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Saddle-point scaling method for ionizing collisions

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Scaling laws have been derived for total single-ionization cross sections from the classical picture of saddle-point ionization. The results agree with experimental data for the projectile-charge dependence of the energy position of cross-section maxima and for the values of the cross-section maxima.

The study of collisions of fast multiply charged ions with hydrogen and helium atoms plays an important role in the development of magnetically confined thermonuclear fusion devices. In particular, one collisional process of interest is the single-ionization reaction

$$A^{q+}+X\rightarrow A^{q+}+X^{+}+e^{-}\ , \tag{1}$$

where X denotes H or He. Extensive measurements have been carried out for reaction 1 for many ionic species. The experimental investigations have shown that the magnitude and energy dependence of single-ionization cross sections seem to depend only on the ionic charge and not on particular ionic species.

To illustrate the general behavior of the projectile-charge dependence of ionization cross sections, experimental data for single ionization of helium by H^{+}, He^{2+}, and Li^{3+} are shown in Fig. 1.[1] As one can see, not only does the value of the maximum cross section increase when the projectile charge is increased, but the projectile energy at which the maximum occurs shifts to higher energies. Until now, no theoretical description of this phenomenon existed.

In absence of theoretical guidance, empirical experimental scaling laws have been developed to facilitate computational modeling of fusion plasmas.[1–4] Existing experimental data for C^{q+},O^{q+} + H and C^{q+},O^{q+} + He allow formulation of the following empirical scaling equations for the energy $E_{\max}$ at which the cross-section maximum appears, and for the value of the cross-section maximum $\sigma_{\max}$:

$$E_{\max}=aq^{0.65}\times 10^{4}\ \mathrm{eV/amu}\ , \tag{2}$$

$$\sigma_{\max}=bq^{1.3}\times 10^{-16}\ \mathrm{cm}^{2}\ . \tag{3}$$

The values of a and b are listed in Table I.

Recent experimental work in this laboratory has lead to a simple, theoretical understanding of Eqs. (2) and (3). In examining ionizing collisions, it was observed that a large portion of the ejected electrons are found emerging from the collision with a velocity near half that of the projectile.[5,6] Another intriguing observation is that the maximum in the forward-ejected electron velocity spectrum shifts to smaller velocities when the projectile charge is increased.[7] These observations strongly imply that the ejected electrons are being "stranded" on the Coulomb equiforce, or saddle region of the system. The saddle point moves at a velocity $\mathbf{v}_{\mathrm{SP}}$ given by

$$\mathbf{v}_{\mathrm{SP}}=\frac{\mathbf{v}_P}{1+Q_P^{1/2}/Q_T^{1/2}}\ , \tag{4}$$

where $\mathbf{v}_P$ is the projectile velocity, Q_P is the projectile charge, and Q_T is the charge of the ionized target. In examining Fig. 2, which illustrates the trajectory of the projectile and saddle point in an ionizing collision, one can envision the manner in which an electron can become stranded on the saddle position. If, for instance, the saddle point passes through the target-atom electron charge cloud, moving with a velocity equivalent to the electron's orbital velocity, the electron can, in a sense, "surf" on the saddle. Since the Coulomb force is zero on the saddle position, the electron will emerge from the collision with a

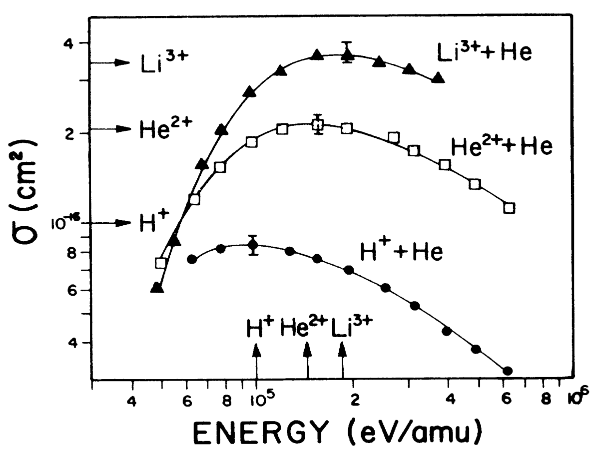

FIG. 1. Total single-ionization cross-sections for H^{+}, He^{2+}, and Li^{3+} incident on helium (Ref. 1). The arrows indicate the energy position and value of the cross-section maximum calculated from Eqs. (5) and (11), after normalization to the He^{2+} + He peak position (using $Z_{\mathrm{eff}}=1.68$ for Q_T).

TABLE I. Values of the scaling constants a and b are listed with the corresponding collision pairs.

Collision pair	a	b
C^{q+}+H	4.3	1.66
O^{q+}+H	4.14	1.75
C^{q+},O^{q+}+He	10	0.843

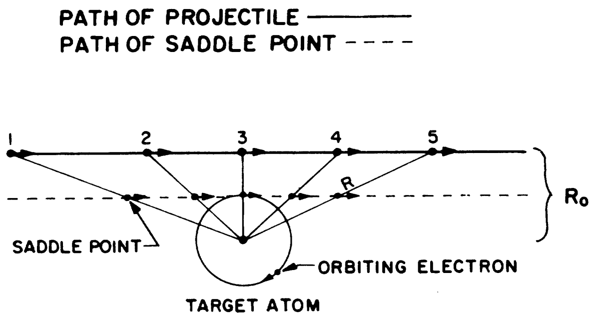

FIG. 2. Illustration of the trajectory of the projectile and saddle point of an ionizing collision. The numbers represent successive positions as the projectile passes the target atom.

velocity near its initial orbital velocity. In order to match the saddle velocity to the electron's orbital velocity, the projectile should have an incident energy E_P given in amu by

$$E_P = 1836 E_{\mathrm{KE}}(1+Q_P^{1/2}/Q_T^{1/2})^2 = A(1+Q_P^{1/2}/Q_T^{1/2})^2 , \quad (5)$$

where E_{KE} is the electron's orbital kinetic energy. If this "saddle matching" phenomenon is valid, then one would expect to observe a maximum in the total single-ionization cross section at the projectile energy given by Eq. (5). In addition, since the saddle point moves with a slower velocity when the projectile charge is increased, the projectile must have a higher incident velocity to maintain matching of its saddle velocity with the orbiting electron; hence, the cross-section maximum shifts to higher energies.

Using conservation of energy and the position of the saddle point $\mathbf{r}_{\mathrm{SP}}$ given by

$$\mathbf{r}_{\mathrm{SP}} = \gamma \mathbf{R}; \quad \gamma = \frac{1}{1+Q_P^{1/2}/Q_T^{1/2}} , \quad (6)$$

where $\mathbf{R}$ is the internuclear separation, the effect of projectile charge on the value of the ionization cross section can be determined. The potential energy of the system is

$$\phi = -\frac{Q_T}{|\mathbf{r}|} - \frac{Q_P}{|\mathbf{R}-\mathbf{r}|} . \quad (7)$$

By substituting the position of the saddle point $\mathbf{r}_{\mathrm{SP}}$ for $\mathbf{r}$ in Eq. (7), the potential energy of the saddle position ϕ_{SP} becomes

$$\phi_{\mathrm{SP}} = -\frac{Q_T}{|\mathbf{R}|\gamma} - \frac{Q_P}{|\mathbf{R}|(1-\gamma)} = -\frac{Q_T}{R\gamma} - \frac{Q_p}{R(1-\gamma)} . \quad (8)$$

If the distance of closest approach between the projectile and target atom is R_0, then the minimum potential energy of the saddle point is given by

$$\phi_{\mathrm{SP}}^{\min} = -\frac{Q_T}{R_0\gamma} - \frac{Q_P}{R_0(1-\gamma)} . \quad (9)$$

When the projectile is at $-\infty$, the potential energy of the saddle point is zero. As the projectile approaches the target atom, the potential energy of the saddle decreases and reaches a minimum value at the distance of closest approach. Then the potential energy of the saddle point rises as the projectile travels outward. From a classical viewpoint, the only way that the electron can be ionized is if the minimum value of the potential energy of the saddle point, at closest approach, is less than or equal to the binding energy of the electron. Hence, the saddle point must, at least, pass "under" the electron. The projectile charge dependence of the cross section can be obtained from Eq. (9). Setting the minimum value of the saddle's potential energy equal to the binding energy of the electron E_B, and solving for R_0, the distance of closest approach, results in

$$R_0 = \frac{1}{E_B}\left[\frac{Q_T}{\gamma} + \frac{Q_P}{(1-\gamma)}\right] = \frac{1}{E_B}(Q_T^{1/2}+Q_P^{1/2})^2 . \quad (10)$$

Therefore, the total cross-section is simply

$$\sigma = \pi R_0^2 = \frac{\pi}{E_B^2}(Q_T^{1/2}+Q_P^{1/2})^4 = B(Q_T^{1/2}+Q_P^{1/2})^4 . \quad (11)$$

Since electron binding energies are known, one can directly calculate the maximum cross sections from Eq. (11). But in this model it is assumed that the electron is on the same side of the target nucleus as the saddle point when the projectile passes; thus Eq. (11) will yield an upper bound for the cross section of interest. In principle, the absolute cross sections can be obtained by multiplying Eq. (11) by $\Omega/4\pi$, where Ω is the solid angle subtended by a region centered around the saddle point as it "grazes" the electron charge cloud. Nonetheless, this model is suitable for obtaining scaling laws for ionization cross sections since Ω is independent of projectile charge.

Comparison of this classical model with experiment is shown in Figs. 1, 3, and 4. In Fig. 1, Q_T was set equal to 1.68, corresponding to the effective charge of the target nucleus as seen by the electron ($Z_{\mathrm{eff}}=1.68$ was obtained by using Slater's rules).[8] Using $Q_T=1.68$ results in a slightly better fit than $Q_T=1$, when normalizing on the $He^{2+}+He$ curve. In Fig. 3 the constant A was determined by trial and error, to obtain the best "eyeball" fit and yielded $A=12.35$ keV/amu. Using the value of A in Eq. (5) results in an electron orbital kinetic energy of 6.73 eV, which is not unreasonable since the most probable E_{KE} for H is 4.53 eV (the classical E_{KE} is 13.6 eV). Actually, one must include polarization effects of the target atom by the projectile when determining the most probable E_{KE}. However, it must be noted that this model is not intended to give absolve values; the intent is to establish scaling laws for ionization cross sections.

In order to compare these results to the empirical scaling laws, Eqs. (2) and (3), it was necessary to determine the power scaling of E_P from Eq. (5). This was accomplished by plotting $\ln E_P$ versus $\ln Q_P$, for $Q_P=1-8$. A least-squares fit determined the exponent of Q_P (with $Q_T=1$) from

$$E_P = A(1+Q_P^{1/2})^2 \simeq aQ_P^x , \quad (12)$$

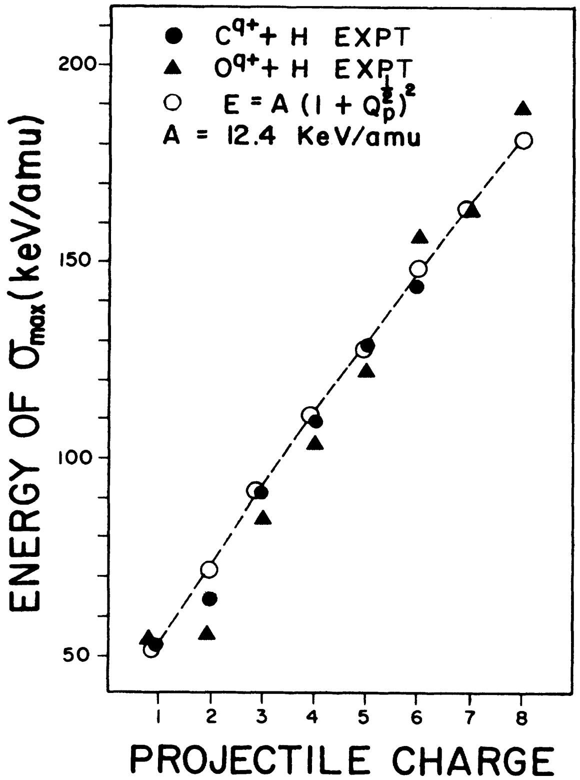

FIG. 3. The projectile energy at which the cross-section maximum occurs is plotted vs projectile charge for the system $C^{q+}+H$, and $O^{q+}+H$. Closed circles and triangles represent the experimental data of Ref. 4. Open circles represent the calculated energy positions from Eq. (5) and are normalized to produce the best fit.

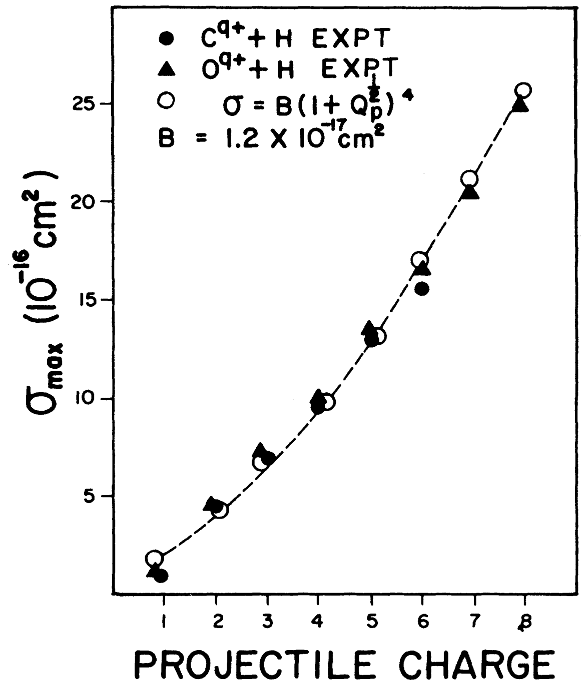

FIG. 4. Maximum cross-section values vs projectile charge for C^{q+}, $O^{q+}+H$. The open circles represent cross sections calculated from Eq. (11), after normalization.

and yielded $x=0.63\pm0.02$, which agrees very well with the empirical experimental scaling law. (The error in x results from the standard deviation of the slope of $\ln E_P$ plotted versus $\ln Q_P$.) When Q_T is set equal to 1, Eqs. (5) and (11) yield

$$E_P=A(1+Q_P^{1/2})^2;\quad A=(1836)E_{KE}\ , \tag{13}$$

$$\sigma=B(1+Q_P^{1/2})^4;\quad B=\frac{\pi}{E_B^2}\ . \tag{14}$$

As can be seen, the cross section scales as the square of the energy position

$$\sigma\simeq E_P^2=A^2(1+Q_P^{1/2})^4\ . \tag{15}$$

Examination of the empirical scaling Eqs. (2) and (3) shows that the experimental cross section also scales as the square of the energy position

$$\sigma_{max}=bq^{1.3}\simeq E_{max}^2=a^2q^{2(0.65)}\ . \tag{16}$$

From this classical viewpoint, it appears that the saddle point "selects" electrons to be ionized from the target atom; electrons which have an orbital velocity near the saddle velocity are predominantly ionized. Since there exists a probability distribution of the electron's orbital velocity within the target atom, the ionization cross-section curves are, in a sense, a crude mapping of this distribution. When a projectile passes a target atom, the electrons that have the same velocity as the saddle point are preferentially ionized, since the Coulomb force on these electrons drops to zero when the saddle passes under them. When the charge of the projectile is increased, the slower moving saddle point ionizes the slower moving electrons; hence, one observes an inward shift in the ejected-electron velocity spectrum. Since the saddle position shifts further inward toward the target atom, when the projectile charge is increased, the projectile doesn't have to pass as close as another with lesser charge to induce ionization; the ionization cross section increases when the projectile charge increases.

In conclusion, it appears that there exists two conditions for which ionization is favorable. The first one is that the "saddle point" of the system must travel at a speed near the electron's most probable orbital velocity. The second condition is that the saddle point must pass "through" the target electron charge cloud. Not only do these conditions give an intuitive picture of ionization, but also yield scaling laws which agree very well with, what have until now been, an empirical experimental law. Thus, the saddle-point mechanism appears to be a much more global phenomenon than previously expected, and the empirical scaling laws seem to be a direct consequence of this.

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