models.

Fig. 5. Reduced (σ_c/q versus $E/q^{0.5}$) charge transfer cross sections

The available experimental values for the multiply charged ions collisions follow the curve of the Fig. 5 (see for example the experimental data review of Gilbody /13/); this is an indication that the CTMC method is valid for the calculation of σ_c in this energy region provided that q is not too small.

For reduced energies greater than 0.5 MeV/amu it is not sure that the universal curve of the Fig. 5 is still valid. It is also possible to observe in this figure that for reduced energies smaller than 50 keV/amu the points corresponding to each energy for various q values are forming individual curves departing from the universal one when q is diminishing.

The reduced charge transfer cross sections for the ions Ne^{10+} and Ne^{9+} are compared in the Fig. 6 with results for Cu^{18+} , Co^{16+} , Mn^{14+} , Cr^{13+} , V^{12+} , V^{11+} , and C^{6+} , also obtained by the CTMC method. For the presented elements and ionization stages the same universal curve stays valid. Nevertheless, our results for the ions of Ne are not sufficient to conclude generally on the behavior of the reduced cross sections. Toward this aim, evaluations including heavier species (see further in this paper) and light elements are under way.

Fig. 6. Collision cross section for $q > 5$, $Z = 6$ to 18, in reduced coordinates

3.2 - Ionization

The dependence of the calculated ionization cross sections σ_i on the energy is shown graphically in the Fig. 7. It can be seen in this figure that

Fig. 7. Calculated ionization cross section versus collision energy

the dependence of σ_i on the ionization stage q becomes less important in the medium energy range (20 to 80 keV/amu) for sufficiently charged projectiles. The ionization curves are crossing in this region and subsequently σ_i becomes smaller when the ionization stage q increases (multicharged ions). This is explained by the preference of the hydrogen electron to be captured in a bound level of the projectile for big q and small energy.

Another way to present our results for H ionization by neon ions is in form of σ_i versus q curves, as given in Fig. 8 for various energies ($E = 50$,

Fig. 8. Ionization cross sections dependence on the projectile ionization stage q .

80, 100, 150 and 500 keV/amu). The maxima corresponding to each energy are not situated according to the empirical law which has been proposed by Gillespie /14/ for energies $E \geq 30$ keV/amu. In fact, he proposed an empirical formula for σ_i which leads to maxima corresponding approximately to $q_m = 0.1xE[\text{keV/amu}]$ for the case of hydrogen target. For 100, 80 and 50 keV/amu this formula gives a q_m equal to 10, 8 and 5 correspondingly.

The influence of the ionization stage on the collision process is shown under another aspect in the Fig. 9, where the reduced total cross section for electron loss $\sigma_t = \sigma_t/q$ is given as a function of the energy. In this figure, values for hydrogen-like projectiles (H^+ , He^{++} , C^{4+}) calculated by the same model are also included. It is to be noted that with increasing q the initial q^2 dependence changes to a q dependence. This is because for low q the ionization (varying as q^2) dominates but for high q the charge transfer (varying as q) becomes more important.

Fig. 9. Reduced cross section of hydrogen electron loss as a function of the projectile ionization state.

4 - Na- AND Mg-LIKE ($Z = 22$ to 29) METALLIC IONS

Calculations have been done for metallic ions (Ti, V, Cr, Mn, Fe, Co, Ni and Cu) with 11 and 12 electrons (iso-electronic series of Na and Mg). The observations for the energy range given in §3 are also valid here. The results are presented schematically in Figs. 10a to 10h.

The general form of the curves is similar to those for neon ions. The ionization cross section for energies smaller than 20 keV/amu become often too small to be calculated within the classical approximation. The cross sections given for the Na- and Mg-like ion of each element are slightly different. The addition of one electron results to an increase of the corresponding cross section except for ionization in the intermediate energy region. Also, the cross sections are increasing with Z . The σ_i maximum in units of πa_0^2 is increasing from 37 ($Z = 2$) to 68 ($Z = 29$) for an energy between 200 and 300 keV/amu. In the same units, σ_e for 10 keV/amu is increasing from 68 to 108.

5 - Ti, Cr, Fe AND Mo IONS COLLISIONS

In order to investigate the variation of the cross sections with increasing q and because such cross sections are needed for plasma modeling and diagnostics, we have done extensive calculations for collisions of Ti, Cr and Fe ions with H in a extended energy region ($E = 0.1$ to 1000 keV/amu). The results will be presented in their entirety in /8/. We present here only a brief review of the obtained cross sections.

Fig. 11. Cross sections of Ti ions colliding with H.

Some of the results obtained for Ti ions colliding with hydrogen are presented in the Fig. 11. Calculations for the lower ionization stages was necessary because the corresponding cross sections are departing from the hydrogen-like values. Ionization cross sections calculated for the $q = 1$ and $q = 2$ ionization stages have peculiar forms. Again the validity of these cross sections is questionable and further calculations on the basis of other theoretical methods are under way.

Selected results for Fe are shown in Fig. 12. Values for energies lower than 10 keV/amu will be given in /8/. The general form of the curves is similar to the neon case, although for lower q it is easier here to see the

Fig. 12. Cross sections of Fe ions colliding with H.

difference from the hydrogen-like curves. We have also calculated cross sections for Mo ions (Mo^{26+} and Mo^{42+}) which are of course hydrogen-like. The values obtained for Mo^{26+} lead to a curve in the Fig. 12. which cannot be differentiated from the curve corresponding to 26 times ionized iron. All potentials used were of the T-F type described earlier, except for totally stripped Fe and Mo. The expected crossings of the σ_i for various q are very noticeable. The obtained numerical values are in good agreement with the evaluated data collected in a recent review paper /15/.

Ionization cross sections for Fe and Mo ions collisions with H for energies of 50 to 500 keV/amu are presented in the Fig. 13 in order to show

Fig. 13. q dependence of ionization cross sections of Fe and Mo ions colliding with H.

their q dependence for $q = 3$ to 42. It can also be seen here that any low giving maxima q for each collision energy proportional to the energy value could be valid only for restricted energy regions.

6 - MODEL POTENTIALS ANALYSIS AND n CAPTURE

We have seen that in calculating with the CTMC method the cross sections of collisions of an ion N^{q+} with an hydrogen atom, three local potentials are used for the determination of the classical trajectories:

V_H , the potential of the H^+ core reacting with the electron e^-

V_N , the potential of the ion N^{q+} reacting with the hydrogen core H^+

V_e , the potential of the ion N^{q+} reacting with the electron e^-

Let r_{He} , r_{NH} and r_{Ne} be the distances between the three ions. $V_H = -1/r_{He}$ is perfectly defined and V_N plays an important role only at very low velocities. In our region of interest the approximation $V_H = q/r_{NH}$ is largely sufficient. Hence the problem of defining the potential V_e constitutes the main difficulty.

For partially ionized atoms there is two kinds of potentials allowing the description of the excited electron spectrum of the ion $N^{(q-1)+}$:

- Model potentials $V_e = -Y$ giving solutions of the equation $(T + V_e^n)Y = EY$ which reproduce both the excited states of the electron and the energy levels of the ion core (as usually, T stays here for the kinetic energy). The wave functions constituting the solution corresponding to this model potential and the real wave functions with the same quantum numbers n and l have the same nodes. If such a model potential is used for the study of the charge transfer it is necessary to divide each partial capture by the occupation rate of the considered level. An electron which could be captured in a occupied level is

then eliminated although in the reality it is simply canalized to an available bound level.

- Pseudo-potentials V_{eP} giving solutions of the equation $(T + V_{eP})Y = EY$ which reproduce only the states that the excited electron could access. In particular this potential V_{eP} must contain a repulsive part for short distances and low quantum numbers l which prevents the electron to occupy a state of the core. It is evident that in this case it is impossible to have a direct correspondence of the real quantum numbers with the calculated ones. In their general quantum formalism the potentials V_{eP} are depending on the angular momentum of the considered electron and are evidently non local.

In the case of CTMC calculations it seems that only the pseudo-potentials are giving satisfactory results. It is further possible to simplify the problem using a local potential independent from the angular momentum, $V_{eP} = V_e(r_{Ne})$ which must then satisfy the following conditions:

i) The lower energy is the ground level energy of the ion $N^{(q-1)+}$; given the form of the Eq. (2) this energy is $Z_e^2/2$.

ii) For very small distances we must return to the core charge, which insures that for very high energies the repulsive effect of the core could be neglected.

iii) For big distances the potential becomes hydrogen-like with charge q .

Note that the very fact of using a potential independent of the angular momentum implies that only the dependence on the final energy could be studied directly.

In order to determine precisely the excitation levels we have combined the WKB approximation with a complete solution of the Dirac equation on the potential V_e . The WKB treatment allows for controlling the number of nodes of the wavefunctions, situated outside the ion N^{q+} radius. Because of the inconsistency of the local potential $V_e(r_{Ne})$ we still have to waive the ambiguity concerning the quantum numbers. In so doing we have introduced the condition that for high excitation energies the levels have to coincide with those of an hydrogen-like ion with charge $q-1$. I.e. for the energy levels of the ion Fe^{13+} we can without ambiguity identify the level $n = 20$; departing from this level we find that the lower level corresponds to $n = 3$. This evidently constitutes an additional verification of the expression used for the potential. The energy levels of this ion (Fe^{13+}) can be seen in the Fig. 14 together with the levels of the corresponding hydrogen-like ion. Note that our results are different from those given previously in /4/, partly because of the different convention on the l distribution.

Because of the use of a momentum independent pseudo-potential as was previously noted, we are restricted here to calculate only the n -dependant electron capture. Let $E(n)$ be the lower energy among all $E(n,l)$. We consider that the electron is captured in the level n if its classical energy E_c verifies the inequality

$$0.5(E(n+1) + E(n)) \geq E_c \geq 0.5(E(n) + E(n-1))$$

and if there is no lower limit when $n = 1$.

Considering M classical trajectories and noting by P_N the number of trajectories leading to a capture of the electron to the level n and by r_{TOT} the total cross section we obtain the following definitions:

- partial cross section $r(n) = r_{tot} / M_R$
- inverse of the $1/n$ mean value $N \text{ moy} = \left[\left(\sum \frac{1}{i} P_i \right) / M_R \right]^{-1}$
- inverse of the $1/n^2$ mean value $N^2 \text{ moy} = \left[\left(\sum \frac{1}{i^2} P_i \right) / M_R \right]^{-1}$
- mean energy $E \text{ moy} = \sum E_i P_i / M_R$
- mean square energy $E^2 \text{ moy} = \sum P_i E_i^2 / M_R$
- statistical uncertainty $s(n) = r(n) \sqrt{\frac{M_R - P_i}{M_R (M_R - 1)}}$

with $M_R = \sum P_i$. The definition of $N \text{ moy}$ allows to circumvent the influence of the statistical errors over the high quantum numbers.

Fig. 14. The levels of the $\text{Fe}^{13+} + e^-$ ion in comparison with those corresponding to a Coulomb potential.

Table 2 is giving some of our results obtained for neon and the hydrogen-like ions H^+ , He^{++} and C^{6+} for energies of 25, 80 and 200 keV/amu. A comparison of our results with results obtained also with the CTMC method by Olson and Schultz /16/ is given in the Fig. 15. It can be seen that the two calculations are in good agreement.

Table 2. Calculated n-resolved Charge Transfer Cross Sections for Ion Collisions with Hydrogen.

Ne 2+, 25keV/a				
partial cross section				
n	r	s		
1	0.000	0.000		
2	0.675	0.017		
3	5.078	0.042		
4	0.785	0.018		
5	0.228	0.010	N moy.	3.050
6	0.098	0.006	N^2 moy.	8.842
7	0.056	0.005	E moy.	0.464
8	0.032	0.004	E^2 moy.	0.336
9	0.027	0.003	r tot	7.040
10	0.011	0.002		
11	0.009	0.002		
12	0.005	0.001		
13	0.008	0.002		
14	0.002	0.001		
15	0.005	0.001		
16	0.003	0.001		
17	0.003	0.001		
18	0.001	0.001		
19	0.003	0.001		
20	0.001	0.001		

Ne 3+, 25keV/a				
partial cross section				
n	r	s		
1	0.000	0.000		
2	2.124	0.035		
3	8.981	0.067		
4	1.686	0.032		
5	0.418	0.016	N moy.	2.955
6	0.172	0.010	N^2 moy.	8.226
7	0.078	0.007	E moy.	0.737
8	0.053	0.006	E^2 moy.	0.706
9	0.043	0.005	r tot	13.650
10	0.022	0.004		
11	0.011	0.003		
12	0.009	0.002		
13	0.012	0.003		
14	0.005	0.002		
15	0.006	0.002		
16	0.004	0.002		
17	0.003	0.001		
18	0.003	0.001		
19	0.002	0.001		
20	0.003	0.001		

Ne 2+, 80keV/a				
partial cross section				
n	r	s		
1	0.0	0.0		
2	0.1064	0.0049		
3	0.4094	0.0095		
4	0.1900	0.0065		
5	0.0852	0.0044	N moy.	3.478
6	0.0517	0.0034	N^2 moy.	10.62
7	0.0334	0.0027	E moy.	0.396
8	0.0287	0.0025	E^2 moy.	0.244
9	0.0206	0.0022	r tot	0.96
10	0.00630	0.0012		
11	0.0043	0.0010		
12	0.0045	0.0010		
13	0.0027	0.0008		
14	0.0027	0.0008		
15	0.002	0.0007		
16	0.002	0.0007		
17	0.0014	0.0006		
18	0.0009	0.0005		
19	0.0007	0.0004		
20	0.0007	0.0004		

Ne 3+, 80keV/a				
partial cross section				
n	r	s		
1	0	0		
2	0.348	0.012		
3	1.09	0.02		
4	0.772	0.017		
5	0.433	0.013	N moy.	3.796
6	0.253	0.010	N^2 moy.	12.169
7	0.149	0.008	E moy.	0.488
8	0.118	0.007	E^2 moy.	0.257
9	0.09	0.006	r tot	3.508
10	0.056	0.005		
11	0.037	0.004		
12	0.029	0.003		
13	0.019	0.003		
14	0.016	0.002		
15	0.015	0.002		
16	0.011	0.002		
17	0.008	0.002		
18	0.009	0.002		
19	0.005	0.001		
20	0.007	0.002		

Table 2. Calculated n-resolved Charge Transfer Cross Sections for Ion Collisions with Hydrogen (continued).

Ne 5+, 25keV/a				
partial cross section				
n	r	s		
1	0.0	0.0		
2	1.27	0.036		
3	13.65	0.108		
4	8.69	0.090		
5	1.63	0.041	N moy.	3.36
6	0.45	0.022	N ² moy.	10.66
7	0.19	0.014	E moy.	1.07
8	0.11	0.011	E ² moy.	1.35
9	0.05	0.008	r tot	26.24
10	0.04	0.006		
11	0.03	0.006		
12	0.03	0.005		
13	0.02	0.005		
14	0.01	0.003		
15	0.01	0.003		
16	0.01	0.002		
17	0.0	0.002		
18	0.01	0.003		
19	0.01	0.003		
20	0.0	0.001		

Ne 10+, 25keV/a				
partial cross section				
n	r	s		
1	0.0	0.0		
2	0.0	0.0		
3	0.01	0.004		
4	1.16	0.048		
5	15.67	0.169	N moy.	5.81
6	29.39	0.22	N ² moy.	33.07
7	7.16	0.117	E moy.	1.51
8	1.55	0.055	E ² moy.	2.49
9	0.6	0.035	r tot	56.21
10	0.29	0.024		
11	0.13	0.016		
12	0.08	0.013		
13	0.03	0.008		
14	0.03	0.008		
15	0.02	0.006		
16	0.01	0.006		
17	0.01	0.004		
18	0.01	0.004		
19	0.01	0.004		
20	0.01	0.004		

Ne 5+, 80keV/a				
partial cross section				
n	r	s		
1	0.0	0.0		
2	0.528	0.032		
3	2.149	0.065		
4	2.584	0.070		
5	2.038	0.063	N moy.	4.636
6	1.331	0.051	N ² moy.	17.566
7	0.894	0.042	E moy.	0.657
8	0.600	0.035	E ² moy.	0.743
9	0.445	0.030	r tot	12.18
10	0.304	0.025		
11	0.238	0.022		
12	0.181	0.019		
13	0.159	0.018		
14	0.121	0.016		
15	0.103	0.014		
16	0.075	0.012		
17	0.048	0.010		
18	0.040	0.009		
19	0.046	0.010		
20	0.046	0.010		

Ne 10+, 80keV/a				
partial cross section				
n	r	s		
1	0.0	0.0		
2	0.0	0.0		
3	0.12	0.037		
4	0.91	0.102		
5	3.63	0.202	N moy.	7.925
6	5.93	0.255	N ² moy.	54.83
7	6.82	0.272	E moy.	0.912
8	4.78	0.230	E ² moy.	1.294
9	3.98	0.211	r tot	39.76
10	2.55	0.170		
11	2.34	0.163		
12	1.74	0.141		
13	1.29	0.122		
14	0.91	0.102		
15	0.77	0.094		
16	0.70	0.090		
17	0.46	0.073		
18	0.40	0.068		
19	0.31	0.060		
20	0.30	0.059		

Table 2. Calculated n-resolved Charge Transfer Cross Sections for Ion Collisions with Hydrogen (continued).

He 2 + , 25keV/a					
partial cross section					
n	r	s			
1	0.16	0.015			
2	7.35	0.092			
3	1.53	0.046			
4	0.33	0.022			
5	0.13	0.014	N moy.	2.162	
6	0.046	0.008	N ^ 2 moy.	4.409	
7	0.035	0.007	E moy.	0.454	
8	0.026	0.006	E ^ 2 moy.	0.263	
9	0.015	0.005	r tot	9.665	
10	0.012	0.004			
11	0.010	0.004			
12	0.007	0.003			
13	0.006	0.003			
14	0.000	0.000			
15	0.001	0.001			
16	0.001	0.001			
17	0.003	0.002			
18	0.000	0.000			
19	0.000	0.000			
20	0.001	0.001			

C 6+, 25keV/a					
partial cross section					
n	r	s			
1	0.0	0.0			
2	0.03	0.017			
3	3.91	0.181			
4	21.17	0.414			
5	6.47	0.232	N moy.	4.105	
6	1.27	0.103	N^2 moy.	16.28	
7	0.39	0.057	E moy.	1.105	
8	0.18	0.039	E^2 moy.	1.388	
9	0.07	0.024	r tot	33.75	
10	0.06	0.022			
11	0.05	0.021			
12	0.02	0.012			
13	0.02	0.012			
14	0.03	0.015			
15	0.0	0.0			
16	0.01	0.008			
17	0.03	0.015			
18	0.01	0.008			
19	0.01	0.008			
20	0.02	0.012			

He 2 + , 200keV/a				
partial cross section				
n	r	s		
1	0.015	0.0014		
2	0.025	0.0019		
3	0.010	0.0012		
4	0.004	0.0007		
5	0.002	0.0005	N moy.	1.787
6	0.001	0.0003	N ^ 2 moy.	2.558
7	0.000	0.0001	E moy.	0.782
8	0.000	0.0002	E ^ 2 moy.	1.684
9	0.000	0.0001	r tot	0.057
10	0.000	0.0000		
11	0.000	0.0000		
12	0.000	0.0000		
13	0.000	0.0002		
14	0.000	0.0000		
15	0.000	0.0000		
16	0.000	0.0001		
17	0.000	0.0000		
18	0.000	0.0000		
19	0.000	0.0000		
20	0.000	0.0001		

C 6+, 200keV/a					
partial cross section					
n	r	s			
1	0.0	0.0			
2	0.04	0.004			
3	0.18	0.007			
4	0.21	0.008			
5	0.17	0.007	N moy.	4.88	
6	0.11	0.006	N ^2 moy.	18.88	
7	0.09	0.005	E moy.	0.95	
8	0.06	0.004	E ^2 moy.	1.90	
9	0.05	0.004	r tot	1.12	
10	0.04	0.003			
11	0.03	0.003			
12	0.02	0.003			
13	0.01	0.002			
14	0.02	0.002			
15	0.01	0.002			
16	0.01	0.002			
17	0.01	0.002			
18	0.0	0.001			
19	0.01	0.001			
20	0.01	0.001

Fig. 15. n - resolved partial cross sections for C and Ne stripped ions

Our results show that N_{moy} , the square root of N^2_{moy} and also the position of maximum n_m are very close at 25 keV and they spread with increasing energy. N_{moy} varies with the energy much faster than n_m . This is due to the spread of the levels distribution for higher energy.

Also, comparison with the results for hydrogen-like ions show an important difference only for the cases $q = 1$ and $q = 2$. Could this observation be verified to other cases, it would mean that the results for the hydrogen-like ions are also valid for partially ionized species; consequently, the forbidden levels have a negligible contribution.

For a low energy Olson is giving in /17/ a q -dependence of n_m (and then of N_{moy}) proportional to $q^{3/4}$. The formalism developed by Bell /18/, is giving for small velocities and high q a $\sqrt{q}$ dependence for E_{moy} , i.e. again a $q^{3/4}$ dependence for N_{moy} . In the Fig. 16 the quantities $N_{moy}/q^{3/4}$ and $2E_{moy}/\sqrt{q}$ are given for the ions of neon and for H^+ , He^{++} and C^{6+} . The aforementioned relations for N_{moy} and E_{moy} are well valid beginning with $q = 5$. For $q = 1$ and $q = 2$ the results are totally different both for neon and for H^+ , He^{++} and C^{6+} . It still has to be verified if this is due to the energy being too high or to a restriction of the applicability only to higher q as suggested by Bell.

Finally, it has been verified that neither the results obtained with the OBK approximation, nor the Eikonal correction proposed by Eichler and Chan /19/ could be of use in this energy range.

Fig. 16. q - dependence of N moy and E moy.

7 - HYDROGEN IONIZATION DEPENDENCE ON EXCITED LEVELS

We obtained results for ionization of excited hydrogen by fully stripped ions of $Z = 1, 2, 6, 10, 13, 18$ and 26 . Preliminary results for $n = 1$ and 2 , have been presented at the First Research Coordination Meeting of the IAEA Coordinated Research Programme (CRP) on "Atomic and Molecular Data for Fusion Edge Plasmas" held in Vienna in September 1990 (see /20/). It has been shown that the behavior of $n = 1$ and $n = 2$ levels of hydrogen is quite different. As expected, for proton projectiles the discrepancy for $n = 2$ with the first Born approximation is reduced in comparison with previous calculations from Rivarola and collaborators.

8 - CONCLUSIONS AND PROSPECTIVES OF CONTINUATION OF THIS WORK

Evaluation of cross sections for various ions collisions with hydrogen was performed with a statistical error lower than 5%. It has to be appreciated however, that in absence of sufficient experimental data, the confidence of these values has still to be tested by comparison with results from other theoretical methods and using them in models for description and diagnostics of confined and astrophysical plasmas.

The work on metallic impurities continue with evaluation of cross sections for collisions at lower energies and with He targets in collaboration with the Atomic and Molecular Data Unit of the IAEA. Results were discussed in the IAEA Advisory Group Meeting on "A+M Data for Metallic Impurities in Fusion Plasmas", Vienna, May 1990 and are now in press /8/.

Because of the availability of experimental data for argon ions collisions, we are looking forward to calculate cross sections involving these ions. Cross sections involving neon and light elements ions as projectiles will also be investigated for lower collision energies in the frame of the aforementioned CRP of the IAEA on edge plasmas. Our CTMC code was modified in order to calculate cross sections of collisions involving He targets and a number of heavy and light ion projectiles for lower energies. Results on neon ions will be eventually used for developing a collisional - radiative model for diagnostics of Tokamak plasmas. The possibilities of collaboration with the Spectroscopy Group of the CEA Nuclear Fusion Department at Cadarache for the elaboration of such a model are presently investigated.

Work in progress includes CTMC calculations of ionization and charge transfer cross sections also for heavier species. Preliminary results for I_{α}

ions colliding with hydrogen were presented recently /21/. These calculations are part of our contribution within the SPQR group working on various aspects of inertial fusion research.

9 - ACKNOWLEDGMENTS

Development of this work could not be possible without the precious help of Professor M.R.C. McDowell. We are missing him.

Big part of the numerical calculations was effectuated at the "Paris-Sud Informatique" (PSI) mainframe of the University of Paris-Sud at Orsay. Contribution and encouragement from the Spectroscopy Group of the CEA Nuclear Fusion Department at Cadarache is also acknowledged.

REFERENCES

- /1/ Janev, R.K. and Katsonis, K., Nucl. Fusion 27 (1987) 1493.
- /2/ Olson, R.E. and Salop, A., Phys. Rev. A 16 (1977) 531.
- /3/ Olson, R.E., "Electron Capture between Multiply Charged Ions and One Electron Targets", in "Electronic and Atomic Collisions", N. Oda and K. Takayanagi Edts., North Holland, Amsterdam (1980) 391.
- /4/ McDowell, M.R.C. and Janev, R.K., J. Phys. B 18 (1985) L295.
- /5/ McDowell, M.R.C. and Janev, R.K., J. Phys. B 17 (1984) 2295.
- /6/ Katsonis, K. and Maynard, G., "Evaluation of Atomic Data for Fusion at Orsay", Report GA-4/244, GAPHYOR, Orsay, September (1980).
- /7/ Katsonis, K. and Maynard, G., "Ionisation et Transfert de Charge des Ions Ne avec des Atomes d'Hydrogène", Report GA-5/245, GAPHYOR, Orsay, November (1980).
- /8/ Janev, R.K., Katsonis, K. and Maynard, G., Phys. Scripta (1991), Katsonis, K., Maynard, G. and Janev, R.K., Phys. Scripta (1991), Maynard, G., Janev, R.K. and Katsonis, K., Phys. Scripta (1991), in press
- /9/ Janev, R.K., Presnyakov, L.P. and Shevelko, V.P., "Physics of Highly Charged Ions" J. Springer, Berlin (1985).
- /10/ Carlson, T.A., Nestor, C.W., Wasserman, N. and McDowell, J.D., At. Data 2 (1970) 63.
- /11/ Knudsen, H., "Electron Capture and Target Ionization by Medium and High-Velocity Multiply Charged Ions" in "Physics of Electronic and Atomic Collisions", S. Datz Edt., (1982) 657.
- /12/ Janev, R.K. and Hvelplund, P., Comm. Atom. Mol. Phys. 11 (1981) 75.
- /13/ Gilbody, H.B., Adv. Atom. Molec. Phys. 22 (1985) 143.
- /14/ Gillespie, G.H., J. Phys. B., 15 (1982) L729.
- /15/ Phaneuf, R.A., Janev, R.K. and Hunter, H.T., "Charge Exchange Processes Involving Iron Ions", Nucl. Fusion SS (1987) p. 7.
- /16/ Olson, R.E. and Schultz, D.R., Phys. Scripta 28 (1989).
- /17/ Olson, R.E., Phys. Rev. A24 (1981) 1726.
- /18/ Bell, G.I., Phys. Rev. 90 (1953) 548.
- /19/ Eichler and Chan, Phys. Rev. 28 (1979) 113.
- /20/ Janev, R.K. Edt. "First Coordination Meeting on Atomic and Molecular Data for Fusion Edge Plasmas" IAEA Report, Vienna, September (1990).
- /21/ Katsonis, K. and Maynard, G., "Echange de Charge entre Niveaux Excités d'Ions Multichargés Rapides et H. Conséquences pour la Charge Effective dans un Plasma Dense" in "SFP, Deuxième Congrès de la Division Plasma", Orsay (1990).