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1980 J. Phys. B: At. Mol. Phys. 13 4233

(http://iopscience.iop.org/0022-3700/13/21/016)

J. Phys. B. Atom. Molec. Phys. **13** (1980) 4233–4244. Printed in Great Britain

Single-electron excitation and ionisation processes in atom–multicharged-ion collisions

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Received 22 April 1980

Abstract. The single-electron excitation and ionisation processes in collisions of atoms with multiply charged ions are considered using the dipole approximation for the atom–ion interaction and a close-coupling method based on atomic states. In the case of ionisation the application of the close-coupling method is simplified by the introduction of an effective oscillator strength for the coupling of the discrete initial state with the continuum.

1. Introduction

The inelastic collision processes of multiply charged ions with neutral atoms have recently become an important field of research in connection with the role they play in thermonuclear fusion plasmas (see e.g. Harrison 1978, Drawin 1978) and in astrophysics (Steigman 1975). Much work, both experimental and theoretical, has already been devoted to the charge exchange processes of this type (see e.g. the recent reviews of Olson (1980) and Salzborn and Müller (1980)). Contrary to this, the excitation and ionisation processes in atom–multicharged-ion collisions have so far been relatively little investigated. This is particularly true for the low and intermediate collision energy regions.

On the theoretical side, atomic ionisation due to a highly charged particle impact has been considered within the context of inner-shell collision phenomena (see e.g. Crasemann 1975, Hansteen 1975). However, the types of approximations used in this context, such as the plane-wave Born approximation (or its time-dependent analogue, the semiclassical approximation), binary encounter approximation, etc, are not really adequate for treating the single-electron impact ionisation in atom–multicharged-ion collisions (Salop and Eichler 1979). For this purpose the first Magnus (or sudden) approximation (Salop and Eichler 1979), the classical-trajectory Monte-Carlo method (Olson and Salop 1977, Olson *et al* 1977, Olson 1978) and the Glauber method (Golden and McGuire 1976), each applied in the region of its validity have proved to be much more adequate.

The excitation process in collisions of multiply charged (or fully stripped) ions with atoms has been theoretically treated mostly by the high-energy approximations (see e.g. McDowell and Coleman 1970), and specific cross section calculations have been done only for singly and doubly charged ions.

0022-3700/80/214233+12$01.50

In the present paper we shall consider the single-electron excitation and ionisation processes

$$A + B^{Z+} \rightarrow A^* + B^{Z+} \tag{1}$$

$$\rightarrow A^+ + B^{Z+} + e \tag{2}$$

where A is a ground-state atom and B^{Z+} is a multicharged ion with charge Z. We exclude from our consideration the excitation and ionisation processes which result from a many-electron transition in the system (Auger processes). In the adiabatic energy region ($v \ll v_0$, v is the relative collision velocity and $v_0 \simeq 2{\cdot}2 \times 10^8$ cm s^{-1} is the atomic velocity unit), processes (1) and (2) are characterised by cross sections which are much smaller than the corresponding charge exchange cross section. At the intermediate energies ($v \sim 1$–$2v_0$), however, processes (1) and (2) become competitive to the charge exchange and at still higher energies ($v \gg v_0$) they are dominant inelastic processes in an atom–multicharged-ion collision. Therefore, our present study of the processes (1) and (2) will be mainly confined to the intermediate and high-energy region. At these energies the electronic transitions involved in the single-electron excitation and ionisation processes can be considered as being caused by the ion–atom interaction (we use atomic units from now on)

$$V(\boldsymbol{r}, \boldsymbol{R}) = -\frac{Z}{|\boldsymbol{R}(t) - \boldsymbol{r}|} \tag{3}$$

where $\boldsymbol{r}$ is the radius vector of the active electron with respect to the centre of the atom and R is the ion–atom (internuclear) distance. Since Z in equation (3) may be large, the use of a perturbational treatment in the electron transition problem is not appropriate. More adequate for the purposes of transition probability and cross section calculations is the use of the close-coupling method, based on an atomic basis expansion of the electron wavefunction. However, the direct numerical solution of the corresponding close-coupled equations, even when they are truncated to a reasonably small number, is an extremely difficult task. Besides, on the basis of such numerical solutions one cannot obtain any general analytical properties of the considered processes in a sufficiently wide range of variation of the parameters (e.g. scaling laws, etc). In order to get information on the general features of the excitation and ionisation cross sections, we shall confine ourselves in the present paper to the case of strong coupling of only two states and then use an analytical method for solving the electron transition problem. In the case of ionisation we shall also consider a third state, in order to account for the transitions into the continuum through intermediate discrete states. To get the results for the transition probabilities and the cross sections in a closed analytical form, we shall restrict ourselves to the dipole approximation for the interaction potential, namely

$$V(\boldsymbol{R}, \boldsymbol{r}) \simeq -Z\frac{\boldsymbol{d} \cdot \boldsymbol{R}}{R^3} \tag{4}$$

where $\boldsymbol{d}$ is the dipole moment. Although our derivations are of a general character, the practical cross section calculations of the excitation and ionisation processes will be, in the framework of the present paper, restricted to collisions of hydrogen atoms with fully stripped ions.

In § 2 we consider in detail the $ns \rightarrow n'p$ excitation processes, whereas the ionisation process is considered in § 3. In § 4 we give the conclusions.

2. Excitation

The solution of the problem of $ns \to n'p$ atomic transitions, caused by the potential (4), requires the solving of three coupled equations for the amplitudes of the states ns, $n'p$ ($m = 0$) and $n'p$ ($|m| = 1$), where m is the magnetic quantum number. If one makes use of the perturbed rotating-atom (PRA) approximation introduced by Bates (1959), then the system of coupled equations reduces to two (the transition with $|\Delta m| = 1$ does not take place), and the problem is considerably simplified. However, the PRA approximation is inadequate for a more detailed description of the excitation process and, in particular, it overestimates the cross section by a factor greater than two in the high-energy region. Therefore, we shall treat the problem of $ns \to n'p$ transitions keeping the axis of quantisation fixed. In that case, the system of coupled equations for the amplitudes a, b_0 and b_1 of the states ns, $n'p$ ($m = 0$) and $n'p$ ($|m| = 1$), respectively, and with the ion–atom interaction in the form of equation (4), has the form (Bates 1959, Presnyakov 1964a):

$$i\frac{da}{dt} = \frac{Z\lambda}{R^2}(\cos\theta b_0 + \sin\theta b_1)\exp(-i\omega t) \tag{5a}$$

$$i\frac{db_0}{dt} = \frac{Z\lambda}{R^2}\cos\theta\exp(i\omega t)a \tag{5b}$$

$$i\frac{db_1}{dt} = \frac{Z\lambda}{R^2}\sin\theta\exp(i\omega t)a \tag{5c}$$

$$\cos\theta = \frac{vt}{R} \qquad \sin\theta = \frac{\rho}{R} \qquad \lambda = \left(\frac{f_{01}}{2\omega}\right)^{1/2} \tag{6}$$

where ω is the energy difference between the $|ns\rangle \equiv |0\rangle$ and $|n'p\rangle \equiv |1\rangle$ states, f_{01} is the oscillator strength of the $ns \to n'p$ transition and ρ is the impact parameter. In solving the coupled equations (5) with the usual initial conditions $a(-\infty) = 1$ and $b_{0,1}(-\infty) = 0$ we first use the transformation from the amplitudes $a(t)$ and $b_i(t)$ ($i = 0, 1$) to the new functions $k_i(t) = -ib_i(t)/a(t)$ (Presnyakov 1964a). The resulting equations for the functions $k_i(t)$ are then solved by the approximate method due to Vainshtein *et al* (1962). Denoting $|k_i(+\infty)|^2$ by P_i, one obtains the following result for the $ns \to n'p$ transition probability $W(\rho)$

$$W(\rho) = W_0(\rho) + W_1(\rho) \tag{7}$$

$$W_0(\rho) = |b_0(+\infty)|^2 = \frac{P_0}{1 + P_0 + P_1} \tag{8a}$$

$$W_1(\rho) = |b_1(+\infty)|^2 = \frac{P_1}{1 + P_0 + P_1} \tag{8b}$$

$$P_0 = \left(\int_{-\infty}^{+\infty} dt \frac{Z\lambda vt}{R^3}\sin\left\{\int_0^t \left[\omega^2 + 4\left(\frac{Z\lambda}{R^2(t')}\right)^2\right]^{1/2} dt'\right\}\right)^2 \tag{9a}$$

$$P_1 = \left(\int_{-\infty}^{+\infty} dt \frac{Z\lambda\rho}{R^3}\cos\left\{\int_0^t \left[\left(\frac{\omega}{2}\right)^2 + \left(\frac{Z\lambda}{R^2(t')}\right)^2\right]^{1/2} dt' + \frac{\omega t}{2}\right\}\right)^2. \tag{9b}$$

An important property of the transition probability (7)–(9) is that it is properly normalised and has non-singular behaviour for $\rho \to 0$. This property of the probability

$W(\rho)$ remains valid also in the perturbational limit ($\frac{1}{2}\omega \gg Z\lambda/R^2$), when P_0 and P_1 go over into the well known result (Seaton 1964)

$$P_0 = \left[\frac{2Z\lambda\omega}{v^2} K_0\left(\frac{\omega\rho}{v}\right)\right]^2 \qquad P_1 = \left[\frac{2Z\lambda\omega}{v^2} K_1\left(\frac{\omega\rho}{v}\right)\right]^2 \tag{10}$$

where $K_0(x)$ and $K_1(x)$ are the MacDonald functions. If we introduce in equations (9) the scaling transformations

$$\rho = \frac{Z\lambda}{v} y \qquad vt = \frac{Z\lambda}{v} x \tag{11}$$

and define parameter β by the relation

$$\beta = \frac{Z\lambda\omega}{v^2} \tag{12}$$

then P_0 and P_1 can be put in the form

$$P_0 = \left[\int_{-\infty}^{+\infty} \frac{x\,\mathrm{d}x}{(x^2+y^2)^{3/2}} \sin\left(\int_0^x [\beta^2 + 4(x'^2+y^2)^{-2}]^{1/2}\,\mathrm{d}x'\right)\right]^2 \tag{13a}$$

$$P_1 = \left[\int_{-\infty}^{+\infty} \frac{y\,\mathrm{d}x}{(x^2+y^2)^{3/2}} \cos\left(\int_0^x [(\tfrac{1}{2}\beta)^2 + (x'^2+y^2)^{-2}]^{1/2}\,\mathrm{d}x' + \tfrac{1}{2}\beta x\right)\right]^2 \tag{13b}$$

i.e. $P_0 = P_0(y|\beta)$ and $P_1 = P_1(y|\beta)$. It follows from equations (7), (8) and (13) that the excitation cross section can be represented in the form

$$\sigma_{ex} = 2\pi \int_0^\infty \rho\,\mathrm{d}\rho\, W(\rho, v, Z\lambda, \omega)$$

$$= 2\pi\left(\frac{Z\lambda}{v}\right)^2 \int_0^\infty y\,\mathrm{d}y \frac{P_0(y|\beta) + P_1(y|\beta)}{1 + P_0(y|\beta) + P_1(y|\beta)} \tag{14}$$

$$= 2\pi(Z\lambda/v)^2 Q(\beta) = 2\pi(Z\lambda/\omega) D(\beta) \tag{15}$$

where

$$D(\beta) = \beta Q(\beta). \tag{16}$$

The values of the function $Q(\beta)$ have been calculated previously for several particular values of β (Presnyakov 1964b, Vinogradov 1966). We have calculated the function $D(\beta)$ in a wide region of the parameter β and the results are given on table 1. For $\beta > 2$

Table 1. Values of the function $D(\beta)$ for $0{\cdot}04 \leqslant \beta \leqslant 2$.

β	$D(\beta)$	β	$D(\beta)$
0·04	0·202	0·200	0·401
0·05	0·221	0·25	0·406
0·066	0·268	0·28	0·410
0·083	0·291	0·333	0·399
0·100	0·332	0·500	0·385
0·143	0·365	1·00	0·212
0·1666	0·381	2·00	0·132

(adiabatic energy region) and for $\beta \ll 0{\cdot}01$ (the region of validity of Born approximation) the function $D(\beta)$ can be approximated by the following expressions:

$$D(\beta) \simeq \frac{\beta}{2}\left(1 - \frac{1}{8\beta^{3/2}}\right) \exp[-(2\beta)^{1/2}] \qquad \beta > 2 \tag{17}$$

$$D(\beta) \simeq 4\beta \ln(1{\cdot}4/\beta) \qquad \beta \ll 0{\cdot}01. \tag{18}$$

By using expression (18) for $D(\beta)$ in equation (15), one obtains

$$\sigma_{ex}^{(B)} = 8\pi\left(\frac{Z\lambda}{v}\right)^2 \ln\left(\frac{1{\cdot}4v^2}{Z\lambda\omega}\right) \tag{19}$$

which also follows from the general Bethe–Born theory (see e.g. Landau and Lifshitz 1974).

Note that in equation (15) for σ_{ex} the factor in front of $D(\beta)$ does not depend on velocity. As can be seen from table 1, the excitation cross section reaches its maximum for $\beta_m = 0{\cdot}28$, which corresponds to the velocity

$$v_m \simeq 1{\cdot}89(Z\lambda\omega)^{1/2}. \tag{20}$$

The cross section value in the maximum is given by

$$\sigma_{ex,m} \simeq 0{\cdot}82\pi Z\lambda/\omega \tag{21}$$

and linearly depends on Z. Thus, the maximum of the excitation cross section scales like Z, whereas its velocity position scales as $Z^{1/2}$. The reduced excitation cross section $\tilde{\sigma}_{ex} = \sigma_{ex}\omega/Z\lambda$ when plotted against the reduced energy $\tilde{E} = \beta^{-1}$ in amu is represented by a universal curve

$$\tilde{\sigma}_{ex}(\tilde{E}) = 2\pi D(\beta^{-1}). \tag{22}$$

By using formula (15) for σ_{ex}, the tabulated values $D(\beta)$, and expressions (17) and (18), one can easily calculate the cross section for the $ns \to n'p$ excitation transitions in the dipole close-coupling approximation.

As an illustration of the results obtained we have calculated the cross sections for the $1s \to n'p$ transitions ($n' = 2, 3, 4, 5$) in $H(1s) + Z$ collisions ($Z = 1, 2, 4, 6, 8, 10$). The results are shown in figures 1–3.

The use of the dipole approximation in treating the $ns \to n'p$ transitions within the three-state close-coupling scheme has resulted in a simple parametrisation of the excitation cross section (see equation (15)) and simple scaling laws (equation (22)). An attempt at going beyond the dipole approximation (which is equivalent to the inclusion of the distortion effects) immediately leads to the appearance of the diagonal matrix elements of the interaction in the probability terms P_0 and P_1. In that case a simple parametrisation of the excitation cross section cannot be obtained. Estimates of the influence of distortion effects on the excitation cross section have shown that they are important only in the adiabatic region and that the cross section in the region of its maximum and above it not considerably changed. Since in the present paper we are interested mainly in the intermediate and high-energy regions, where the excitation and ionisation cross sections are of the order of the charge exchange cross section or greater, we shall not go into a detailed discussion of the excitation process in the low-energy region.

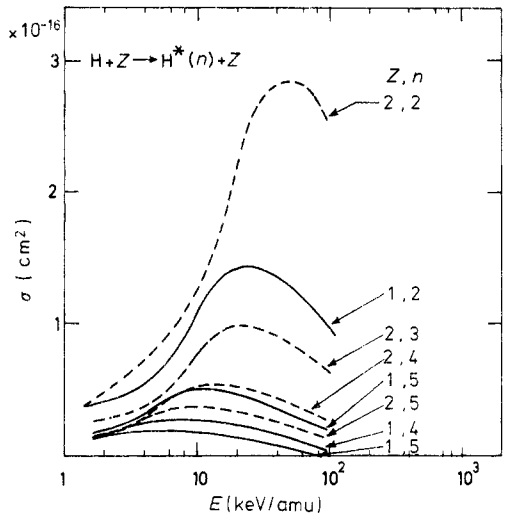

Figure 1. Cross sections for the H(1s) + Z → H(np) + Z excitation (Z = 1, 2; n = 2 – 5) in the dipole two-state close-coupling approximation.

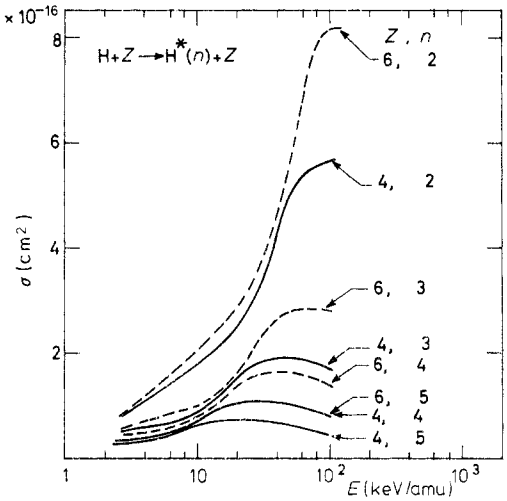

Figure 2. Same as in figure 1, except for Z = 4 and Z = 6.

3. Ionisation

The problem of ionisation in atom–multicharged-ion collisions is much more complex than that of excitation. The reason is that the corresponding system of coupled differential equations of the close-coupling method in the case of ionisation is transformed into a system of coupled integro-differential equations, which is much more difficult to solve. At high collision velocities ($v \gg 1$), one would expect theoretical methods like the plane-wave Born approximation, the sudden approximation, etc, to be valid for the ion–atom ionisation problem. However, for highly charged ions ($Z \gg 1$) the validity region of the above high-energy approximations is restricted to extremely high energies.

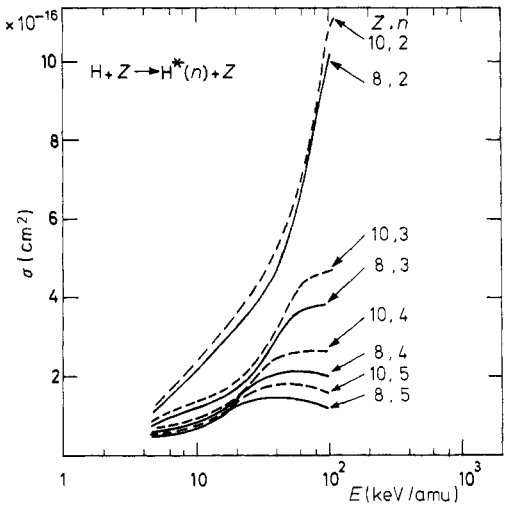

Figure 3. Same as in figure 1, except for $Z = 8$ and $Z = 10$.

In the present section we propose an approach to the ionisation problem in atom–multicharged-ion collisions, based on the close-coupling method and on the introduction of an effective oscillator strength for the transitions into the continuum. Using the concept of the effective oscillator strength (van Regemorter 1962), we replace the continuous spectrum by an effective energy level and then we can use the close-coupling method as in the case of transitions within the discrete spectrum.

Let us define the effective continuum oscillator strength by the expression

$$f_{\text{eff}} = \kappa f_{\text{cont}} \tag{23}$$

where

$$f_{\text{cont}} = \tfrac{2}{3}\int_0^\infty f_{0\epsilon}(\epsilon)\,\mathrm{d}\epsilon \tag{24}$$

is the 'ordinary' continuum oscillator strength and κ is a factor which accounts for the contribution of the higher multipoles in the total ionisation cross section. The numerical values of f_{cont} and κ can be determined on the basis of quantum-mechanical calculations of the oscillator strengths, presented, for instance, in the book of Vainshtein *et al* (1979). For the hydrogen atom, for example, $f_{\text{cont}} = 0{\cdot}4350$ and $\kappa = 1{\cdot}5$. In accordance with definition (6), the strength of the effective dipole potential for the ionisation process is given by

$$\lambda_{\text{eff}} = \left(\frac{f_{\text{eff}}}{2\omega_{\text{ion}}}\right)^{1/2} \tag{25}$$

where ω_{ion} is the ionisation potential of the atom, ($\omega_{\text{ion}} = \frac{1}{2}$ for H, and, consequently $\lambda_{\text{eff}}(\text{H}) = 0{\cdot}808$). The calculation of the ionisation cross section, corresponding to the transition $n\text{s} \to \epsilon\text{p}$ (ϵ is the electron energy in the continuum) can now be performed by using the same formulae as in the case of $n\text{s} \to n'\text{p}$ excitation (see equations (15), (17), (18) and table 1) with $\lambda = \lambda_{\text{eff}}$. We have performed such calculations for the $n\text{s} \to \epsilon\text{p}$ ionisation transition in $\text{H}(1\text{s}) + \text{H}^+$ collisions and the result is shown in figure 4 (the

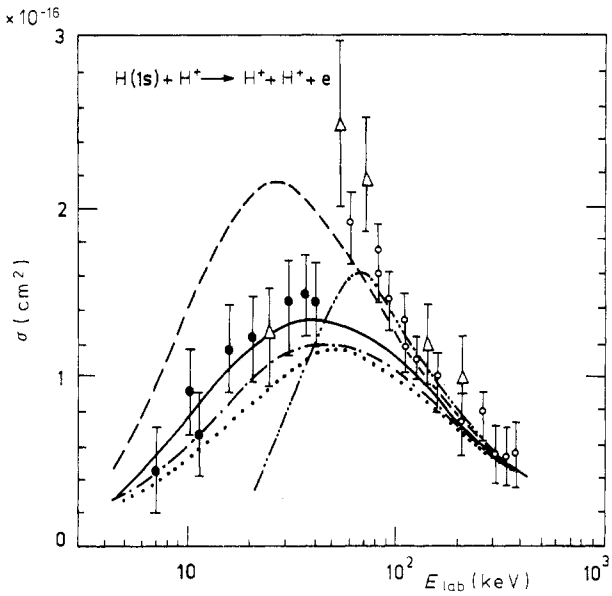

Figure 4. Cross sections for the $H(1s)+H^+ \rightarrow H^+ + H^+ + e$ reaction. Experimental points: ● are data of Fite *et al* (1960); ○ are data of Gilbody and Ireland (1964); △ are data of Park *et al* (1977). Theoretical calculations: the full curve is the result of dipole close-coupling approximation with inclusion of transitions via the 2p resonant state; the single-dotted chain curve is the result of dipole two-state close-coupling approximation ($1s \rightarrow \epsilon p$ transitions only); the broken curve is the first Born approximation result of Bates and Griffing (1953); the double-dotted chain curve is the result of Olson and Salop (1977) obtained by the classical trajectory Monte-Carlo method and the dotted curve is the result of Glauber theory (Golden and McGuire 1975).

single-dotted chain curve). The experimental data in this figure are those of Fite *et al* (1960), Gilbody and Ireland (1964) and Park *et al* (1977), whereas the theoretical curves are due to Bates and Griffing (1953) (Born approximation; broken curve), Olson and Salop (1977) (classical-trajectory Monte-Carlo calculations; double-dotted chain curve) and Golden and McGuire (1975) (Glauber theory; dotted curve). The comparison of the theoretical and experimental results shows that the effective-dipole close-coupling approximation gives a satisfactory agreement with the experimental data in the whole energy range considered, except in the region around the cross section maximum. Our dipole close-coupling approximation result lies systematically below the experimental data, since the transitions into the continuum through intermediate discrete states have not been included in the treatment. To account for these multi-step transitions, we shall use the analytical method developed earlier (Poluektov and Presnyakov 1968, 1970). Taking account of only one intermediate state leads to the following expression for the ionisation probability

$$W_{\text{ion}} = W_{0\rightarrow 1} + \tfrac{1}{4} W_{0\rightarrow i} W_{i\rightarrow 1} \tag{26}$$

where $|0\rangle$ and $|1\rangle$ are the initial and final (continuous) states and $|i\rangle$ is the intermediate state. In the atom–multicharged-ion collisions, the dominant contribution to the two-step ionisation comes from the transitions through the resonance level (e.g. $|i\rangle = |2p\rangle$ in the case of a hydrogen atom), since the probability $W_{0\rightarrow i}$ of its excitation is

considerably larger than those for other states (see figures 1–3). The analysis of the expressions for $W_{0\to i}$ and $W_{i\to 1}$ (see e.g. equations (7)–(10)) shows that for $\beta \ll 1$ and $\beta \gg 1$ one has

$$\tfrac{1}{4}W_{0\to i}W_{i\to 1} \ll W_{0\to 1} \qquad (\beta \gg 1, \beta \ll 1). \tag{27}$$

In the intermediate velocity region, where the cross section maximum lies, the ionisation probability $W_{i\to 1}$ is close to $\frac{1}{2}$ for all the values of the impact parameter. Therefore, the second term in equation (26) in this region can be approximated by

$$\tfrac{1}{4}W_{0\to i}W_{i\to 1} \simeq \tfrac{1}{8}W_{0\to i} \qquad (\beta_{0i}, \beta_{i1} > 0{\cdot}5) \tag{28}$$

where β_{0i} and β_{i1} are the parameters β (see equation (12)) for the $0\to i$ and $i\to 1$ transitions, respectively.

Using relations (27) and (28), the ionisation cross section now can be represented in the form

$$\sigma_{\text{ion}} = \sigma_{0\to 1} + \tfrac{1}{8}\sigma_{0\to i} \tag{29}$$

or, by virtue of equation (15),

$$\sigma_{\text{ion}} = 2\pi Z\left(\frac{\lambda_{\text{eff}}}{\omega_{\text{ion}}}D(\beta_{01}) + \frac{1}{8}\frac{\lambda_{0i}}{\omega_{0i}}D(\beta_{0i})\right) \tag{30}$$

where λ_{eff} has been defined previously.

In principle, expression (30) for σ_{ion} should be summed over all intermediate states i. However, with respect to the resonant state, all other intermediate states give a very small contribution to σ_{ion} ($\lesssim 5\%$), which can be neglected.

We have calculated the ionisation cross section for the $H(1s)+H^+$ system by using formula (30) with $|2p\rangle$ as an intermediate state. The result is shown in figure 4 (the full curve). From the figure we see that the agreement with experimental data is improved, especially in the region of the cross section maximum. We note, however, that the correction in the ionisation cross section, introduced by inclusion of the transitions through the 2p intermediate state, is only about 10–20% with respect to the values obtained in the dipole two-state close-coupling approximation.

Considering the agreement between the results of the developed ionisation theory and those of the experiments satisfactory, we have performed cross section calculations for the process $H(1s)+Z\to H^+ + Z + e$, for $Z = 2$, 4, 5, 8, 10, 14, 18, 24 and 32. The results are shown in figures 5 and 6 (full curves). The broken curves in these figures represent the results obtained by Olson and Salop (1977) and Olson *et al* (1977) by the classical-trajectory Monte-Carlo (CTMC) method. The chain curves for $Z = 2$ and $Z = 6$ represent the result of the sudden approximation (Salop and Eichler 1979) and the dotted curve for $Z = 2$ is the result of Glauber theory (Golden and McGuire 1976). As seen from the figures, the CTMC results in the region below the cross section maximum are considerably lower than those predicted by the effective-dipole close-coupling theory, which is similar to the $H(1s)+H^+$ case (see figure 4).

The scaling properties of the ionisation cross section are approximately the same as those for excitation. The maximum of the ionisation cross section occurs at $v_{\text{m}} \simeq 1{\cdot}89(Z\omega_{\text{ion}}\lambda_{\text{eff}})^{1/2}$ and has the value

$$\sigma_{\text{ion,m}} \simeq 0{\cdot}82\pi Z\left(\frac{\lambda_{\text{eff}}}{\omega_{\text{ion}}} + \frac{1}{8}\frac{\lambda_{0i}}{\omega_{0i}}\right) \tag{31}$$

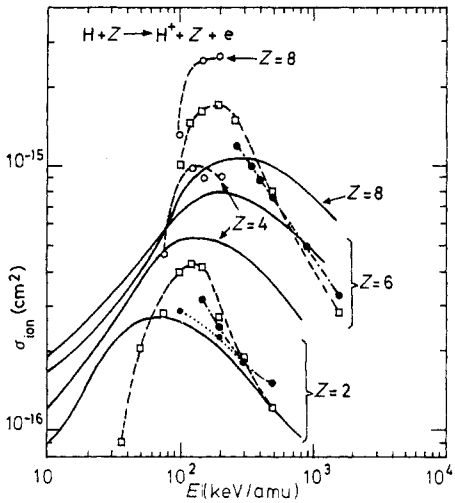

Figure 5. Cross sections for the $H(1s)+Z \rightarrow H^+ + Z + e$ reaction ($Z = 2, 4, 6, 8$). Solid curves: dipole close-coupling calculations with inclusion the transitions via the 2p intermediate state; – –□– – and – –○– –: results of the classical-trajectory Monte-Carlo calculations of Olson and Salop (1977) for $E \leqslant 200$ keV/amu and Olson (as quoted in Salop and Eichler 1979) for $E \geqslant 200$ keV/amu; chain curves for $Z = 2$ and 6 are the results of the sudden approximation (Salop and Eichler 1979); and dotted curve for $Z = 2$ is the result of Glauber theory (Golden and McGuire 1976).

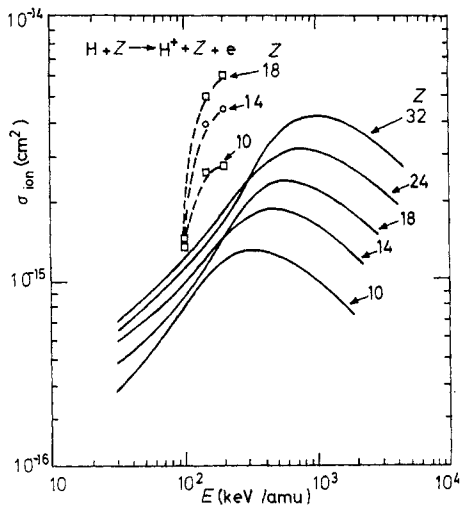

Figure 6. Same as in figure 5, except for $Z = 10$, 14, 18, 24 and 32.

where ω_{ion} and $\omega_{0i} = \omega_{\text{res}}$ are the atom ionisation and resonance frequencies, respectively. For the $H(1s)+Z$ case, one has $v_{\text{m}}^{(\text{H})} \simeq 1{\cdot}2Z^{1/2}$ and $\sigma_{\text{ion,m}}(\text{H}) \simeq 1{\cdot}53\pi Z$. In the region $v \gg v_{\text{m}}$ ionisation cross section has the usual Born approximation scaling (see equations (15), (18) and (27))

$$\sigma_{\text{ion}}^{(\text{B})} \simeq 8\pi\left(\frac{Z\lambda_{\text{eff}}}{v}\right)^2 \ln\left(\frac{1{\cdot}4v^2}{Z\lambda_{\text{eff}}\omega_{\text{ion}}}\right) \qquad v \gg (Z\lambda_{\text{eff}}\omega_{\text{ion}})^{1/2} \tag{32}$$

whereas in the adiabatic region σ_{ion} behaves as

$$\sigma_{\text{ion}} \simeq \pi\left(\frac{Z\lambda_{\text{eff}}}{v}\right)^2 \exp\left(-\frac{1}{v}(2Z\lambda_{\text{eff}}\omega_{\text{ion}})^{1/2}\right) \qquad v \ll (Z\lambda_{\text{eff}}\omega_{\text{ion}})^{1/2}. \quad (33)$$

As seen from the above formulae, in different velocity regions the ionisation cross section obeys different Z-scaling laws. It is worthwhile noting that the cross section maximum scales linearly with Z, i.e. in the same way as the charge exchange cross section in the intermediate energy region (where it gets its maximum value). From the above formulae it is also evident that the most natural reduced energy parameter for the case of ionisation is $\tilde{E} = \alpha E/Z$, where α is a constant. In the effective-dipole two-state close-coupling approximation for the process (i.e. only direct ionisation transitions taken into account) α may be taken in the form $\alpha = (\lambda_{\text{eff}}\omega_{\text{ion}})^{-1}$ and then a natural reduced form of the ionisation cross section is

$$\tilde{\sigma}_{\text{ion}} = \frac{\sigma_{\text{ion}}\omega_{\text{ion}}}{Z\lambda_{\text{eff}}}.$$

4. Conclusions

In the present paper we have considered the excitation and the ionisation processes in atom–multicharged-ion collisions. The main attention has been focused on the intermediate and high-energy regions, where these processes dominate the inelastic atom–multicharged-ion collision. The multi-electron transition (Auger-type) processes, which are important in the complex target atom case, have been excluded from our consideration. Within these restrictions, we have described the inelastic excitation and ionisation processes by using a dipole approximation for the ion–atom interaction potential and by using the close-coupling method based on an atomic basis set expansion. For excitation only the $n\text{s} \to n'\text{p}$ transitions have been considered, whereas for ionisation both $n\text{s} \to \epsilon\text{p}$ and $n\text{s} \to n'\text{p} \to \epsilon\text{s}$ transitions have been included in the treatment. The complex ionisation close-coupling problem has been simplified by using the concept of the effective continuum oscillator strength. In both the excitation and ionisation problems, the dipole close-coupling cross sections have been obtained in relatively simple analytical forms, which allows us to deduce general information on their scaling properties. With slight generalisation the developed treatment can also be extended to $nl \to n'l'$ and $nl \to \epsilon l'$ transitions.

An important feature of the presented theory is that it preserves the correct behaviour of the inelastic transition probability in the limit of small impact parameters. Therefore, no cut-off or matching procedures of any kind need be introduced in the small impact parameter region (as in the perturbational and sudden approximation treatments).

The accuracy of the results which the present theory provides is different for the cases of excitation and ionisation. In the case of excitation, the cross section in the adiabatic energy region (well below the cross section maximum on the velocity scale) is accurate only to within a factor of two, because of the strong $n'\text{p}$–$n'\text{s}$ coupling, not taken into account in our treatment. The possible inclusion of this coupling into the consideration would also require the inclusion of the Stark splitting and level shift effects, which would make the treatment rather complex. In the intermediate and high-energy regions all these effects are much less pronounced and, consequently, our

treatment should give much more accurate results for the excitation cross section. In the case of ionisation, the $\epsilon s \rightarrow \epsilon p$ continuum state coupling is rather small and the Stark splitting problem is absent. Therefore, the accuracy of the cross section predictions of our theory is expected to be high in the whole energy range (see e.g. figure 4).

Acknowledgment

One of us (RKJ) would like to express his gratitude to the International Atomic Energy Agency, Vienna, Austria, for the financial support under the Contract No 2043/R1/RB.

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