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Ionization of hydrogen atoms by multiply charged ions at low energies: The scaling law

R. K. Janev,[1] G. Ivanovski,[2] E. A. Solov'ev[2,*]
[1]*International Atomic Energy Agency, P.O. Box 100, A-1400 Vienna, Austria*
[2]*Faculty of Natural Sciences and Mathematics, St. Cyril and Methodius University, P.O. Box 162, 91000 Skopje, Macedonia*
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Using the adiabatic superpromotion model of low-energy atomic collisions, a simple scaling relationship is derived for the ionization cross section of hydrogen atoms colliding with multiply charged ions. Detailed ionization-cross-section calculations for the systems $H(1s)+He^{2+}$, C^{6+}, and O^{8+} have been performed and used to determine three numerical constants in the cross-section-scaling relationship. The scaled cross section represents well the available data for fully stripped ions with charge $Z \geq 2$ in the energy region below the cross-section maximum.

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The adiabatic superpromotion model for low-energy atomic collisions [1–3] continues to attract attention both from the point of view of its further development [4,5] and its systematic application to various atomic collision processes [6–12]. The model is based on the dynamical adiabatic approach to the low-energy dynamics of a one-electron–two-Coulomb-center collision system and represents its exact adiabatic limit. The close-coupling problem for the dynamical (velocity-dependent) molecular states is reduced in this limit [with an accuracy of $O(v^2)$, v being the relative collision velocity] to a large set of independent two-state close-coupling problems in isolated regions of internuclear distance R. It has been shown [1,3] that these nonadiabatic (radial-coupling) regions are associated with the branching points of the adiabatic potential energy of the system analytically continued in the complex R plane ("hidden crossings"). By knowing the elementary transition probabilities at the branching points (as well as the rotational transition probabilities at small and large internuclear distances), the evolution matrix of the system can be constructed in a simple manner [5–12].

The branch points of the adiabatic potential-energy surfaces in the complex R plane connect pairwise adiabatic states with same symmetry and form infinite series. In the (Z_1,e,Z_2) system, Z_1,Z_2 being the nuclear charges (we assume that neither the difference nor the ratio of these charges is too small), there are two types of branch point series [1,2], labeled by S and T. The first branching points of these series, connecting pairwise and *successively* adiabatic states of the same symmetry, also form infinite series, called S and T superseries. It has been shown [1] that the S superseries provide strong (diabatic) channels for promotion of the system to the continuum ("superpromotion") on the incoming stage of the collision, while the T superseries provide such superpromotion ionization channels during the receding of nuclei [4,9]. It has been also shown [4] that there is a close connection between the S and T superpromotion ionization channels with the unstable electron trajectories in the classical treatment of the one-electron–two-Coulomb-center problem: the S series are related to unstable trajectories of the electrons located on the top of the centrifugal barrier, while the T series are related to the unstable trajectories of electrons located on the top of the potential barrier between the nuclei ("saddle-point electrons" [13]). The relative importance of the two ionization mechanisms in the $H(1s)+H^+$ and $H(1s)+He^{2+}$ systems has been investigated in Ref. [9].

In the present article we investigate the low-energy ionization in the system $H(1s)+A^{Z+}$, where A^{Z+} is a completely stripped ion of charge $Z \geq 2$. We shall derive approximate analytic expressions for the contributions of S and T superpromotion mechanisms to the total ionization cross section and show that for $Z>2$ the T superpromotion is dominant. Moreover, it appears that the ionization cross section due to this mechanism exhibits scaling properties with respect to both Z and the collision velocity v. A simple cross-section relationship is found in which a few numerical constants are determined from the numerically calculated (within the adiabatic superpromotion model) ionization cross sections for the $H(1s)+He^{2+},C^{6+},O^{8+}$ collision systems. We note that the detailed numerical calculations for these systems have shown that the contribution of the S superpromotion channels to the total ionization channels is much smaller than that from the T channels in the entire energy range investigated (0.4–80 keV/amu) and that it rapidly decreases with increasing Z.

Let us first estimate the contribution of S superpromotion channels to the ionization cross section (see also Ref. [1]). The branch points $R^{(s)}_{N+i,lm}$ of the S superseries (Nlm are the united atom spherical quantum numbers) are all located in a small domain of the complex R plane near the coordinate origin (i.e., $|R^{(s)}_{N+i,lm}| \simeq |R^{(s)}_{N+i+1,lm}|$). They are distributed according to the relation $\mathrm{Re}R^{(s)}_{N+i,lm} > \mathrm{Re}R^{(s)}_{N+i+1,lm}$, and for $N \to \infty$ the limit point of the series is [3] (atomic units are used throughout, unless explicitly stated otherwise)

$$R^{(s)}_{lm} \simeq \frac{(l+1/2)^2}{Z} \exp\left[\frac{i\pi(m+1)}{2l+1}\right] . \quad (1)$$

*Permanent address: Department of Theoretical Physics, Institute of Physics, St. Petersburg University, St. Petersburg 198904, Russia.

(In this analysis we disregard the higher-order S superseries [5].) The ionization probability along a given S_{lm} superseries (starting with the state $N=l+1$) is the product of the two state transition probabilities along the series

$$P_{lm}^{(s)}=\prod_{N=l+1}^{\infty} p_{Nlm}^{(s)},\quad p_{Nlm}^{(s)}=\exp\left[-\frac{2}{v}\Delta_{Nlm}^{(s)}\right], \tag{2}$$

where $\Delta_{Nlm}^{(s)}$ is the generalized Massey parameter defined by (we use the straight-line trajectory approximation, $R^2=b^2+v^2$, with b denoting the impact parameter)

$$\Delta_{Nlm}^{(s)}(b)=\left|\mathrm{Im}\int_{\mathrm{Re}R_c^{(s)}}^{R_c^{(s)}}\frac{\Delta E_{Nlm;N+1,lm}(R)dR}{(1-b^2/R^2)^{1/2}}\right| \simeq\Delta_{Nlm}^{(s)}(0)\left[1+\frac{b^2}{2|R_c^{(s)}|^2}\right], \tag{3}$$

with R_c denoting the branching point $R_{Nlm}^{(s)}$. [The integration in (3), for both $\Delta_{Nlm}^{(s)}(b)$ and $\Delta_{Nlm}^{(s)}(0)$, is carried out along a contour in the complex R plane encompassing the branch point $R_c^{(s)}$.] To a good approximation, $\Delta_{Nlm}^{(s)}(0)$ can be approximated by [3]

$$\Delta_{Nlm}^{(s)}(0)\simeq\Delta E_{Nlm;N+1,lm}(\mathrm{Re}R_c)\mathrm{Im}R_c\ , \tag{4}$$

where for the higher values of N the quantity $\Delta E_{Nlm;N+1,lm}$ can be determined from the united atom energy spectrum ($\Delta E\simeq Z^2/N^3$, for $Z\gg1$). Using Eqs. (2), (3), and (4), and replacing the sum $\sum_N\Delta_{Nlm}^{(s)}$ [appearing in Eq. (2) from the product] by an integral, the S_{lm}-channel ionization probability is obtained in the form (see also [1])

$$P_{lm}^{(s)}\simeq\exp\left[-\frac{Z^2}{vN_0^2}\mathrm{Im}R_{lm}^{(s)}\left[1+\frac{b^2}{2|R_{lm}^{(s)}|^2}\right]\right],\quad N_0=l+1\ . \tag{5}$$

The ionization cross section $\sigma_{lm}^{(s)}$ is now obtained by integrating $P_{lm}^{(s)}$ over the impact parameters. In view of the inverse proportionality of $|R_{lm}^{(s)}|$ with Z [see Eq. (1)], the second, b-dependent term in the exponent of $P_{lm}^{(s)}$ gives a negligible contribution and the ionization cross section is obtained in the form

$$\sigma_{lm}^{(s)}\simeq\frac{2\pi v(l+1/2)^2N_0^2}{Z^3\sin\left[\frac{\pi(m+1)}{2l+1}\right]}\times\exp\left[-\frac{Z(l+1/2)^2}{vN_0^2}\sin\left[\frac{\pi(m+1)}{2l+1}\right]\right],\quad N_0=l+1\ . \tag{6}$$

This expression shows that $\sigma_{lm}^{(s)}$ decreases rapidly with increasing Z. The cross section $\sigma_{lm}^{(s)}$ increases with increasing l, and for given l it decreases with m. (Note that the branching point $R_{00}^{(s)}$ has $\mathrm{Re}R_{00}^{(s)}<0$ and the S_{00} series does not lead to superpromotion [1,3,5].) It is also worthwhile to note that the ionization cross sections $\sigma_{lm}^{(s)}$ can be represented in a reduced (scaled) form. By taking $N_0^2\simeq(l+1/2)^2$ and introducing the scaled quantities

$$\tilde{\sigma}^{(s)}=\frac{Z^2}{N_0^4}\sigma_{lm}^{(s)}\ ,\quad \tilde{v}_s=\frac{v}{Z\sin\left[\frac{\pi(m+1)}{2l+1}\right]}\ , \tag{7}$$

the reduced cross section $\tilde{\sigma}^{(s)}$ can be represented as

$$\tilde{\sigma}^{(s)}=2\pi\tilde{v}_s\exp(-1/\tilde{v}_s)\ . \tag{8}$$

Let us now estimate the contribution $\sigma^{(T)}$ of the T-superpromotion channels to the low-energy ionization cross section in the system $\mathrm{H}(1s)+A^{Z+}$, $Z\geq2$. As the numerical calculations for $Z=2$, 6, and 8 demonstrate, the series $T_{1s\sigma}$ gives the dominant contribution to $\sigma^{(T)}$ down to very low collision energies (~0.5 keV/amu). The ionization probability for this channel can be written as

$$P_{1s\sigma}^{(T)}=2(1-p_{000}^{(T)})\prod_{i=0}^{\infty}p_{0i0}^{(T)} =2(1-p_{000}^{(T)})\times\exp\left[-\frac{2}{v}\sum_{i=0}^{\infty}\Delta_{0i0}^{(T)}(0)\left[1+\frac{b^2}{2|R_{0i0}^{(T)}|^2}\right]\right], \tag{9}$$

where the indices n_1n_2m in $p_{n_1n_2m}^{(T)}$ denote the parabolic quantum numbers of the electron in the separated atom limit, and $\Delta_{n_1n_2m}^{(T)}(0)$ is given by an expression similar to (3) (with $b=0$) except that the branching point R_c is now a T-type branching point, $R_c^{(T)}$. The superpromotion series $T_{1s\sigma}$ obviously includes branching points which couple adiabatic states correlating at $R\rightarrow\infty$ with Stark states localized either on the proton ($R_c^{(T,1)}$ points) or on the projectile nucleus ($R_c^{(T,Z)}$ points). Accurate analytic expressions for the T-branching points in the general case are extremely difficult to obtain. Approximate expressions for $R_c^{(T,1)}$ and $R_c^{(T,Z)}$ have been obtained for the case $Z\gg1$ [9,14,15], which for the $n_1=m=0$ case considered here can be simplified as

$$R_{0n_20}^{(T,1)}\simeq a_1Z^{1/2}[n^{(1)2}+ia_2n^{(1)}(1+a_3)]\ , \tag{10a}$$

$$R_{0n_20}^{(T,Z)}\simeq\frac{b_1}{Z}[n^{(Z)2}+ib_2n^{(Z)}(1+\lambda Z^{1/4})]\ , \tag{10b}$$

where $n^{(1)}$ and $n^{(Z)}$ are the principal quantum numbers of the asymptotic states located on the proton and the nucleus Z, respectively, a_1 and b_1 are numerical constants, and a_2, b_2, and λ are constants which contain a much weaker dependence on the quantum numbers and Z than those indicated in Eq. (10). To a good approximation, the generalized Massey parameter $\Delta^{(T)}(0)$ can be represented as [7]

$$\Delta_{0i0}^{(T)}(0)\simeq\frac{\pi}{4}\Delta E_{i,i+1}(\mathrm{Re}R_c^{(T)})\mathrm{Im}R_c^{(T)}\ , \tag{11}$$

in which $\Delta E_{i,i+1}$ can be approximately calculated from the Coulomb energy spectrum in the separated atom limit. With this in mind, it is obvious that the dominant

contribution to the sum in Eq. (9) gives the subsum of $\Delta_{0i0}^{(T,Z)}$. Disregarding the contribution of the b-containing terms in this subsum (which after integration over b will anyway be negligible), the sum can be calculated by integration (the initial level being $i \simeq Z$, due to the quasiresonance with the hydrogen ground-state energy) and making use of Eqs. (11) and (10b). The ionization probability (9) can then be written as

$$P_{1s\sigma}^{(T)} \simeq \left\{1-\exp\left[-\frac{2}{v}\Delta_{000}^{(T,1)}(0)\left[1+\frac{b^2}{2|R_{000}^{(T,1)}|^2}\right]\right]\right\} \times \exp\left[-\frac{c}{v}(1+\lambda Z^{1/4})\right], \quad (12)$$

where $c=\frac{1}{2}\pi b_1 b_2$. Integrating this expression over impact parameters up to $\mathrm{Re}R_{000}^{(T,1)}$, and retaining only the leading term, one obtains for $\sigma^{(T)}$

$$\sigma^{(T)}=a\frac{Zv}{(1+2\lambda Z^{1/4})}\exp\left[-\frac{c}{v}(1+\lambda Z^{1/4})\right], \quad (13)$$

where $a=2\pi a_1^2/c$. Although derived for the $T_{1s\sigma}$ superseries, this expression for $\sigma^{(T)}$ is approximately valid for the total contribution to the ionization cross section from all T-superpromotion channels since the contribution from other T_{nlm} superseries can be, to the first approximation, accounted for in the constants a, c, and λ. The contribution from the T_{Nlm}-superpromotion channels with $m \geq 1$, opened through the rotational couplings at small R, may slightly increase the preexponential v dependence of $\sigma^{(T)}$. A notable feature of $\sigma^{(T)}$ is the weak dependence of the adiabatic exponent on Z. By comparing the expressions (6) and (13) it is evident that for large values of Z (practically already at $Z=2$) $\sigma^{(T)}$ is much larger than $\sigma^{(S)}$, as confirmed by the numerical calculations.

The expression (13) for $\sigma^{(T)}$ has obvious scaling properties. By introducing the reduced quantities

$$\tilde{\sigma}^{(T)}=\frac{\sigma^{(T)}}{Z}, \quad \tilde{v}=vf_z, \quad f_z=\frac{1+\lambda}{1+\lambda Z^{1/4}}, \quad (14)$$

the expression(13) can be written in the form

$$\tilde{\sigma}^{(T)}=a\tilde{v}\exp(-c/\tilde{v}), \quad (15)$$

or in terms of the reduced energy $\tilde{E}=25\tilde{v}^2$ keV/amu, as

$$\tilde{\sigma}^{(T)}=A\tilde{E}^{0.5}\exp(-C/\tilde{E}^{0.5}), \quad (16)$$

where $\tilde{E}=Ef_z^2$ (keV/amu). [f_Z has been chosen in the form given by Eq. (14) for normalization to the proton impact case, $f_1=1$.]

Unlike the case of S superpromotion, the theoretical determination of the constants a, c, and λ in Eq. (13) is a highly difficult task, if solvable at all. The basic difficulty consists in the accurate determination of the positions of branching points $R_c^{(T)}$, i.e., the solution of the quasiangular equation for the electronic motion along the elliptic coordinate $\eta=(r_1-r_2)/R$ in the region around the top of the potential in this equation [1,3,4,14] (r_1 and r_2 being the electron distances from the two Coulomb centers). Summation over all the T-superpromotion channels (some of them open through the rotational transitions at small R) would further complicate the problem. For that reason, we have chosen to determine the constants a, c, and λ in Eq. (13) from the cross sections for the collision systems $H(1s)+He^{2+}$, C^{6+}, O^{8+}, obtained by calculating the entire evolution matrix with all molecular states having $N \leq 10$. The number of included molecular states in the case of the $H(1s)+He^{2+}$ system is 165 and they are radially coupled via 178 S- and T-type branching points. In the case of $H(1s)+C^{6+}$ and $H(1s)+O^{8+}$ systems 220 molecular orbitals were included in the basis, coupled via 246 and 232 branching points, respectively. The rotational transitions within each of the (N,l) manifolds in the united atom region have been calculated by numerical integration of the corresponding close-coupled equations as formulated in Ref. [16]. The rotational couplings at large internuclear distances have also been included in the calculational scheme as described in [6,12]. The entire procedure of the calculations [determination of the branching points in the complex R plane, calculation of the contour integrals (3), construction of the evolution matrix, calculation of the channel probabilities and cross sections] is automated and contained in the computer-program package ARSENY. The ionization cross sections for the $H(1s)+He^{2+}$, C^{6+}, O^{8+} systems calculated by using this program in the region of validity of the method are given in Table I.

The determination of the constant λ has been done by the condition of coincidence of the reduced cross sections σ/Z for all three collision systems considered, while the constants A and C in Eq. (16) have been obtained by a fitting procedure. The resulting values for A, C, and λ are

$$A=0.847\times10^{-16}\ \mathrm{cm}^2, \quad C=8.55, \quad \lambda=0.275. \quad (17)$$

With these values for A, C, and λ, Eq. (16) represents the

TABLE I. Ionization cross sections for $H(1s)+He^{2+}$, C^{6+}, O^{8+} collisions (in units of 10^{-16} cm^2). The numbers in brackets denote multiplicative powers of ten.

E (keV/amu)	$H(1s)+He^{2+}$	$H(1s)+C^{6+}$	$H(1s)+O^{8+}$
0.4	8.77[−7]	7.51[−6]	1.35[−6]
0.6	1.43[−5]	8.32[−5]	1.69[−5]
0.8	7.73[−5]	3.39[−4]	1.02[−4]
1.0	2.47[−4]	8.66[−4]	3.67[−4]
1.4	1.15[−3]	3.12[−3]	1.90[−3]
2.0	4.63[−3]	1.07[−2]	8.14[−3]
3.0	1.47[−2]	3.63[−2]	3.46[−2]
4.0	3.85[−2]	7.87[−2]	8.44[−2]
6.0	9.97[−2]	2.10[−1]	2.49[−1]
8.0	1.67[−1]	3.95[−1]	4.81[−1]
10.0	2.60[−1]	6.24[−1]	7.57[−1]
14.0	4.43[−1]	1.18	1.38
20.0	7.89[−1]	2.17	2.36
30.0	1.66	3.98	4.23
40.0	1.88	5.82	6.33
60.0		9.25	
80.0		12.20	

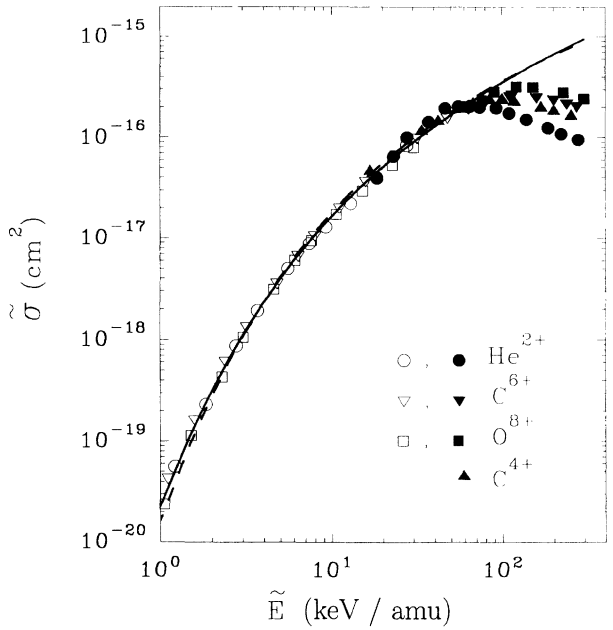

FIG. 1. Reduced ionization cross section vs reduced energy. The solid curve represents the scaled cross section given by Eq. (18). The dashed curve represents the scaled cross section given by Eqs. (16) and (17). The open symbols are the scaled data of Table I; the closed symbols are scaled experimental (for He^{2+}, Ref. [17]) and recommended (for C^{4+}, C^{6+}, and O^{8+}, Ref. [18]) ionization cross-section data.

reduced cross sections from Table I with an rms deviation of 5% (and maximum deviation of about 25% at the lowest reduced energies).

A slightly improved representation of the calculated reduced ionization cross sections for these three systems can be achieved if the exponent of the factor $\tilde{E}^{0.5}$ in Eq. (16) is treated as a free parameter [to account, for instance, for the effects of the $m \geq 1$ T-superpromotion channels, see the discussion below Eq. (13)]. In that case, the best fit to the reduced cross-section data is obtained by the expression (the last two high-energy points for He^{2+} and O^{8+} were excluded from the fitting procedure as unreliable)

$$\tilde{\sigma} = 0.44\tilde{E}^{0.615}\exp(-7.58/\tilde{E}^{0.5}) \times 10^{-16}\ \text{cm}^2\ , \qquad (18)$$

with λ having the same value as before. The expression (18) fits the reduced cross-section data with an rms deviation of 2–3 % and a maximum deviation of 10% at lowest reduced energies.

The numerically calculated reduced cross-section values and the cross section (18) are shown in Fig. 1 by open symbols and a solid curve, respectively. In the higher-energy part of this figure we also show the reduced experimental cross sections for $H(1s)+He^2$ [17], and the reduced "recommended" cross sections for $H(1s)+C^{4+}$, $H(1s)+C^{6+}$, and $H(1s)+O^{8+}$ from Ref. [18] (closed symbols). It is seen from the figure that Eq. (18) represents a smooth extrapolation of the experimental or recommended cross-section data in the energy region below the corresponding cross-section maximum. The dashed line in Fig. 1 represents the results of Eq. (17) with the values of parameters A, B, λ given by Eq. (17). This figure also shows the upper energy limit of the validity of Eq. (18). Taking into account that the ionization cross-section maximum in the $H(1s)+A^{Z+}$ system takes place at $E_m \simeq 50Z^{0.65}$ keV/amu [18], an approximate upper limit for the validity of Eq. (18) can be set at $\tilde{E}_c \simeq E_m f_z^2$. Since this limit increases with increasing the ionic charge Z, the solid curve in Fig. 1 can be extended indefinitely, providing an upper limit (envelope) for the reduced ionization cross sections with $Z \geq 2$.

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